Identifying causal effects in maximally oriented partially directed acyclic graphs

Emilija Perković
Department of Statistics
University of Washington, USA
perkovic@uw.edu

October 9, 2019

Abstract

We develop a necessary and sufficient causal identification criterion for maximally oriented partially directed acyclic graphs (MPDAGs). MPDAGs as a class of graphs include directed acyclic graphs (DAGs), completed partially directed acyclic graphs (CPDAGs), and CPDAGs with added background knowledge. As such, they represent the type of graph that can be learned from observational data and background knowledge under the assumption of no latent variables. Our identification criterion can be seen as a generalization of the g-formula of Robins (1986). We further obtain a generalization of the truncated factorization formula for DAGs (Pearl, 2009) and compare our criterion to the generalized adjustment criterion of Perković et al. (2017).

1 INTRODUCTION

The gold standard method for answering causal questions are randomized controlled trials. In some cases, however, it may be impossible, unethical, or simply too expensive to perform a desired experiment. For this purpose, it is of interest to consider whether a causal effect can be identified from observational data.

Remarkably, Jaber et al. (2019) recently gave an answer to this question in the form of a graphical algorithm that is necessary and sufficient for identifying causal effects from observational data that allows for hidden confounders. The class of graphs that Jaber et al. (2019) consider is fully characterized by conditional independences in the observed probability distribution of the data.

Surprisingly, however, identifying causal effects from observational data under the assumption of no hidden variables is still an open problem. The most relevant recent work on this topic is the generalized adjustment criterion of Perković et al. (2017, 2018) which is sufficient but not necessary for the identification of causal effects.

In this paper, we develop a necessary and sufficient graphical criterion for identifying causal effects under the assumption of no hidden variables. We refer to our identification criterion (Theorem 3.5) as the causal identification formula. Our result gives a closed-form solution to the causal identification problem. Furthermore, our criterion allows the inclusion of additional background knowledge in the form of certain partial causal orderings (see Meek, 1995).
The causal identification formula can be seen as a generalization of the g-formula of Robins (1986). Consequently, we also obtain a generalization of the truncated factorization formula (Pearl, 2009), i.e. the manipulated density formula (Spirtes et al., 2000) in Corollary 3.7.

The g-formula is one of the causal identification methods that has seen considerable use in practice (see e.g. Taubman et al., 2009; Young et al., 2011; Westreich et al., 2012). Until now, however, it was not possible to apply the g-formula to graphs learned from observational data.

From a theoretical perspective, it is of interest to note that the proof of our causal identification formula does not consider intervening on additional variables in the graph. This is in contrast to most current necessary and sufficient graphical results for causal identification including Jaber et al. (2019).

Furthermore, even though the generalized adjustment criterion of Perković et al. (2017) is not complete for causal identification, we characterize a special case in which it is “almost” complete (Proposition 4.2). All omitted proofs can be found in the Appendix.

**Related Work.** Directed acyclic graphs (DAGs, e.g. Pearl, 2009) are used to reason about the underlying causal system. If the causal DAG is known and all variables in the causal system are observed, then all causal effects can be identified and estimated from observational data (see e.g. Robins, 1986; Pearl, 1995; Pearl and Robins, 1995; Galles and Pearl, 1995). If some variables in the causal DAG are not observed, certain causal effects are not identifiable from the observational data even when the causal DAG is known. But the complete set of identifiable causal effects is well understood (see e.g. Tian and Pearl, 2002; Shpitser and Pearl, 2006; Huang and Valtorta, 2006; Richardson et al., 2017; Jaber et al., 2019).

In general, however, it is not possible to learn the underlying causal DAG from observational data. When all variables in the causal system are observed, one can at most learn a completed partially directed acyclic graph (CPDAG, Meek, 1995; Andersson et al., 1997; Spirtes et al., 2000; Chickering, 2002). A CPDAG represents a Markov equivalence class of DAGs (see Section 2 for definitions).

If in addition to observational data one has background knowledge of the partial orderings of some variables, data from previous experiments, or specific model restrictions, one can obtain a maximally oriented partially directed acyclic graph (MPDAG) which uniquely represents a refinement of the Markov equivalence class of DAGs (Meek, 1995; Scheines et al., 1998; Hoyer et al., 2008; Hauser and Bühlmann, 2012; Eigenmann et al., 2017; Wang et al., 2017; Rothenhäusler et al., 2018). Since DAGs and CPDAGs can be seen as special types of MPDAGs, we will use MPDAGs to refer to all three of these types of graphs.

When latent variables are present, one can at most learn a partial ancestral graph (PAG) over the set of observed variables from the observed data (Richardson and Spirtes, 2002; Spirtes et al., 2000; Zhang, 2008a,b). PAGs represents an equivalence class of DAGs over the full set of observed and unobserved variables.

The topic of identifying causal effects in MPDAG and PAGs has generated a wealth of research in recent years. Perković et al. (2015, 2018) and Perković et al. (2017) build on prior work of Pearl (1993); Shpitser et al. (2010); van der Zander et al. (2014) and Maathuis and Colombo (2015) to develop a graphical criterion that identifies all causal effects in MPDAGs and PAGs that are identifiable through covariate adjustment. Their criterion is sufficient, but not necessary for identifying causal effects in MPDAGs and PAGs.

