Discovering Ancestral Instrumental Variables for Causal Inference From Observational Data
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Abstract—Instrumental variable (IV) is a powerful approach to inferring the causal effect of a treatment on an outcome of interest from observational data even when there exist latent confounders between the treatment and the outcome. However, existing IV methods require that an IV is selected and justified with domain knowledge. An invalid IV may lead to biased estimates. Hence, discovering a valid IV is critical to the applications of IV methods. In this article, we study and design a data-driven algorithm to discover valid IVs from data under mild assumptions. We develop the theory based on partial ancestral graphs (PAGs) to support the search for a set of candidate ancestral IVs (AIVs), and for each possible AIV, the identification of its conditioning set. Based on the theory, we propose a data-driven algorithm to discover a pair of IVs from data. The experiments on synthetic and real-world datasets show that the developed IV discovery algorithm estimates accurate estimates of causal effects in comparison with the state-of-the-art IV-based causal effect estimators.

Index Terms—Causal inference, confounding bias, instrumental variables (IVs), latent confounders, maximal ancestral graph (MAG).

I. INTRODUCTION

A FUNDAMENTAL problem for inferring from observational data the causal effect of a treatment \( W \) (a.k.a. exposure, intervention, or action) on an outcome \( Y \) of interest is the presence of a latent (a.k.a. unobserved or unmeasured) confounder, each of which is a common cause of \( W \) and \( Y \) [1], [2]. It is especially challenging to obtain unbiased estimation of the causal effect of \( W \) on \( Y \) when there is a latent confounder. Instrumental variables (IVs) are a powerful tool to address this challenge, primarily used in data analysis (e.g., financial big data) by statisticians, economists, and social scientists [3], [4], [5]. It is possible to eliminate the confounding bias by leveraging a valid IV [6].

The standard IV approach requires a predefined IV (denoted as \( S \)) that meets the following three conditions: 1) \( S \) is a cause of \( W \); 2) there is no confounding bias for the effect of \( S \) on \( Y \) (a.k.a. exogeneity); and 3) the effect of \( S \) on \( Y \) is entirely mediated through \( W \) (a.k.a. the exclusion restriction) [7]. For example, \( S \) in the causal graph in Fig. 1(a) is a standard IV as it meets all the three conditions. The second and third conditions have to be justified by domain knowledge [2] and hence IV-based methods are mostly classified as empirical methods in literature [8], [9].

Data-driven approach to identifying standard IVs is impractical. Instrumental inequality [8], [10] has been proposed to test an IV in data, but it is a necessary condition, not a sufficient condition. Under a set of strong assumptions on the data distribution, a semi-IV that can be tested in data has been introduced by [11]. However, there is not a practical algorithm rooted in the above concepts. By assuming that at least half of the covariates are valid IVs, Kang et al. [12] proposed an algorithm, sisVIVE (some invalid, some valid IV estimator), to estimate the causal effect in data. Hartford et al. [13] extended the sisVIVE algorithm by employing a deep-learning-based IV estimator. The main challenge of the two algorithms is that their strong assumption is often unsatisfied in many real-world applications.

To relax the last two conditions (i.e., the exogeneity and exclusion restriction) of a standard IV, a graphical criterion [2], [14] is proposed to identify an observed variable \( S \) as an IV [i.e., the conditional IV (CIV)], conditioning on a set of observed variables \( Z \) from a given directed acyclic graph (DAG, which represents the causal relations of all measured and unmeasured variables). CIV allows a confounding bias between \( S \) and \( Y \), and \( S \) have multiple causal paths to \( Y \). A path with direct edges all pointing to \( Y \).

Fig. 1. (a) \( S \) is a standard IV for \( W \to Y \). (b) \( S_1 \) and \( S_2 \) are valid IVs w.r.t. \( W \to Y \), conditioning on \( Z = [X_3] \).

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Zander et al. [15] have revised CIV to Ancestral IV (AIV) to avoid the situation where void CIVs may be identified based on the original definition (see Section 2-B for details). AIV identification needs a DAG too.

IV.tetrad [9] is the only existing data-driven CIV method. IV.tetrad is based on CIV and it requires two valid CIVs in the covariate set. The tetrad condition is used to discover the pair of CIVs in data and it assumes that the conditioning sets of the pair of CIVs are the same and equal to the set of remaining covariates (i.e., the original covariate set excluding the pair of CIVs). This tetrad condition leads to a wrong identification when the set of remaining covariates contains a collider. For example, $S_1$ and $S_2$ in Fig. 1(b) are a pair of CIVs. The conditioning sets for $S_1$ and $S_2$ are the same, both equal to $\{X_3\}$, but not as assumed in the IV.tetrad, i.e., $\{X_1, X_2, X_3\}$. When $X_1$ is used in the conditioning set, path $S_1 \rightarrow X_1 \leftarrow U_2 \rightarrow Y$ is opened and $S_1$ does not instrumentize $W$ conditioning on $\{X_1, X_2, X_3\}$ any more. Hence, the tetrad condition does not find the right CIV pairs and leads to a biased causal effect estimation.

This work improves IV.tetrad in the following ways, which are also our contributions.

1. We generalize the tetrad condition so that each AIV in the pair conditions on its own conditioning set, and this rectifies the current tetrad condition which fails to find the right pair when the covariate set contains a collider.
2. We develop the theory for identifying the set of candidate AIVs in a reduced space for efficient search for a pair of AIVs.
3. We propose a data-driven algorithm for estimating causal effects from data with latent variables based on the above developed theorems. Extensive experiments on synthetic and real-world datasets have shown the effectiveness of the algorithm.

II. BACKGROUND

A. Graph Terminology

A graph $G = (V, E)$ is composed of a set of nodes $V = \{V_1, \ldots, V_n\}$, representing random variables, and a set of edges $E \subseteq V \times V$, representing the relations between nodes. In this article, we consider a simple graph $G$ where between any two nodes there is at most one edge.

Two nodes are adjacent if there exists an edge between them. For an edge, $V_i \rightarrow V_j$, $V_i$ and $V_j$ are its head and tail, respectively, and $V_i$ is known as a parent of $V_j$ (and $V_j$ is a child of $V_i$). We use Adj($V_i$), Pa($V_i$), and Ch($V_i$) to denote the sets of all adjacent nodes, parents, and children of $V_i$, respectively. A path $\pi$ is a sequence of nodes $(V_1, \ldots, V_n)$ such that for $1 \leq i \leq n-1$, the pair $(V_i, V_{i+1})$ is adjacent. A path $\pi$ from $V_i$ to $V_j$ is a directed or causal path if all edges along it are directed toward $V_j$, and $(V_i, V_j)$ are called endpoint nodes, other nodes are non-endpoint nodes. If there is a directed path $\pi$ from $V_i$ to $V_j$, $V_i$ is known as an ancestor of $V_j$ and $V_j$ is a descendant of $V_i$. The sets of ancestors and descendants of a node $V$ are denoted as An($V$) and De($V$), respectively.

A DAG is a direct graph (i.e., a graph containing only directed edges $\rightarrow$) without directed cycles (i.e., a directed path whose two endpoints are the same node). A DAG is often used to represent the data generation mechanism or causal mechanism underlying the data, with all variables, both observed and unobserved (if any) included in the graph.