On the other hand, Jaber et al. (2019) build on previous work of Tian and Pearl (2002); Shpitser and Pearl (2006); Huang and Valtorta (2006) to develop a recursive graphical
algorithm that is both necessary and sufficient for identifying causal effects in PAGs. The identification algorithm of Jaber et al. (2019) is not designed with MPDAGs in mind and hence, does not exploit the additional information they provide. In fact, naively simplifying the strategies used by Jaber et al. (2019) for causal identification in PAGs would not lead to a complete causal identification algorithm in MPDAGs. See the motivating examples (Examples 3.8 and 4.3) for an illustration of this.

2 PRELIMINARIES

We use capital letters (e.g. \( X \)) to denote nodes in a graph as well as random variables that these nodes represent. Similarly, bold capital letters (e.g. \( \textbf{X} \)) are used to denote both sets of nodes in a graph as well as the random vectors that these nodes represent.

Nodes, Edges And Subgraphs. A graph \( \mathcal{G} = (\mathbf{V}, \mathbf{E}) \) consists of a set of nodes (variables) \( \mathbf{V} = \{X_1, \ldots, X_p\} \) and a set of edges \( \mathbf{E} \). The graphs we consider are allowed to contain directed (\( \rightarrow \)) and undirected (\( \sim \)) edges and at most one edge between any two nodes. An induced subgraph \( \mathcal{G}_\mathbf{V'} = (\mathbf{V'}, \mathbf{E}') \) of \( \mathcal{G} = (\mathbf{V}, \mathbf{E}) \) consists of \( \mathbf{V}' \subseteq \mathbf{V} \) and \( \mathbf{E}' \subseteq \mathbf{E} \) where \( \mathbf{E}' \) are all edges in \( \mathbf{E} \) between nodes in \( \mathbf{V}' \). An undirected subgraph \( \mathcal{G}_\text{undir} = (\mathbf{V}, \mathbf{E}') \) of \( \mathcal{G} = (\mathbf{V}, \mathbf{E}) \) consists of \( \mathbf{V} \) and \( \mathbf{E}' \subseteq \mathbf{E} \) where \( \mathbf{E}' \) are all undirected edges in \( \mathbf{E} \).

Paths. A path \( p \) from \( X \) to \( Y \) in \( \mathcal{G} \) is a sequence of distinct nodes \( \{X, \ldots, Y\} \) in which every pair of successive nodes is adjacent. A path consisting of undirected edges in an undirected path. A causal path from \( X \) to \( Y \) is a path from \( X \) to \( Y \) in which all edges are directed towards \( Y \), that is, \( X \rightarrow \cdots \rightarrow Y \). Let \( p = (X = V_0, \ldots, V_k = Y) \), \( k \geq 1 \) be a path in \( \mathcal{G} \), \( p \) is a possibly causal path if no edge \( V_i \leftarrow V_j, 0 \leq i < j \leq k \) is in \( \mathcal{G} \). Otherwise, \( p \) is a non-causal path in \( \mathcal{G} \) (see Definition 3.1 and Lemma 3.2 of Perković et al., 2017) (Lemma A.4 in the Appendix). For two disjoint subsets \( \mathbf{X} \) and \( \mathbf{Y} \) of \( \mathbf{V} \), a path from \( \mathbf{X} \) to \( \mathbf{Y} \) is a path from some \( X \in \mathbf{X} \) to some \( Y \in \mathbf{Y} \). A path from \( \mathbf{X} \) to \( \mathbf{Y} \) is proper (w.r.t. \( \mathbf{X} \)) if only its first node is in \( \mathbf{X} \).

Partially Directed And Directed Cycles. A causal path from \( X \) to \( Y \) and the edge \( Y \rightarrow X \) form a directed cycle. A partially directed cycle is formed by a possibly causal path from \( X \) to \( Y \), together with \( Y \rightarrow X \).

Ancestral Relationships. If \( X \rightarrow Y \), then \( X \) is a parent of \( Y \). If there is a causal path from \( X \) to \( Y \), then \( X \) is an ancestor of \( Y \), and \( Y \) is a descendant of \( X \). If there is a possibly causal path from \( X \) to \( Y \), then \( X \) is a possible ancestor of \( Y \). We use the convention that every node is a descendant, ancestor, and possible ancestor of itself. The sets of parents, ancestors, possible ancestors and descendants of \( X \) in \( \mathcal{G} \) are denoted by \( \text{Pa}(X, \mathcal{G}) \), \( \text{An}(X, \mathcal{G}) \), \( \text{PossAn}(X, \mathcal{G}) \) and \( \text{De}(X, \mathcal{G}) \) respectively. For a set of nodes \( \mathbf{X} \subseteq \mathbf{V} \), we let \( \text{Pa}(\mathbf{X}, \mathcal{G}) = (\cup_{X \in \mathbf{X}} \text{Pa}(X, \mathcal{G})) \setminus \mathbf{X} \), whereas, \( \text{An}(\mathbf{X}, \mathcal{G}) = \cup_{X \in \mathbf{X}} \text{An}(X, \mathcal{G}) \), \( \text{PossAn}(\mathbf{X}, \mathcal{G}) = \cup_{X \in \mathbf{X}} \text{PossAn}(X, \mathcal{G}) \), and \( \text{De}(\mathbf{X}, \mathcal{G}) = \cup_{X \in \mathbf{X}} \text{De}(X, \mathcal{G}) \).

Colliders, Shields, And Definite Status Paths. If a path \( p \) contains \( X_i \rightarrow X_j \leftarrow X_k \) as a subpath, then \( X_j \) is a collider on \( p \). A path \( \langle X_i, X_j, X_k \rangle \) is an unshielded triple if \( X_j \) and \( X_k \) are not adjacent. A path is unshielded if all successive triples on the path are unshielded. A node \( X_j \) is a definite non-collider on a path if the edge \( X_i \leftarrow X_j \), or the edge \( X_j \rightarrow X_k \) is on \( p \), or if \( X_i - X_j - X_k \) is a subpath of \( p \) and \( X_i \) is not adjacent to \( X_k \). A node is of definite status on a path if it is a collider, a definite non-collider or an endpoint on the path. A path \( p \) is of definite status if every node on \( p \) is of definite status.

D-connection And Blocking. A definite status path \( p \) from \( X \) to \( Y \) is \( d \)-connecting given a node set \( Z \) (\( X, Y \notin Z \)) if every definite non-collider on \( p \) is not in \( Z \), and every
collider on \( p \) has a descendant in \( Z \). Otherwise, \( Z \) blocks \( p \). If \( Z \) blocks all definite status paths between \( X \) and \( Y \) in MPDAG \( \mathcal{G} \), then \( X \) is \( d \)-separated from \( Y \) given \( Z \) in \( \mathcal{G} \) (Lemma C.1 of Henckel et al., 2019).

**DAGs, PDAGs.** A directed graph contains only directed edges. A partially directed graph may contain both directed and undirected edges. A directed graph without directed cycles is a directed acyclic graph (DAG). A partially directed acyclic graph (PDAG) is a partially directed graph without directed cycles.

**Markov Equivalence And CPDAGs.** (c.f. Meek, 1995; Andersson et al., 1997) All DAGs that encode the same \( d \)-separation relationships are Markov equivalent and form a Markov equivalence class of DAGs, which can be represented by a completed partially directed acyclic graph (CPDAG).

**MPDAGs.** A PDAG \( \mathcal{G} \) is a maximally oriented PDAG (MPDAG) if and only if the graphs in Figure 1 are not induced subgraphs of \( \mathcal{G} \). Both a DAG and a CPDAG are types of MPDAG (Meek, 1995).

**\( \mathcal{G} \) And \( [\mathcal{G}] \).** A DAG \( \mathcal{D} \) is represented by MPDAG \( \mathcal{G} \) if \( \mathcal{D} \) and \( \mathcal{G} \) have the same adjacencies, same unshielded colliders and if for every directed edge \( X \to Y \) in \( \mathcal{G} \), \( X \to Y \) is in \( \mathcal{D} \) (Meek, 1995). If \( \mathcal{G} \) is a MPDAG, then \( [\mathcal{G}] \) denotes the set of all DAGs represented by \( \mathcal{G} \).

**Partial Causal Ordering.** Let \( \mathcal{D} = (V, E) \) be a DAG. A total ordering, \( \prec \), of nodes \( V' \subseteq V \) is consistent with \( \mathcal{D} \) and called a causal ordering of \( V' \) if for every \( x_i, x_j \in V' \), such that \( x_i \prec x_j \) and such that \( x_i \) and \( x_j \) are adjacent in \( \mathcal{D} \), \( x_i \to x_j \) is in \( \mathcal{D} \). There can be more than one causal ordering of \( V' \) in a DAG \( \mathcal{D} = (V, E) \). For example, in DAG \( X_i \leftarrow X_j \to X_k \) both orderings \( X_j < X_i < X_k \) and \( X_j < X_k < X_i \) are consistent.

Let \( \mathcal{G} = (V, E) \) be an MPDAG. Since \( \mathcal{G} \) may contain undirected edges, there is generally no causal ordering of \( V' \), for a node set \( V' \subseteq V \) in \( \mathcal{G} = (V, E) \). Instead, we define a partial causal ordering, \( \prec \), of \( V' \) in \( \mathcal{G} \) as a total ordering of pairwise disjoint node sets \( A_1, \ldots, A_k \), \( k \geq 1, \bigcup_{i=1}^{k} A_i = V' \), that satisfies the following: if \( A_i < A_j \) and there is an edge between \( A_i \in A_i \) and \( A_j \in A_j \) in \( \mathcal{G} \), then \( A_i \to A_j \) in \( \mathcal{G} \).

**Do-intervention.** We consider interventions \( do(X = x) \) (for \( X \subseteq V \)) or \( do(x) \) for shorthand, which represent outside interventions that set \( X \) to \( x \).

**Observational And Interventional Densities.** A density \( f \) of \( V \) is consistent with a DAG \( \mathcal{D} = (V, E) \) if it factorizes as \( f(v) = \prod_{V_i \in V} f(v_i | pa(v_i, D)) \) (Pearl, 2009). A density \( f \) that is consistent with \( \mathcal{D} = (V, E) \) is also called an observational density.

Let \( X \) be a subset of \( V \) and \( V' = V \setminus X \) in a DAG \( \mathcal{D} \). A density over \( V' \) is denoted by \( f(V' | do(x)) \), or \( f_X(v') \), and called an interventional density consistent with \( \mathcal{D} \) if there is an observational density \( f \) consistent with \( \mathcal{D} \) such that \( f(V' | do(x)) \) factorizes as

\[
  f(V' | do(x)) = \prod_{V_i \in V'} f(v_i | pa(v_i, D)), \tag{1}
\]
Figure 2: (a) MPDAG $\mathcal{C}$, (b) MPDAG $\mathcal{G}$.

for values $\text{pa}(v, D)$ of $\text{Pa}(V, D)$ that are in agreement with $x$. If $X = \emptyset$, we define $f(v|\text{do}(\emptyset)) = f(v)$. Equation (1) is known as the truncated factorization formula (Pearl, 2009), manipulated density formula (Spirtes et al., 2000) or the g-formula (Robins, 1986). A density $f$ of $V$ is consistent with a MPDAG $\mathcal{G} = (V, E)$ if $f$ is consistent with a DAG in $[\mathcal{G}]$.