Ancestral graphs are used to represent the data generation mechanisms that may involve latent variables, with only observed variables included in the graphs [16], [17]. An ancestral graph may contain three types of edges: $\rightarrow$, $\leftrightarrow$ (it is used to represent that a common cause of two observed variables is a latent variable), and $\leftrightarrow$ (the circle tail denotes the orientation of the edge is uncertain), and we use “$\leftrightarrow$” to denote any of the three types. $C$ is a collider on the path $\pi$ if $\pi$ contains a subpath $\leftrightarrow \leftrightarrow$. In an ancestral graph, a path is a collider path if every non-endpoint node on it is a collider. A path of length one is a trivial collider path.

In a graph, an almost directed cycle occurs when $V_i \leftrightarrow V_j$ is in the graph and $V_j \in An(V_i)$. An ancestral graph is a graph that does not contain directed cycles or almost directed cycles [16]. In an ancestral graph, a path from $V_i$ to $V_j$ is a possibly directed or causal path if there is not an arrowhead pointing in the orientation of $V_i$. In this case, $V_j$ is a possible ancestor of $V_i$, $V_i$ is a possible descendant of $V_j$. The sets of possible ancestors and descendants of $V$ are denoted as PossAn($V$) and PossDe($V$), respectively.

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

Definition 1 (Markov Property [2]): A DAG $G = (V, E)$ and the joint probability distribution of $V$ (prob($V$)), $G$ satisfies the Markov property if for $\forall V_i \in V$, $V_i$ is probabilistically independent of all of its non-descendants, given $Pa(V_i)$.

Definition 2 (Faithfulness [1]): A DAG $G = (V, E)$ is faithful to a joint distribution prob($V$) over the set of variables $V$ if and only if every independence present in prob($V$) is entailed by $G$ and satisfies the Markov property. A joint distribution 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 prob($V$).

A DAG $G = (V, E)$ satisfies both assumptions, the probability distribution prob($V$) can be factorized as: prob($V$) = $\prod_i$ prob($V_i$|$Pa(V_i)$). Thus, together Markov property and faithfulness establish a close relationship between the causal graph and the data distribution.

Definition 3 (Causal Sufficiency [1]): In a data, for every pair of observed variables $(V_i, V_j)$ in $V$, all their common causes are also in $V$.

In a DAG, d-separation is a well-known graphical criterion that is used to read off the identification of conditional independence between variables entailed in the DAG when the Markov property, faithfulness, and causal sufficiency are satisfied [1], [2].

Definition 4 (d-Separation [2]): 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 1) $\pi$ contains a chain $V_i \rightarrow V_k \rightarrow V_j$ or a fork $V_i \leftarrow V_k \rightarrow V_j$ such that the middle node $V_k$ is in $Z$. 

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or 2) \(\pi\) contains a collider \(V_k\) such that \(V_i\) is not in \(Z\) and no descendant of \(V_k\) is in \(Z\). A set \(Z\) is said to d-separate \(V_i\) from \(V_j\) if \(V_i \perp_{d} V_j \mid Z\) if and only if \(Z\) blocks every path between \(V_i\) and \(V_j\). Otherwise they are said to be d-connected by \(Z\), denoted as \(V_i \parallel_{d} V_j \mid Z\).

Property 1: Two observed variables \(V_i\) and \(V_j\) are d-separated given a conditioning set \(Z\) in a DAG if and only if \(V_i\) and \(V_j\) are conditionally independence given \(Z\) in data [1]. if \(V_i\) and \(V_j\) are d-connected, \(V_i\) and \(V_j\) are conditionally dependent.

However, a system may involve the latent variables (the latent variable is an unmeasured common cause of two nodes) in most situations since there is not a close world. Ancestral graphs are proposed to represent the system that may involve latent variables [16], [17]. In our work, we utilize the maximal ancestral graph (MAG) and introduce it as follows.

Definition 5 (Maximal Ancestral Graph [16]): An ancestral graph \(M = (V, E)\) is a MAG when every pair of nonadjacent nodes \(V_i\) and \(V_j\) in \(M\) is m-separated by a set \(Z \subseteq V \setminus \{V_i, V_j\}\).

It is worth noting that a DAG satisfies both conditions of a MAG, so a DAG is also a MAG without bidirected edges [17]. An important concept in a DAG is d-separation, which captures the conditional independence relationships between variables based on Markov property [2]. A natural extension of the d-separation to an ancestral graph is m-separation [16].

Definition 6 (m-Seperation [16]): 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 \(V_k, V_l, V_s\) such that the middle node \(V_k\) is a non collider on \(\pi\) and \(V_k \in Z\); or \(\pi\) contains \(V_i \leftrightarrow V_k \leftrightarrow V_l\) such that \(V_k \notin Z\) and no descendant of \(V_k\) is in \(Z\). Two nodes \(V_i\) and \(V_j\) are said to be m-separated by \(Z\) in \(M\), denoted as \(V_i \perp_{m} V_j \mid Z\) if every path between \(V_i\) and \(V_j\) are m-separated by \(Z\); otherwise they are said to be m-connected by \(Z\), denoted as \(V_i \parallel_{m} V_j \mid Z\), where \(\perp_{m}\) denotes m-separation and \(\parallel_{m}\) denotes m-connection. In a DAG, m-separation/m-connection reduces to d-separation/d-connection. The Markov property of the ancestral graph is captured by m-separation.

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

Definition 7 (Markov Equivalent MAGs [18]): Two MAGs \(M_1\) and \(M_2\) with the same nodes are said to be Markov equivalent, denoted \(M_1 \sim M_2\), if for all triple nodes \(X, Y, Z\), \(X, Y\), and \(Z, X\) and \(Y\) are m-separated by \(Z\) in \(M_1\) if and only if \(X\) and \(Y\) are m-separated by \(Z\) in \(M_2\).

A set of Markov equivalent MAGs can be encoded uniquely by a partial ancestral graph (PAG) [17].

Definition 8 (PAG [17]): Let \([M]\) be the Markov equivalence class of a MAG \(M\). The PAG \(P\) for \([M]\) is a partial mixed graph such that 1) \(P\) has the same adjacent relations among nodes as \(M\) does and 2) 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 9 (Visibility [17]): Given a MAG \(M = (V, E)\), a directed edge \(V_i \rightarrow V_j\) is visible if there is a node \(V_k \notin Adj(V_j)\), such that either there is an edge between \(V_i\) and \(V_k\) that is into \(V_j\), or there is a collider path between \(V_k\) and \(V_j\) that is into \(V_i\) and every node on the path is a parent of \(V_j\). Otherwise, \(V_i \rightarrow V_j\) is invisible.

The visible edge is a critical concept in a MAG [17], [19]. A DAG over measured and unmeasured variables can be mapped to a MAG with measured variables. From a DAG over \(X \cup U\) where \(X\) is a set of measured variables and \(U\) is a set of unmeasured variables, following the construction rule specified in [18], one can construct a MAG with nodes \(X\) such that all the conditional independence relationships among the measured 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.

B. Instrumental Variable

Let \(W\) be the treatment variable, \(Y\) the outcome, and \(X\) be the set of all other variables. As in the literature, we consider that \(X\) contains pretreatment variables only, i.e., for any \(X \in X, X \notin (De(W) \cup De(Y))\) [9], [20], [21]. In the rest of the article, we assume that in the joint distribution, the relationships between a variable \(X\) and its parents are linear, i.e., \(x_i = \beta_0 + \sum_{j \in P(a(x_i))} \beta_{ij} x_j\) where \(\beta_{ij}\) can be interpreted as the average causal effect of \(X_j\) on \(X_i\). In this work, we would like to estimate the average causal effect of \(W\) on \(Y\), denoted as \(\beta_{wy}\), from data with latent confounders. We follow the convention in causal inference literature, that is, the data distribution is said to be compatible with the underlying causal DAG \(\mathcal{G}\), i.e., the assumptions of Markov property and faithfulness are satisfied.

The goal of this work is to quantify the average causal effect of \(W\) on \(Y\), i.e., \(\beta_{wy}\), even when there exist unmeasured variables between \(W\) and \(Y\), based on observational data, by extending the existing IV techniques.

In this section, we introduce the background information related to IVs.

Definition 10 (Standard IV [22], [23]): A variable \(S\) is said to be an IV w.r.t. \(W \rightarrow Y\), if 1) \(S\) has a causal effect on \(W, 2) S\) affects \(Y\) only through \(W\) (i.e., \(S\) has no direct effect on \(Y\)), and 3) \(S\) does not share common causes with \(Y\).

The last two conditions of a standard IV are untestable and strict. In practice, \(S\) may have other causal paths to \(Y\), and \(S\) is often confounded with \(Y\) by other measured variables. The concept of CIV in DAG is proposed to relax the conditions of a standard IV.

Definition 11 (Conditional IV in DAG [2], [14]): Given a DAG \(\mathcal{G} = (X \cup U \cup \{W, Y\}, E)\), where \(X\) and \(U\) are measured and unmeasured variables, respectively. A variable \(S \in X\) is said to be a CIV w.r.t. \(W \rightarrow Y\), if there exists a set of measured variables \(Z \subseteq X\) such that 1) \(S \parallel_{d} W \mid Z, 2) S \parallel_{d} Y \mid Z\) in \(\mathcal{G}_W\) where \(\mathcal{G}_W\) is obtained by removing \(W \rightarrow Y\) from \(\mathcal{G}\), and 3) \(W \otimes Y \not\in De(Y)\).

For a CIV \(S\) as defined in Definition 11, \(Z\) is known to instrumentalize \(S\) in the given DAG. However, a variable may be a CIV when it has zero causal effect on \(W\), and this might

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result in a misleading conclusion. To mitigate this issue, AIV in DAG is proposed.

**Definition 12 (Ancestral IV in DAG [15]):** Given a DAG \( \mathcal{G} = (\mathbf{X} \cup \mathbf{U} \cup \{W, Y\}, \mathbf{E}) \), where \( \mathbf{X} \) and \( \mathbf{U} \) are measured and unmeasured variables, respectively. A variable \( S \in \mathbf{X} \) is said to be an AIV w.r.t. \( W \rightarrow Y \), if there exists a set of measured variables \( \mathbf{Z} \subseteq \mathbf{X} \setminus \{S\} \) such that (1) \( S \perp W \mid \{Z, \mathbf{Z}\} \), (2) \( \mathbf{Z} \) consists of an \( \mathcal{A}(Y) \) or \( \mathcal{A}(S) \) or both and \( \forall Z \in \mathbf{Z}, Z \notin \mathcal{D}(Y) \).

An AIV in DAG is a CIV in DAG, but a CIV may not be an AIV. AIV is a restricted version of CIV [15]. However, the applications of standard IV, CIV, and AIV are established in a complete causal DAG \( \mathcal{G} \), which greatly limits their capacity in real-world applications.

Recently, Cheng et al. [24] proposed the concept of AIV in MAG and the theorem for identifying a conditioning set \( \mathbf{Z} \) that instrumentalizes a given AIV in PAG. However, the work by Cheng et al. [24] assumes an AIV in MAG has been given, and the focus is on finding the conditioning set for the AIV in MAG from data. Our work in this article aims to find an AIV in MAG from data, which makes it possible for a complete data-driven search for AIVs.

**Proposition 1 (AIV in MAG [24]):** 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 \( \mathbf{U} \subseteq \mathbf{U} \), and the MAG \( \mathcal{M} = (\mathbf{X} \cup \{W, Y\}, \mathbf{E}) \) is mapped from \( \mathcal{G} \) based on the construction rules [18]. Then if \( S \) is an AIV conditioning on a set of measured variables \( \mathbf{Z} \subseteq \mathbf{X} \setminus \{S\} \) in \( \mathcal{G} \), \( S \) is an AIV conditioning on a set of measured variables \( \mathbf{Z} \subseteq \mathbf{X} \setminus \{S\} \) in \( \mathcal{M} \).

**Theorem 1 (Conditioning Set of a Given AIV in PAG [24]):** 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 \( \mathbf{U} \subseteq \mathbf{U} \), and let \( \mathcal{M} = (\mathbf{X} \cup \{W, Y\}, \mathbf{E}) \) be the MAG mapped from \( \mathcal{G} \). From data, the mapped MAG \( \mathcal{M} \) is represented by a PAG \( \mathcal{P} = (\mathbf{X} \cup \{W, Y\}, \mathbf{E}'') \). For a given AIV \( S \) which is a cause or spouse of \( W \), the set PossAn(\( S \cup Y \) \( \setminus \{W, S\} \)) in the learned PAG is a set that instrumentalizes \( S \) in the DAG \( \mathcal{G} \).

where PossAn(\( S \cup Y \)) is the union of the set of the possible ancestors of \( S \) and the set of the possible ancestors of \( Y \) in the causal DAG \( \mathcal{G} \). It is worth noting that Theorem 1 and the work in [24] are to discover the conditioning set for a given AIV, rather than discovering AIVs and the conditioning set simultaneously. Hence, discovering an AIV and its conditioning set simultaneously from data remains unresolved, and it is the problem to be addressed in this work.

### III. Discovering AIVs Based on Graphical Causal Modeling

In this section, we first introduce the generalized tetrad condition. Next, we propose a set of candidates’ AIVs in MAG. Then, we propose a theorem to guarantee that the generalized tetrad condition can be used to discover valid AIVs from data if there exists a pair of AIVs. Finally, we develop a practical data-driven algorithm for estimating \( \beta_w \) from data.

**A. Generalized Tetrad Condition**

Let \( S_i \) and \( S_j \) be a pair of CIVs given the conditioning set \( \mathbf{X} \setminus \{S_i, S_j\} \). Let \( \sigma_{s_i y z x}(\sigma_{s_j y z x}) \) denote the partial covariance of \( S_i(S_j) \) and \( Y \) given \( \mathbf{Z} \), and \( \sigma_{s_{iujw}}(\sigma_{s_{jujw}}) \) denote the partial covariance of \( S_i(S_j) \) and \( W \) given \( \mathbf{Z} \). Then, we have \( \beta_{wz} = \sigma_{s_{iujw}}/\sigma_{s_{iujw}} = \sigma_{s_{jujw}}/\sigma_{s_{jujw}} \), which gives us the following tetrad condition [9]:

\[
\sigma_{s_{iujw}}\sigma_{s_{jujw}} - \sigma_{s_{iujw}}\sigma_{s_{iujw}} = 0.
\]

The tetrad condition can be tested from data directly. It is a necessary condition for discovering valid CIVs, which means a pair of variables that are not valid CIVs can also satisfy the tetrad condition. However, the tetrad condition requires a conditioning set that instrumentalizes a pair of AIVs, and in this case, the tetrad condition may result in a biased estimate as discussed in the Introduction.