A density $f(v'|\text{do}(x))$ of $V' \subset V$, $X = V \setminus V'$ is an interventional density consistent with an MPDAG $\mathcal{G} = (V, E)$ if it is an interventional density consistent with a DAG in $[\mathcal{G}]$. Let $Y \subset V'$, and let $f(v'|\text{do}(x))$ be an interventional density consistent with an MPDAG $\mathcal{G} = (V, E)$ for some $X \subset V$, $V' = V \setminus X$, then $f(y|\text{do}(x))$ denotes the marginal density of $Y$ calculated from $f(v'|\text{do}(x))$.

**Probabilistic implications of d-separation.** Let $f$ be any density over $V$ consistent with an MPDAG $\mathcal{G} = (V, E)$ and let $X, Y$, and $Z$ be pairwise disjoint node sets in $V$. If $X$ and $Y$ are d-separated given $Z$ in $\mathcal{G}$, then $X$ and $Y$ are conditionally independent given $Z$ in the observational probability density $f$ consistent with $\mathcal{D}$ (Lauritzen et al., 1990; Pearl, 2009).

### 3 RESULTS

The causal effect of a set of treatments $X$ on a set of responses $Y$ is a function of the interventional density $f(y|\text{do}(x))$. For example, under the assumption of a Bernoulli distributed treatment variable $X$, the causal effect of $X$ on a singleton response $Y$ may be defined as the difference in expectation of $Y$ under $\text{do}(X = 1)$ and $\text{do}(X = 0)$, that is, $E[Y|\text{do}(X = 1)] - E[Y|\text{do}(X = 0)]$ (Chapter 1 in Hernán and Robins, 2019). We define an identifiable causal effect below.

**Definition 3.1 (Identifiability of Causal Effects).** Let $X$ and $Y$ be disjoint node sets in an MPDAG $\mathcal{G} = (V, E)$. The causal effect of $X$ on $Y$ is identifiable in $\mathcal{G}$ if $f(y|\text{do}(x))$ is uniquely computable from any observational density consistent with $\mathcal{G}$. Meaning, there are no two DAGs $\mathcal{D}^1, \mathcal{D}^2$ in $[\mathcal{G}]$ such that

1. $f_1(v) = f_2(v) = f(v)$, where $f$ is an observational density consistent with $\mathcal{G}$, and
2. $f_1(y|\text{do}(x)) \neq f_2(y|\text{do}(x))$, where $f_1(\cdot|\text{do}(x))$ is an interventional density consistent with $\mathcal{D}^1$ and $f_2(\cdot|\text{do}(x))$ is an interventional density consistent with $\mathcal{D}^2$.

Definition 3.1 is analogous to the Definition 3 of Galles and Pearl (1995) and Definition 1 of Jaber et al. (2019).

### 3.1 A Necessary Condition For Identification

We present a necessary condition for the identifiability of causal effects in MPDAGs in Proposition 3.2. The condition in Proposition 3.2 is denoted as amenability by Perković et al. (2015, 2017).
Proposition 3.2. Let $X$ and $Y$ be disjoint node sets in an MPDAG $G = (V, E)$. If there is a proper possibly causal path from $X$ to $Y$ that starts with an undirected edge in $G$, then the causal effect of $X$ on $Y$ is not identifiable in $G$.

Consider MPDAG $C$ in Figure 2a. Since $X \rightarrow Y$ is in $C$, by Proposition 3.2, the causal effect of $X$ on $Y$ is not identifiable in $C$. This is intuitively clear since both $X \rightarrow Y$ and $X \leftarrow Y$ are DAGs represented by $C$. The DAG $X \leftarrow Y$ implies that there is no causal effect of $X$ on $Y$. Conversely, the DAG $X \rightarrow Y$ implies that there is a causal effect of $X$ on $Y$.

The condition in Proposition 3.2 is somewhat less intuitive for non-singleton $X$. Consider MPDAG $G$ in Figure 2b and let $X = \{X_1, X_2\}$ and $Y = \{Y\}$. The path $X_1 - X_2 \rightarrow Y$ in $G$ is a possibly causal path from $X_1$ to $Y$ that starts with an undirected edge. However, $X_1 - X_2 \rightarrow Y$ is not a proper possibly causal path from $X$ to $Y$, since it contains $X_2$ in addition to $X_1$. Hence, the necessary condition for identifiability is satisfied with respect to $X, Y$, and $G$.

Intuitively Proposition 3.2 only considers proper possibly causal paths because if the proper possibly causal paths from $X$ to $Y$ start with a directed edge out of $X$, then any non-proper possibly causal definite status path from $X \in X \rightarrow Y$ to $Y \in Y$ is blocked given $X \cup \{X\}$. Hence, in this case, the causal effect of $X$ on $Y$ only “propagates” through the proper possibly causal paths from $X$ to $Y$.

3.2 Partial Causal Ordering In Maximal PDAGs

For our main result, it is necessary to determine a partial causal ordering for a set of nodes in an MPDAG. In order to compute a partial causal ordering of nodes in an MPDAG, we first define buckets. Definition 3.3 is similar to the definition of buckets in PAGs of Jaber et al. (2018a).

**Definition 3.3 (Buckets and bucket decomposition).** Let $B$ and $D$ be node sets in an MPDAG $G = (V, E)$ such that $B \subseteq D$. Then

1. $B$ is a bucket in $D$ if
   - there is an undirected path between any pair of distinct nodes in $B$ in $G$, and
   - there is no pair of nodes $B \in B$ and $D \in D \setminus B$ such that there is an undirected path between $B$ and $D$ in $G$.