We consider a more general setting, where a pair of AIVs \( S_i \) and \( S_j \) have different conditioning sets \( \mathbf{Z}_i \subseteq \mathbf{X} \setminus \{S_i\} \) and \( \mathbf{Z}_j \subseteq \mathbf{X} \setminus \{S_j\} \), respectively, and \( \mathbf{Z}_i \) and \( \mathbf{Z}_j \) do not need to be equal. Let \( \sigma_{s_{iujw}}(\sigma_{s_{jujw}}) \) denote the partial covariance of \( S_i(S_j) \) and \( Y \) given \( \mathbf{Z}_i(\mathbf{Z}_j) \), and \( \sigma_{s_{iujw}}(\sigma_{s_{jujw}}) \) denote the partial covariance of \( S_i(S_j) \) and \( W \) given \( \mathbf{Z}_i(\mathbf{Z}_j) \). Then we have \( \beta_{wz} = \sigma_{s_{iujw}}/\sigma_{s_{iujw}} = \sigma_{s_{jujw}}/\sigma_{s_{jujw}} \), which gives us the following generalized tetrad condition:

\[
\sigma_{s_{iujw}}\sigma_{s_{jujw}} - \sigma_{s_{iujw}}\sigma_{s_{iujw}} = 0.
\]

In the DAG (b) in Fig. 1, \( \mathbf{Z}_1 = \emptyset \) instrumentalizes \( S_1 \) and \( \mathbf{Z}_2 = \{X_3\} \) instrumentalizes \( S_2 \). Hence, the pair of AIVs satisfies the generalized tetrad condition, i.e., \( \sigma_{s_{iujw}}\sigma_{s_{iujw}} - \sigma_{s_{iujw}}\sigma_{s_{iujw}} = 0 \).

In the following, we will show that the generalized tetrad condition can be used for finding a pair of AIVs in data if there exists a pair of AIVs. In comparison with the tetrad condition used in IV.tetrad [9], the search space of the generalized tetrad condition is larger since \( S_1, S_j, Z_i, \) and \( Z_j \) all vary. In Section III-B, we will develop a lemma to reduce the search space.

**B. Theory for Discovering AIVs in MAG**

We aim to develop a practical solution for discovering AIVs directly from data by leveraging the property of a MAG. In this work, we assume that there exist a pair of AIVs and their conditioning sets, and each AIV can be used to obtain an unbiased estimation of the causal effect from data with latent variables.

We first categorize AIVs into direct AIVs and indirect AIVs. When \( S \) is an AIV and it is an adjacent node of the treatment in the given DAG, its ancestral or adjacent nodes may be AIVs. We call \( S \) a direct AIV and the AIVs which are ancestral or adjacent nodes of \( S \) indirect AIVs if they satisfy Definition 12. For instance, Fig. 2 provides possible configurations of direct AIV and indirect AIV represented in MAGs relative to the invisible edge \( W \rightarrow Y \). In MAGs (a) and (b), \( S \) is a direct AIV, w.r.t. \( W \rightarrow Y \). In MAGs (c) and (d), \( S_i \) is an indirect AIV w.r.t. \( W \rightarrow Y \) since its validity relies on the direct AIV \( S \). Note that \( S_i \) is independent of \( W \) due to the collider at \( S \).

We consider direct AIVs as, in practice, indirect AIVs may not be collected in a dataset since it is independent of
the treatment. Practitioners collect relevant variables that are associated with both $W$ and $Y$. In the following discussions, all AIVs are direct AIVs. We have the following conclusion for discovering the direct AIVs in a MAG $M$.

**Lemma 1 (Direct AIV in MAG):** Given a DAG $G = (X \cup U \cup \{W, Y\}, E')$ with the edges $W \rightarrow Y$ and $W \leftarrow U \rightarrow Y$ in $E'$, and $U \subseteq U$, and let $\mathcal{M} = (X \cup \{W, Y\}, E) be the MAG mapped from $G$. If $S$ is a direct AIV in the DAG $G$, then $S \in \text{Adj}(Y) \setminus \{W\}$ in MAG $M$.

**Proof:** First, the edges $W \rightarrow Y$ and $W \leftarrow U \rightarrow Y$ in the given DAG are represented by an invisible edge $W \rightarrow Y$ in the mapped MAG $M$ since there is an inducing path relative to $U$ between $W$ and $Y$ [17], [18]. For an $S \subseteq X$ to be an eligible direct AIV in the DAG $G$, there are only two cases in the mapped MAG $M$. The first case is that $S$ has an edge $S \rightarrow W$, then $S$ must have an edge into $Y$, i.e., $S \in \text{Adj}(Y) \setminus \{W\}$, since otherwise $W \rightarrow Y$ in $M$ is visible, which contradicts the invisible edge $W \rightarrow Y$ in $M$. The second case is that $S$ has a collider path into $W$ and every collider on the path is in $\text{Pa}(Y)$, i.e., $S \| W | \text{Pa}(Y) \setminus \{W\}$, then $S$ must have an edge into $Y$, i.e., $S \in \text{Adj}(Y) \setminus \{W\}$, since otherwise $W \rightarrow Y$ in $M$ is visible, which contradicts the invisible edge $W \rightarrow Y$ in $M$. Therefore, all direct AIVs in the DAG $G$ are included in the set $S = \text{Adj}(Y) \setminus \{W\}$ of the mapped MAG $M$.

**Lemma 1** provides a set of candidate direct AIVs $\text{Adj}(Y) \setminus \{W\}$ and reduces the search space of a direct AIV, i.e., the search space of a direct AIV is reduced from $O(|X|)$ to $O(|\text{Adj}(Y) \setminus \{W\}|)$ where $|\text{Adj}(Y) \setminus \{W\}| \ll |X|$.

Next, we will develop a theorem to show that the generalized tetrads condition in (2) can be used to discover a pair of direct AIVs directly from data with latent variables.

**Theorem 2:** Given a DAG $G = (X \cup U \cup \{W, Y\}, E')$ with the edges $W \rightarrow Y$ and $W \leftarrow U \rightarrow Y$ in $E'$, and $U \subseteq U$, and let $\mathcal{M} = (X \cup \{W, Y\}, E) be the MAG mapped from $G$. Let $P = (X \cup \{W, Y\}, E')$ be the PAG which encodes the set of MAGs Markov equivalent to $\mathcal{M}$. If there exists a pair of direct AIVs $\{S, S_j\} \subseteq X$ in the DAG $G$, then $\{S, S_j\}$ must be in $\text{Adj}(Y) \setminus \{W\}$ in the PAG $P$. Moreover, the two sets, $Z_i = \text{possAn}(S) \cup Y \setminus \{W, S_i\}$ and $Z_{ij} = \text{possAn}(S) \cup Y \setminus \{W, S_i\}$ in the DAG $G$, respectively. Hence, (2) holds for $S_i$ and $S_j$ and their conditioning sets $Z_i$ and $Z_{ij}$.

**Proof:** According to Lemma 1, $\text{Adj}(Y) \setminus \{W\}$ in the mapped MAG $M$ is the set of candidate direct AIVs in the DAG $G$. Hence, the set $\text{Adj}(Y) \setminus \{W\}$ in the PAG $P$ must be the set of candidate direct AIVs because the mapped MAG $M$ is encoded in the PAG $P$. Thus, if $S \in X$ is a direct AIV in the DAG $G$, then $S \in \text{Adj}(Y) \setminus \{W\}$ in the PAG $P$, i.e., $\{S, S_j\} \subseteq S$ holds. According to Theorem 1, $Z_i = \text{possAn}(S) \cup Y \setminus \{W, S_i\}$ and $Z_{ij} = \text{possAn}(S) \cup Y \setminus \{W, S_i\}$ in the PAG $P$ instrumentalize $S_i$ and $S_j$ in the DAG $G$, respectively. Thus, we have $\beta_{ij} = \sigma_{s_i,s_j}/\sigma_{s_i,u,w,z_k} = \sigma_{s_i,s_j}/\sigma_{s_i,u,w,z_j}$. Therefore, $\sigma_{s_i,s_j}/\sigma_{s_i,v,w,z_k} - \sigma_{s_i,v,w,z_j} = 0$, i.e., (2) holds.

**Theorem 2** supports a data-driven algorithm to discover a pair of direct AIVs $\{S, S_j\}$ and their corresponding conditioning sets $Z_i$ and $Z_{ij}$ by utilizing the generalized tetrat condition. In the next section, based on the theorem, we will propose a practical algorithm for estimating $\beta_{ij}$ from data with latent variables.

Note that a significant number of direct AIVs are in both $\text{Adj}(W) \setminus \{Y\}$ and $\text{Adj}(Y) \setminus \{W\}$ in a MAG. Sometimes, they may be missed from $\text{Adj}(Y) \setminus \{W\}$ due to the false discoveries of the structure learning algorithm used [25], [26]. In the corresponding DAG, the direct AIVs are closer to $Y$. To avoid the random fluctuations without sacrificing much efficiency, in our developed practical algorithm, we extend the search space of Lemma 1 to $\text{Adj}(W \cup Y) \setminus \{W, Y\}$ where $\text{Adj}(W \cup Y)$ denotes the union of the set of adjacent nodes of $W$ and the set of adjacent nodes of $Y$. This only adds minor additional costs to the search process.

**C. Practical Algorithm for Estimating $\beta_{ij}$**

We develop a practical data-driven algorithm, AIV.GT (Ancestral IV based on Generalised Tetrat condition), for estimating $\beta_{ij}$ from data with latent variables. The pseudocode of AIV.GT is listed in Algorithm 1.

AIV.GT aims to search for the pair of AIVs from data directly without domain knowledge. The generalised tetrat condition in (2) is held by a pair of AIVs and their conditioning sets as described in Theorem 2 if there is a pair of IVs $\{S, S_j\}$ in data.

To obtain a reliable result, we propose a consistency score to assess which paired variables are the most likely AIVs based on the generalized tetrat condition. Let $\epsilon_{ij} = \{\sigma_{s_i,s_j}, \sigma_{s_i,s_j}, \sigma_{s_i,u,w,z_k}, \sigma_{s_i,u,w,z_j}, |, \delta_{ij} = |\hat{\beta}_i - \hat{\beta}_j|$, where $\hat{\beta}_i$ and $\hat{\beta}_j$ are the estimated causal effects of $W$ on $Y$ using $S_i$ and $S_j$ as an instrument, respectively. The consistency score is defined as $\lambda_{ij} = |\epsilon_{ij} - \delta_{ij}|$.

The justification of the consistency score is that $\epsilon_{ij}$ is expected to be close to 0, and the same with $\delta_{ij}$ if the variables $S_i$ and $S_j$ are AIVs. Theoretically, the pair of variables with either the smallest $\epsilon_{ij}$ or $\delta_{ij}$ is most likely to be the pair of IVs, but in practical cases, a pair of variables passing the
Algorithm 1 AIVs Based on the Generalized Tetrad Condition

1. **Input:** The set of pretreatment variables $X$, the treatment $W$, outcome $Y$, and the dataset $D$; $\alpha = 0.05$
2. **Output:** $\hat{\beta}_{WY}$, the causal effect of $W$ on $Y$, or NA, i.e., lacking knowledge
3. Recover a PAG $\mathcal{P}$ from $D$ using the rfci algorithm
4. Obtain $S = \text{Adj}(W \cup Y) \setminus \{W, Y\}$ from $\mathcal{P}$
5. if $|S| \leq 1$ then
   6. return NA
7. else
   8. for each $S_i \in S$ do
      9. $Z_i \leftarrow \text{PossAn}(S_i \cup Y) \setminus \{S_i, W, Y\}$
     10. $\hat{\beta}_i \leftarrow TSL(S, Y, S_i, Z_i, D)$
     11. end for
8. Initialize $Q = \emptyset$
9. for each pair $(S_i, S_j) \in S$ do
     10. if $\text{Test.tetrad}(W, Y, S_i, S_j, Z_i, Z_j, \mathcal{P}, \alpha)$ then
        11. \[ \epsilon_{ij} = \frac{\sigma_{S_iYWZ} - \sigma_{(S_iW)YZ} - \sigma_{S_jYWZ} + \sigma_{(S_jW)YZ}}{\sqrt{2}} \]
        12. \[ \lambda_{ij} = |\epsilon_{ij} - \delta_{ij}| \text{ where } \delta_{ij} = |\hat{\beta}_i - \hat{\beta}_j| \]
        13. $Q \leftarrow Q \cup \lambda_{ij}$
     14. end if
   15. end for
16. if $|Q| = \emptyset$ then
     17. return NA
   18. end if
19. return $\hat{\beta}_{WY} = \text{mean}(\hat{\beta}_i, \hat{\beta}_j)$
20. where the consistent score $\lambda_{ij}$ is the smallest in $Q$
21. end if
22. end if

Theorem 1. Line 10, the function $TSL(S)$ is the estimator of two-stage least squares (TSLS) using $S_i$ as an IV and conditioning on $Z_i$ for calculating $\hat{\beta}_i$.

The second part of AIV.GT is to discover the pair of AIVs. Line 12 is to initialize the set of consistency scores $Q$. Lines 13–19 are to check the validity of each pair of candidate AIVs based on Theorem 2. If the generalized tetrad condition holds on a pair of candidate AIVs, then calculate their consistency score. Line 14, the function $\text{Test.tetrad}()$ is implemented using the Wishart test w.r.t. the generalized tetrad condition [1], [29]. $\text{Test.tetrad}()$ returns TRUE if and only if the set of candidate pair variables returns a $p$-value greater than the significant level $\alpha$ ($\alpha = 0.05$ in this work). Lines 15–17 are to obtain the consistency score of each paired AIVs satisfying the generalized tetrad condition. In Lines 20 and 21, if $Q$ is an empty set, then no pair of variables has passed the tetrad condition test and the algorithm returns NA. In Lines 22–24, AIV.GT returns the mean causal effect of the pair of variables with the smallest $\lambda_{ij}$ in $Q$.