2. $B = \{B_1, \ldots, B_k\}$, $k \geq 1$, is the bucket decomposition of $D$ if
   - $B_i$, $i \in \{1, \ldots, k\}$, is a bucket in $D$, and
Algorithm 1: Partial causal ordering (PCO)

input: Node set D in MPDAG \( \mathcal{G} = (V, E) \).
output: An ordered list \( B = (B_1, \ldots, B_k) \), \( k \geq 1 \), of the bucket decomposition of D in \( \mathcal{G} \).

1. Let \( \mathcal{G}_{\text{undir}} \) denote the undirected subgraph of \( \mathcal{G} \);
2. Let \( \text{ConComp} \) be the bucket decomposition of \( V \) in \( \mathcal{G}_{\text{undir}} \);
3. Let \( B \) be an empty list;
4. while \( \text{ConComp} \neq \emptyset \) do
   5. Let \( C \in \text{ConComp} \);
   6. Let \( \overline{C} \) be the set of nodes in \( \text{ConComp} \) that are not in \( C \);
   7. if all edges between \( C \) and \( \overline{C} \) are into \( C \) in \( \mathcal{G} \) then
      8. Remove \( C \) from \( \text{ConComp} \);
      9. Let \( B_* = C \cap D \);
     10. if \( B_* \neq \emptyset \) then
       11. Add \( B_* \) to the beginning of \( B \);
     end
   end
end
15. return \( B \);

- \( D = \bigcup_{i=1}^{k} B_i \), and
- \( B_i \cap B_j = \emptyset \), \( i, j \in \{1, \ldots, k\} \), \( i \neq j \).

For a MPDAG \( \mathcal{G} = (V, E) \), a node set \( B \) is a bucket in \( V \) if \( B \) is a connected component in the undirected subgraph of \( \mathcal{G} \).

Consider MPDAG \( \mathcal{G} = (V, E) \) in Figure 3a. The only path in the undirected subgraph \( \mathcal{G}_{\text{undir}} \) of \( \mathcal{G} \) is \( Y_1 - V_1 - X \). Hence, the bucket decomposition of \( V \) is \( \{\{X, V_1, Y_1\}, \{Y_2\}\} \).

Now, consider DAGs in Figure 3b, which are all DAGs represented by \( \mathcal{G} \). The total orderings of \( V \) that are consistent with DAGs in Figure 3b are: \( V_1 < Y_1 < X < Y_2 \), \( Y_1 < V_1 < X < Y_2 \), and \( Y_1 < X < V_1 < Y_2 \). All of these orderings are consistent with the following partial causal ordering \( \{X, V_1, Y_1\} < Y_2 \), which is a total ordering of the buckets in \( \{\{X, V_1, Y_1\}, \{Y_2\}\} \). This motivates Algorithm 1.

Algorithm 1 describes how to obtain an ordered bucket decomposition for a set of nodes \( D \) in a MPDAG \( \mathcal{G} \). In Lemma 3.4, we prove that the ordered list of buckets output by Algorithm 1 is a partial causal ordering of \( D \) in \( \mathcal{G} \).

**Lemma 3.4.** Let \( D \) be a node set in an MPDAG \( \mathcal{G} = (V, E) \) and let \( B = (B_1, \ldots, B_k) \), \( k \geq 1 \), be the output of \( \text{PCO}(D, \mathcal{G}) \). Then for each \( i, j \in \{1, \ldots, k\} \), \( B_i \) and \( B_j \) are buckets in \( D \) and if \( i < j \), it follows that \( B_i < B_j \), i.e. the total ordering of buckets \( (B_1, \ldots, B_k) \) implies a partial causal ordering of \( D \) that is consistent with all DAGs in \( \mathcal{G} \).

Algorithm 1 is similar to the PTO algorithm for PAGs of Jaber et al. (2018a,b). Lemma 3.4 is similar to Lemma 1 of Jaber et al. (2018b) and Proposition 4 of Jaber et al. (2018a).

Consider MPDAG \( \mathcal{G} = (V, E) \) in Figure 3a and let \( D = \{X, Y_1, Y_2\} \). We now explain how the output of \( \text{PCO}(D, \mathcal{G}) \) is obtained.

7
In line 2, the bucket decomposition of $\mathbf{V}$ is obtained, $\text{ConComp} = \{(X, Y_1, V_1), \{Y_2\}\}$ (as noted above). In line 3, $\mathbf{B}$ is initialized as an empty list.

Let $\mathbf{C} = \{X, Y_1, V_1\}$ (line 5). Then $\mathbf{C} = \{Y_2\}$ (line 6). Since $X \rightarrow Y_2$ and $Y_1 \rightarrow Y_2$ are in $\mathcal{G}$, $\mathbf{C}$ does not satisfy the condition in line 7 and hence, $\{X, Y_1, V_1\}$ cannot be removed from $\text{ConComp}$ at this time.

Next, let $\mathbf{C} = \{Y_2\}$ (line 5). Then $\mathbf{C} = \{X, Y_1, V_1\}$ (line 6). Since all edges between $\{Y_2\}$ and $\{X, Y_1, V_1\}$ in $\mathcal{G}$ are into $\{Y_2\}$, Algorithm 1 removes $\{Y_2\}$ from $\text{ConComp}$ in line 8. Since $\mathbf{B}_* = \mathbf{C} \cap \mathbf{D} = \{Y_2\}$ (line 9), Algorithm 1 adds $\{Y_2\}$ to the beginning of list $\mathbf{B}$ (line 11).