**Example 1:** We use the DAG (b) in Fig. 1 as a toy example to illustrate the AIV.GT algorithm. We have its MAG as in Fig. 3(a) and the corresponding PAG as in Fig. 3(b).

We assume that the true $\beta$ and each CIV gets the unbiased estimate.

We have $S = \text{Adj}(W \cup Y) \setminus \{W, Y\} = \{S_1, S_2, X_2, X_3\}$. For each variable in $S$, we have $Z_{S_1} = \{S_2, X_2, X_3\}$, $Z_{S_2} = \{S_1, X_2, X_3\}$, $Z_{S_3} = \{S_1, S_2, X_3\}$, and $Z_{S_4} = \{S_1, S_2, X_3\}$, respectively. Then, AIV.GT gets a set of candidate causal effects $\hat{\beta}_{S_1}$, $\hat{\beta}_{S_2}$, $\hat{\beta}_{S_3}$, and $\hat{\beta}_{S_4}$, respectively. Next, we go through the “for loop” (i.e., Lines 13–19). For these pairs $(S_1, S_2)$, $(S_1, X_2)$, $(S_2, X_2)$, $(X_2, X_3)$, only the pair $(S_1, S_2)$ passes the $\text{Test.tetrad}()$, and $Q \leftarrow 3$. Finally, AIV.GT returns $\hat{\beta}_{WY} = (\hat{\beta}_{S_1} + \hat{\beta}_{S_2})/2$.

**Time Complexity Analysis:** Three factors contribute to the time complexity of AIV.GT. The first contributing factor is the learning of a PAG $\mathcal{P}$ from data and finding $S$ from $\mathcal{P}$, which largely relies on the rfci algorithm. In the worst situation, rfci has a complexity of $O(2^n n)$, where $r$ is the maximum degree of a node in the underlying causal MAG and $n$ is the sample size. In most cases, the average degree of a causal Bayesian network is 2–5 [27], and most of the underlying MAGs are sparse in real-world applications. Hence, the time complexity of rfci is lower [28]. The complexity of Line 4 is $O(1)$ since it reads from $\mathcal{P}$. The second factor is estimating all possible causal effects, i.e., Lines 8–11 in Algorithm 1. Noting that obtaining $Z_i$ takes $O(1)$ and calculating $\hat{\beta}_i$ needs $O(n * p^2)$. Hence, the whole time complexity of this part is $O(|S| * n * p^2)$. The third factor is finding the pair of IVs from $S$ and time complexity.
complexity relies on the size of $S$ (pairwise search for a pair of IVs) and calculating covariance, which all together takes $O(|S|^2 * n * p^2)$. Therefore, the overall complexity of AIV.GT is $O(2^n * n + |S| * n * p^2 + |S|^2 * n * p^2) = O(2^n * n + |S|^2 * n * p^2)$. Therefore, the complexity of AIV.GT is largely attributed to the rfci algorithm and searching for a pair satisfying the generalized tetrad criterion.

IV. EXPERIMENTS

We assess the performance of AIV.GT by comparing it to the state-of-the-art causal effect estimators, first with a simulation study. Then, we conduct experiments on two real-world datasets that have been used for a long time in IV research [30], [31] to show that AIV.GT can be applied in real-world applications.

The estimators compared include: 1) least squares regression (LSR) $Y$ on $(W, X)$; 2) TSLS [32] of $Y$ on $W$ using all variables $X$ as standard IVs; 3) some invalid some valid IV estimator (sisVIVE) [12]; and 4) IV.tetrad method [9]. LSR is not an IV-based method. It is included since it is frequently used in machine learning disregarding bias of latent variables in data, and it is used as a baseline. All other three comparison estimators do not need a nominated IV. TSLS is a standard IV estimator, and it is also used as a baseline. sisVIVE and IV.tetrad are the two most related methods and have been discussed in the Introduction.

**Implementations of Estimators in Sections IV-A and IV-B2:** The method OLS is implemented by the function `cov` in R package `stats`. The TSLS is coded by the functions `cov` in R package `stats` and `solve` in the base. The implementation of LSR is the same with TSLS, i.e., using the functions `cov` and `solve`. The implementation of sisVIVE is based on the function `sisVIVE` in R package `sisVIVE`. The implementation of IV.tetrad is retrieved from the authors’ site: http://www.homepages.ucl.ac.uk/~ucgtlbl/code/iv_discovery. The parameter of `num_ivs` is set to 3 (2 for VitD).

AIV.GT is implemented using the functions rfci, in R package `pcalg`, and the functions in IV.tetrad, respectively. The implementation of AIV.GT is available here: https://github.com/chengdb2016/AIVGT.

**Implementations of Estimators in Section IV-B3:** The implementations of the compared estimators that require a known IV are introduced as follows. The estimator TSLS is implemented by the function `ivreg` in R package `AER` [33]. The implementation of TSLS.CIV is based on the functions `glm` and `ivglm` from R packages `stats` and `ivtools` [31]. FIVR is implemented by the function `instrumental_forest` in R package `grf` [21].

All parameters in FIVR are default. AIViP is implemented by the functions `rfci` in R package `pcalg` [26], `glm` in R package `stats`, and `ivglm` in R package `ivtools` [31].

**Evaluation Metrics and Parameter Setting:** For the simulation study, we have the ground truth of $\beta_{wy}$, so we report the estimation bias: $|\hat{\beta}_{wy} - \beta_{wy}| * 100\%$. In the experiments with real-world datasets, we empirically evaluate all estimators, and then compare AIV.GT with four additional IV-based estimators that require a nominated IV. The significant-level $\alpha$ is set to 0.05 for the functions of `rfci` and `Test.tetrad()` in all experiments.

A. Simulation Study

The goal of this set of experiments is to test the effectiveness of AIV.GT with and without colliders in the covariate set in comparison with various causal effect estimators. We utilize five true DAGs over $X \cup \{W, Y\}$ to generate five synthetic datasets with latent variables. The five true DAGs are shown in Fig. 4. In addition to the variables in the five true DAGs, 20 additional measured variables for each dataset are generated as noise variables that are related to each other but not to the variables in the five DAGs. The additional 20 variables are generated by a multivariate normal distribution. Each synthetic dataset has 2000 samples. To ensure the existence of the pair of CIVs and their conditioning sets (maybe $\emptyset$), we use the ground-truth CIVs and conditioning sets in the TSLS.CIV method to get an estimate. We use the generated datasets with the estimate $\hat{\beta}_{wy}$ closing to the true causal effect. Next, we will separately introduce the details of each synthetic dataset generation based on the five true DAGs in Fig. 4.

The synthetic dataset (a) is generated from the DAG (a) in Fig. 4, and the specifications are as follows: $U_1 \sim Bernoulli(0.5)$ and $S_1, S_2 \sim N(0, 1)$, in which $N(,)$ denotes the normal distribution. The treatment $W$ is generated from $n \times n$ (denotes the sample size) Bernoulli trials using the assignment probability $P(W = 1 | U_1, S_1, S_2) = [1 + exp(1 - 3 * U_1 - 3 * S_1 - 3 * S_2)]$. The potential outcome is generated from $Y_W = 2 + 2 * W + 3 * U_1 + \epsilon_w$ where $\epsilon_w \sim N(0, 1)$.