Now, $\mathbf{C} = \{X, Y_1, V_1\}$ and $\mathbf{C} = \emptyset$ (lines 5 and 6). Hence, $\mathbf{C}$ satisfies condition in line 7 and it is removed from $\text{ConComp}$ in line 8. Then $\mathbf{B}_* = \mathbf{C} \cap \mathbf{D} = \{X, Y_1\}$ (line 9), and $\mathbf{B} = \{(X, Y_1), \{Y_2\}\}$ (line 11). Since $\text{ConComp}$ is now empty, Algorithm 1 outputs $\mathbf{B}$.

### 3.3 Causal Identification Formula

We present our main result in Theorem 3.5. Theorem 3.5 establishes that the condition from Proposition 3.2 is not only necessary, but also sufficient for the identification of causal effects in MPDAGs.

**Theorem 3.5 (Causal identification formula).** Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in an MPDAG $\mathcal{G} = (\mathbf{V}, \mathbf{E})$. If there is no proper possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ in $\mathcal{G}$ that starts with an undirected edge, then for any observational density $f$ consistent with $\mathcal{G}$ we have

$$f(\mathbf{y}|\text{do}(\mathbf{x})) = \int \prod_{i=1}^{k} f(\mathbf{b}_i|\text{pa}(\mathbf{b}_i, \mathcal{G}))d\mathbf{b}, \quad (2)$$

for values $\text{pa}(\mathbf{b}_i, \mathcal{G})$ of $\text{Pa}(\mathbf{b}_i, \mathcal{G})$ that are in agreement with $\mathbf{x}$, where $(\mathbf{B}_1, \ldots, \mathbf{B}_k) = \text{PCD}(\text{An}(\mathbf{Y}, \mathcal{G}_{\mathbf{V}\backslash \mathbf{X}}), \mathcal{G})$ and $\mathbf{B} = \text{An}(\mathbf{Y}, \mathcal{G}_{\mathbf{V}\backslash \mathbf{X}}) \backslash \mathbf{Y}$.

Note that the variables that appear on the right hand side of equation (2) are either in $\text{An}(\mathbf{Y}, \mathcal{G}_{\mathbf{V}\backslash \mathbf{X}}), \mathcal{G})$ or in $\mathbf{X}$, for those $\mathbf{X}$ that have a proper causal path to $\mathbf{Y}$ in $\mathcal{G}$. We refer to equation (2) as the causal identification formula. The causal identification formula takes a form similar to the $g$-formula of Robins (1986).

To explain the reason for the somewhat sudden appearance of the set $\text{An}(\mathbf{Y}, \mathcal{G}_{\mathbf{V}\backslash \mathbf{X}}), \mathcal{G})$ in Theorem 3.5, note that for a DAG $\mathcal{D} = (\mathbf{V}, \mathbf{E})$ it is well known that in order to identify a causal effect of $\mathbf{X}$ on $\mathbf{Y}$ it is enough to consider the set of ancestors of $\mathbf{Y}$, that is $\text{An}(\mathbf{Y}, \mathcal{G})$ (see Theorem 4 of Tian and Pearl, 2002). The causal identification formula further refines this notion by using only those ancestors of $\mathbf{Y}$ that are ancestors of $\mathbf{Y}$ through a path that does not contain $\mathbf{X}$, and nodes in $\mathbf{X}$ that have a proper causal path to $\mathbf{Y}$.

If there is no possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ in an MPDAG $\mathcal{G}$, we can conclude that the causal effect of $\mathbf{X}$ on $\mathbf{Y}$ is zero for any observational density $f$ consistent with $\mathcal{G}$. We formalize this in the following lemma.

**Lemma 3.6.** Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in an MPDAG $\mathcal{G} = (\mathbf{V}, \mathbf{E})$. If there is no possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ in $\mathcal{G}$, then for any observational density $f$ consistent with $\mathcal{G}$ we have

$$f(\mathbf{y}|\text{do}(\mathbf{x})) = f(\mathbf{y}).$$
Lemma 3.6 follows from Lemma 3.2 in Perković et al. (2017) and Rule 3 of the do-calculus of Pearl (2009) (see Lemma A.4 and equation (9) in the Appendix).

Next, we consider the identifiability of \( f(v'|do(x)) \) in \( G = (V, E) \), when \( V' = V \setminus X \).

**Corollary 3.7 (Truncated factorization formula in MPDAGs).** Let \( X \) be a node set in an MPDAG \( G = (V, E) \) and let \( V' = V \setminus X \). If there is no pair of nodes \( V \in V' \) and \( X \in X \) such that \( X - V \) is in \( G \), then for any observational density \( f \) consistent with \( G \) we have

\[
f(v'|do(x)) = \prod_{i=1}^{k} f(v_i|pa(v_i, G)),
\]

for values \( pa(v_i, G) \) of \( Pa(v_i, G) \) that are in agreement with \( x \), where \( (V_1, \ldots, V_k) = PCO(V', G) \). Otherwise, the causal effect of \( X \) on \( V' \) is not identifiable.

Corollary 3.7 follows directly from Theorem 3.5 and is an interesting result in its own right since it can be seen as a direct generalization of the truncated factorization formula in equation (1) to MPDAGs.

### 3.4 Examples

**Example 3.8 (Motivating example).** In this example, the causal effect of \( X \) on \( Y \) is identifiable in an MPDAG \( G = (V, E) \), but there is no truncated factorization formula with respect to \( X \) in \( G \). Furthermore, this example and Example 4.3 discuss a scenario in which the current causal identification strategies are incomplete.