The synthetic dataset (b) is generated from the DAG (b) in Fig. 4, and the specifications are as follows: $U_1 \sim Bernoulli(0.5), S_1, S_2 \sim N(0, 1)$ and $\epsilon_{X_1} \sim N(0, 0.5)$. The measured variable $X_1 = 0.8 * S_2 + \epsilon_{X_1}$. The treatment $W$ is generated by $P(W = 1 | U_1, S_1, S_2) = [1 + exp(1 - 3 * U_1 - 3 * S_1 - 3 * S_2)]$. The potential outcome is generated from $Y_W = 2 + 2 * W + 3 * U_1 + 3 * X_1 + \epsilon_w$. 

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TABLE I
SATISFACTION (TICK)/VIOLATION (CROSS) OF THE ASSUMPTIONS OF A METHOD BY A DATASET. “✓?” MEANS THE PROBLEM OF COLLIDER BIAS SUFFERED BY IV.TETRAD

| Methods  | (a) | (b) | (c) | (d) | (e) |
|----------|-----|-----|-----|-----|-----|
| LSR      | ✓   | ✓   | ✓   | ✓   | ✓   |
| TSLS     | ✓   | ✓   | ✓   | ✓   | ✓   |
| sisVIVE  | ✓   | ✓   | ✓   | ✓   | ✓   |
| IV.tetrad| ✓   | ✓   | ✓?  | ✓?  | ✓?  |
| AIV.GT   | ✓   | ✓   | ✓   | ✓   | ✓?  |

Fig. 5. Estimation bias (%) of the estimators on five synthetic datasets. AIV.GT has the smallest bias on all datasets.

The synthetic dataset (c) is generated from the DAG(c) in Fig. 4, and the specifications are as follows: 
\[ U_1 \sim \text{Bernoulli}(0.5), S_1, S_2, U_2, X_2 \sim N(0, 1) \text{ and } \epsilon_{X_1} \sim N(0, 0.5). \]
The measured variable \( X_1 \) is generated by \( X_1 = 0.3 + S_1 + X_2 + U_2 + \epsilon_{X_1}. \) The treatment \( W \) is generated by \( P(W = 1 | U_1, S_1, S_2) = [1 + \exp(1 - 3 * U_1 - 3 * S_1 - 3 * S_2)]. \) The potential outcome is generated from \( Y_W = 2 + 2 * W + 3 * \epsilon_{S_1} + 3 * U_1 + 3 * S_1 + 2 * X_2 + 2 * X_2 + \epsilon_w. \)

The synthetic dataset (d) is generated from the DAG (d) in Fig. 4, and the specifications are as follows: 
\[ U_1 \sim \text{Bernoulli}(0.5), S_1, S_2, U_2, X_2 \sim N(0, 1) \text{ and } \epsilon_{X_1}, \epsilon_{X_2} \sim N(0, 0.5). \]
The measured variables \( X_1 \) and \( X_2 \) are generated by \( X_1 = 0.3 + S_1 + X_2 + 1.5 * U_2 + \epsilon_{X_1} \) and \( X_2 = 0.8 * \epsilon_{S_2} + \epsilon_{X_2}, \) respectively. The treatment \( W \) is generated by \( P(W = 1 | U_1, S_1, S_2) = [1 + \exp(-3 * U_1 - 3 * S_1 - 3 * S_2)]. \) The potential outcome is generated by \( Y_W = 2 + 2 * W + 3 * U_1 + 2 * S_2 + 2 * U_2 + 2 * X_2 + 2 * X_2 + \epsilon_w. \)

The synthetic dataset (e) is generated from the DAG (e) in Fig. 4, and the specifications are as follows: 
\[ U_1 \sim \text{Bernoulli}(0.5), S_1, S_2, U_2, X_2 \sim N(0, 1) \text{ and } \epsilon_{X_1}, \epsilon_{X_2} \sim N(0, 0.5). \]
The measured variables \( X_1 \), \( X_3 \), and \( X_4 \) are generated by \( X_1 = 0.3 + S_1 + X_2 + 1.5 * U_2 + \epsilon_{X_1} \), \( X_3 = 0.8 * S_2 + \epsilon_{X_1} \), and \( X_4 = 0.8 * S_2 + \epsilon_{X_2}, \) respectively. The treatment \( W \) is generated by \( P(W = 1 | U_1, S_1, S_2) = [1 + \exp(-3 * U_1 - 3 * S_1 - 3 * S_2)]. \) The potential outcome is generated by \( Y_W = 2 + 2 * W + 3 * \epsilon_{S_1} + 2 * U_1 + 2 * S_2 + 2 * U_2 + 2 * X_3 + 2 * X_3 + \epsilon_w. \)

The suitability of datasets with the method requirements is summarized as Table I.

Results: The estimation biases AIV.GT and the four compared estimators on the synthetic datasets are visualized in Fig. 5. From Fig. 5, we have the following observations: 1) The biases of LSR are large on all datasets. This is because it does not consider any bias of latent variables in data; 2) TSLS has a low bias on dataset (a) because \( S_1 \) and \( S_2 \) are standard IVs in this dataset. It has large biases on all other datasets since there are no standard IVs in the datasets; 3) sisVIVE works well on the first three datasets, i.e., (a) - (c), since its requirement (i.e., a half of covariates are IVs) is satisfied. It works poorly on datasets (d) and (e) because the assumption is violated; 4) IV.tetrad has a low bias on the first two datasets, but large biases on the last three datasets because the last three datasets contain colliders in the covariate sets. All datasets satisfy the assumption of IV.tetrad (i.e., a pair of CIVs), but it suffers from the problem of collider bias as identified in this article; and 5) AIV.GT obtains consistent results and has the lowest bias on all datasets.

Moreover, we report the identified AIVs, as well as the conditioning sets by AIV.GT with IV.tetrad methods on the five synthetic datasets in Table II. From Table II, we have 1) AIV.GT identifies the correct pair of AIVs and the conditioning sets on all synthetic datasets and 2) IV.tetrad identifies the correct pair of AIVs and the conditioning sets on the first two datasets, but identifies either the wrong pair of AIVs, the wrong conditioning sets or both on the three other datasets. Note that the wrong conditioning sets contain the collider \( X_1 \) leading to a collider bias. Therefore, AIV.GT can identify the AIVs and conditioning sets more accurately than IV.tetrad.

In sum, AIV.GT is able to identify the correct pair of AIVs and the conditioning sets for obtaining an unbiased \( \hat{\beta}_w \) from data with latent variables when there exists a pair of AIVs. AIV.GT overcomes the collider bias suffered by IV.tetrad.

B. Experiments on Two Real-World Datasets

It is challenging to evaluate the performance of causal effect estimators, including AIV.GT on real-world datasets because the ground truth causal DAG and \( \hat{\beta}_w \) are not available. We select two real-world datasets with empirical estimates available in the literature, including Vitamin D data (VitD) [31], [34] and Schooling returns [30]. The two datasets have been extensively studied and analyzed before and each has a nominated AIV. Therefore, it is credible to choose them as the benchmark datasets to evaluate AIV.GT.