Consider MPDAG \( G \) in Figure 3a and let \( f \) be an observational density consistent with \( G \). Let \( X = \{X\} \) and \( Y = \{Y_1, Y_2\} \). The only possibly causal path from \( X \) to \( Y \) in \( G \) is \( X \rightarrow Y_2 \). Hence, by Theorem 3.5, the causal effect of \( X \) on \( Y \) is identifiable in \( G \).

To use the causal identification formula we first determine that \( An(\{Y_1, Y_2\}, G \setminus \{X\}) = \{Y_1, Y_2\}, \text{ and } PCO(\{Y_1, Y_2\}, G) = (\{Y_1\}, \{Y_2\}) \). Next, \( Pa(Y_1, G) = \emptyset \), and \( Pa(Y_2, G) = \{X\} \). Hence, by Theorem 3.5, \( f(y_1, y_2|do(x)) = f(y_2|x)f(y_1) \).

Now, let \( V' = V \setminus \{X\} \). Since edge \( X - V_1 \) is in \( G \), by Corollary 3.7, there is no truncated factorization formula with respect to \( X \) in \( G \). That is, \( f(v'|do(x)) \) is not identifiable in \( G \).

The strategy of Jaber et al. (2019) for identifying causal effects (in PAGs) relies on the fact that the causal effect of \( X \) on \( Y \) is identifiable in \( G \) if and only if the causal effect of \( V \setminus \text{PossAn}(Y, G_{V \setminus X}) \) on \( \text{PossAn}(Y, G_{V \setminus X}) \) is identifiable (see equation (8) of Jaber et al., 2019).
Note that $V' = \text{PossAn}(Y, G_{V \setminus X})$ and of course, $\{X\} = V \setminus \text{PossAn}(Y, G_{V \setminus X})$. Thus, this is an example where the additional background knowledge enables us identify more causal effects compared to the current strategies.

**Example 3.9.** In this example, the causal effect of $X$ on $Y$ is identifiable in an MPDAG $G$, and there is a truncated factorization formula with respect to $X$ in $G$.

Consider MPDAG $G$ in Figure 4a and let $f$ be an observational density consistent with $G$. The only possibly causal path from $X$ to $Y$ in $G$ is $X \rightarrow Y$. Hence, the causal effect of $X$ on $Y$ is identifiable in $G$. In fact, there is no undirected edge between $X$ and any other node in $G$, so the causal effect of $X$ on $V'$, $V' = \{V_1, V_2, V_3, Y\}$ is also identifiable in $G$. Thus, we can obtain the truncated factorization formula with respect to $X$ in $G$.

We will first determine the causal identification formula for $f(y|do(x))$ in $G$. Hence, we identify that $\text{An}(Y, G_{V \setminus \{X\}}) = \{V_1, V_2, Y\}$. The output of $\text{PCO}(\{V_1, V_2, Y\}, G)$ is $\{\{V_1, V_2\}, \{Y\}\}$. Furthermore, $\text{Pa}(\{V_1, V_2\}, G) = \emptyset$, and $\text{Pa}(Y, G) = \{X, V_1, V_2\}$. Hence, by Theorem 3.5, the causal identification formula for $f(y|do(x))$ in $G$ is $f(y|do(x)) = \int f(y|x, v_1, v_2)f(v_1, v_2)dv_1dv_2$.

In order to use Corollary 3.7, first note that the output of $\text{PCO}(V', G)$ is $\{\{V_1, V_2, V_3\}, \{Y\}\}$. Further, $\text{Pa}(\{V_1, V_2, V_3\}, G) = \emptyset$. The truncated factorization formula for $G$ with respect to $X$ is then $f(V'|do(x)) = f(y|x, v_1, v_2)f(v_1, v_2, v_3)$.

**Example 3.10.** This example shows how the causal identification formula can be used to estimate the causal effect of $X$ on $Y$ in an MPDAG $G$ under the assumption that the observational density $f$ consistent with $G$ is multivariate Gaussian.

Consider DAG $D$ in Figure 4b and let $f$ be an observational density consistent with $D$. Further, let $X = \{X_1, X_2\}$ and $Y = \{Y\}$. Then $\text{An}(Y, G_{V \setminus X}) = \{Y, V_4\}$ and $\text{PCO}(\{Y, V_4\}, D) = (\{V_4\}, \{Y\})$ in $D$.

Since $\text{Pa}(V_4, D) = \{X_1\}$ and $\text{Pa}(Y, D) = \{X_1, X_2, V_4\}$, by Theorem 3.5,

$$f(y|do(x_1, x_2)) = \int f(y|x_1, x_2, v_4)f(v_4|x_1)dv_4.$$

Suppose that the density $f$ consistent with $D$ is multivariate Gaussian. The causal effect of $X$ on $Y$ can then be defined as the vector

$$\left( \frac{\partial E[Y|do(x_1, x_2)]}{\partial x_1}, \frac{\partial E[Y|do(x_1, x_2)]}{\partial x_2} \right)^T.$$