The two datasets have the nominated AIV w.r.t. \( (W, Y) \), but the conditioning sets are unknown. There is not an available algorithm in the literature to discover the conditioning set that instrumentalizes the nominated AIV on both datasets. Therefore, we divide the experiments on both datasets into two parts: 1) experiments on AIV.GT in comparison with four estimators without nominated AIVs and 2) experiments

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comparing AIV.GT with four additional IV estimators that require a nominated IV.

1) Details of the Two Real-World Datasets:

a) Vitamin D (VitD): This dataset was collected from a cohort study of vitamin D status on mortality, i.e., the potential effect of VitD on death, as in [34]. The dataset contains 2571 individuals and five 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) [31]. A measured value of vitamin D less than 30 nmol/L implies vitamin D deficiency. We take the estimated \( \hat{\beta}_{w} = 2.01 \) with 95% confidence interval (0.96, 4.26) from the literature [34] as the reference causal effect.

b) Schoolingreturns: This dataset is from the national longitudinal survey of youth (NLSY) of US young employees, aged range from 24 to 34 [30]. The dataset contains 3010 individuals and 19 variables. The treatment is the education of employees, and the outcome is raw wages in 1976 (in cents per hour). The covariates include experience (years of labor market experience), ethnicity (a factor indicating ethnicity), resident information of an individual, age, nearcollege (whether an individual grew up near a 4-year college), Education in 1966 (education66), marital status, father’s educational attainment (feducation), mother’s educational attainment (meducation), Ordered factor coding family education class (fameducation), and so on. A goal of the studies on this dataset is to investigate the causal effect of education on earnings. We take \( \hat{\beta}_{w} = 13.29\% \) with 95% confidence interval (0.0484, 0.2175) from [35] as the reference causal effect.

2) Comparing AIV.GT With the Estimators Without Requiring a Known IV: We conduct experiments on the two real-world datasets to assess AIV.GT against the four estimators that do not require nominated IV as in Section IV-A with the simulated data. All experimental results are visualized in Fig. 6 for VitD and Schoolingreturns, respectively.

a) Results on VitD: From Fig. 6, we have the following observations: 1) the estimated result of LSR is close to 0 and far away from the 95% confidence interval of the empirical estimation and 2) the estimated results of TSLS, sisVIVE, IV.tetrad, and AIV.GT are close to the reference causal effect 2.01 and fall into the 95% confidence interval.

b) Results on Schoolingreturns: According to Fig. 6, we have the following findings: 1) the estimated result of TSLS is at the bottom of the 95% confidence interval; 2) the estimated results of LSR and sisVIVE fall outside of the empirical interval. It is very likely that their assumptions have not been satisfied; and 3) the estimated results of IV.tetrad and AIV.GT are in the empirical interval. They are consistent with the reference causal effect [35]. The consistency between the results of IV.tetrad and AIV.GT is likely due to the reason that they have found proper conditional settings.

The experiments show that AIV.GT can obtain consistent estimations in both real-world datasets.

3) Comparing AIV.GT With the Estimators With Known IVs: We add the four more comparison methods that require the given IVs, which are 1) TSLS.IV, TSLS with a given IV, 2) TSLS.CIV [36], TSLS with a given CIV S by conditioning on X \ {S}, 3) FIVR, causal random forest for IV regression with a given CIV S and conditioning on X \ {S} [21], and 4) AIVP [24], AIV estimator in PAG.

The two datasets have nominated IVs in the literature. The indicator of filaggrin was used as an IV in VitD [34] and Card [30] used geographical proximity to a college, i.e., nearcollege as an IV in Schoolingreturns. All results of the above four estimators and AIV.GT are visualized in Fig. 7.

a) Results on VitD: AIV.GT discovers \( \hat{\beta}_{w} \) as a pair of AIVs. They are reasonable AIVs since they affect W (vitd, vitamin D status) but do not directly affect Y (death). From Fig. 7, we see that the results of TSLS.IV, AIVP, and AIV.GT are in the middle of 95% empirical interval estimations.

b) Results on Schoolingreturns: AIV.GT discovers the set \{feducation, fameducation\} as a pair of AIVs. They are valid IVs because father’s educational attainment and family education class affect their child’s education, but do not directly affect the child’s income. From Fig. 7, we see that the results of TSLS.IV, AIVP, and AIV.GT are in the middle of the 95% empirical interval of the reference causal effect.

In a word, AIV.GT, which does not need given AIVs, performs better or is comparable with other methods which require a given IV. This shows the potential of the AIV.GT in a broader range of real-world applications.

c) Limitations: The proposed AIV.GT requires that there exist at least a pair of AIVs and the correctness of the recovered PAG. It is important to carefully check whether the recovered PAG is consistent with domain knowledge since learning a PAG from data is error prone. It is recommended to combine other algorithms, such as sensitive analysis [35], [37].
with AIV.GT when there is uncertainty about the existence of a pair of AIVs.

V. RELATED WORK

Latent variables are the major obstacle to estimating causal effect from observational data [2], [38], [39], [40]. When the treatment and outcome are confounded, IV methods [2], [7], [14], [15], [32], [41], [42], [43] provide a solution. Some methods have been developed for standard IV-based causal effect estimation when the IVs are given by domain experts [41], such as the well-known TSLS IV estimator [32] which obtains causal effect using the ratio of two regression coefficients. Recently, Athey et al. [21] developed the generalized random forests to estimate conditional causal effects using nonparametric quantile regression and IV regression (FIVR). The conditional causal effects can be aggregated into the average causal effect and FIVR has been compared in our experiments. We refer readers to [7], [23], and [44] for a review of standard IV-based methods.

When a CIV is given, a proper conditioning set needs to be identified for unbiased causal effect estimation. Cheng et al. [24] have proposed a data-driven method AIViP for identifying such a conditioning set for causal effect estimation with a given CIV. Our work is different from these works since we focus on discovering AIVs and the corresponding conditioning set simultaneously from data and the proposed method is more general than the existing methods.

The CIV approach is very similar to the approach of covariate adjustment since both of them need to identify a proper conditioning set. However, there are essential differences between CIV and covariate adjustment. Most methods for covariate adjustment assume not a latent variable between W on Y [2], [19], [45]. There are four graphical criteria for identifying a proper conditioning set from a causal graph: back-door criterion [2], adjustment criterion [46], generalized back-door criterion [45], and generalized adjustment criterion [19]. There are some data-driven methods based on the four graphical criteria [47], [48], [49]. More detailed discussions for covariate selection can be found in [50], [51], and [37]. There are no works for finding a conditioning set when the pair of (W, Y) are confounded as discussed in this work.

VI. CONCLUSION

Estimating causal effects in the presence of latent variables is a challenging problem. IV is a well-known approach to address this challenge. However, most existing IV methods require strong domain knowledge or assumptions to determine an IV. This restricts the practical use of the IV approach. In this article, we present the theory and a practical algorithm (AIV.GT) for finding valid AIVs and their corresponding conditioning sets from data, to enable data-driven causal effect estimation from data with latent variables. The experiments on synthetic datasets demonstrate that AIV.GT is able to address the challenges of latent variables and outperform the state-of-the-art causal effect estimators. The experimental results on two real-world datasets also show that AIV.GT achieves consistent results with empirical estimates in the literature, implying the practicability of AIV.GT in real-world applications.

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