(Nandy et al., 2017). Hence, consider $E[Y|do(x_1, x_2)]$,

$$E[Y|do(x_1, x_2)] = \int yf(y|do(x_1, x_2))dy$$
$$= \int \int yf(y|x_1, x_2, v_4)f(v_4|x_1)dv_4dy$$
$$= \int E[Y|x_1, x_2, v_4]f(v_4|x_1)dv_4$$
$$= \alpha x_1 + \beta x_2 + \gamma \int v_4f(v_4|x_1)dv_4$$
$$= \beta x_2 + x_1(\alpha + \gamma \delta),$$

where $E[Y|x_1, x_2, v_4] = \alpha x_1 + \beta x_2 + \gamma v_4$ and $E[V_4|x_1] = \delta x_1$ (Theorem 3.2.4 of Mardia et al., 1980, see Theorem A.2 in the Appendix).
Thus, the causal effect of $X$ on $Y$ is equal to $(\alpha + \gamma \delta, \beta)$. Note that consistent estimators for $\alpha$, $\beta$, and $\gamma$ are the least squares estimators of the coefficients of $X_1$, $X_2$, and $V_4$ (respectively) in the regression of $Y$ on $X_1$, $X_2$, and $V_4$. Analogously, the least squares estimator of the coefficient of $X_1$ in the regression of $V_4$ on $X_1$ is a consistent estimator for $\delta$.

### 3.5 Proof of Theorem 3.5

The proof of Theorem 3.5 relies on Lemma D.1 in the Appendix. Lemma D.1 is proven through use of do-calculus rules from Pearl (2009) and some basic probability calculus.

The proofs of Theorem 3.5 and Lemma D.1 at no point require intervening on additional variables in $G$. This is in contrast to the proofs for most other causal identifiability results including the identification algorithms of Tian and Pearl (2002); Shpitser and Pearl (2006) and Jaber et al. (2019), as well as the identification formula in Theorem 60 of Richardson et al. (2017).

Our proof strategy alleviates any concerns of whether such additional interventions are reasonable to assume as possible (see e.g. VanderWeele and Robinson, 2014; Kohler-Hausmann, 2018).

**Proof of Theorem 3.5.** For $i \in \{2, \ldots, k\}$, let $P_i = (\cup_{j=1}^{i-1} B_i) \cap Pa(B_i, G)$. For $i \in \{1, \ldots, k\}$, let $X_{p_i} = X \cap Pa(B_i, G)$.

Then

$$f(y|do(x)) = \int f(b, y|do(x))db$$

$$= \int f(b_1|do(x)) \prod_{i=2}^{k} f(b_i|b_{i-1}, \ldots, b_1, do(x))db$$

$$= \int f(b_1|do(x)) \prod_{i=2}^{k} f(b_i|p_i, do(x))db$$

$$= \int f(b_1|do(x_{p_1})) \prod_{i=2}^{k} f(b_i|p_i, do(x_{p_i}))db$$

$$= \int \prod_{i=1}^{k} f(b_i|pa(b_i, G))db,$$  \hspace{1cm} (6)

The first two equalities follow from the law of total probability. Equations (4), (5), and (6) follow by applying results (ii), (iii), and (iv) in Lemma D.1 in the Appendix. \qed

### 4 COMPARISONS TO STATE OF THE ART

The current state-of-the-art method for identifying causal effects in MPDAGs is the generalized adjustment criterion of Perković et al. (2017) which we state in Theorem 4.1.

**Theorem 4.1 (Adjustment set, Generalized adjustment criterion: Perković et al., 2017).** Let $X, Y$ and $Z$ be pairwise disjoint node sets in an MPDAG $G = (V, E)$. Let $f$ be any observational density consistent with $G$. 
Then Z is an adjustment set relative to (X, Y) in G and we have
\[
f(y|do(x)) = \begin{cases} \int_z f(y|x, z)f(z)dz, & \text{if } Z \neq \emptyset, \\ f(y|x), & \text{otherwise}. \end{cases}
\]
if and only if the following graphical conditions are satisfied:

1. There is no proper possibly causal path from X to Y that starts with an undirected edge in G.
2. \(Z \cap \text{Forb}(X, Y, G) = \emptyset\), where
\[
\text{Forb}(X, Y, G) = \{W' \in V : W' \in \text{PossDe}(W, G), \text{for some } W \notin X \text{ which lies on a proper possibly causal path from } X \text{ to } Y \text{ in } G\}.
\]
3. All proper non-causal definite status paths from X to Y are blocked by Z in G.

The generalized adjustment criterion is sufficient for identifying causal effects in an MPDAG, but it is not necessary. In the following proposition, however, we show that when X and Y are singleton sets, the generalized adjustment criterion identifies all non-zero causal effects of X on Y in a MPDAG G.

**Proposition 4.2.** Let X and Y be distinct nodes in an MPDAG G = (V, E). If Y \(\notin\) Pa(X, G), then the causal effect of X on Y is identifiable in G if and only if there is an adjustment set relative to (X, Y) in G.

Furthermore, Pa(X, G) is an adjustment set relative to (X, Y) in G.

If Y \(\in\) Pa(X, G), then by Lemma 3.6, there is no causal effect of X on Y in MPDAG G. Hence, by Proposition 4.2, the generalized adjustment criterion is “almost” complete for the identification of causal effects of X on Y in MPDAGs.

If X or Y are non-singleton sets in G, however, the generalized adjustment criterion will fail to identify some non-zero causal effects of X on Y. We discuss this further in the two examples below.

**Example 4.3 (Motivating example continued).** Consider MPDAG G in Figure 3a and let X = \{X\}, and Y = \{Y_1, Y_2\} as in Example 3.8.

Path X ← Y_1 is a non-causal path from X to Y that cannot be blocked by any set of nodes disjoint with \{X, Y_1\}. Hence, there is no adjustment set relative to (X, Y) in G. But there is a causal path from X to Y in G and as we have seen in Example 3.8, the causal effect of X on Y is identifiable in G.

**Example 4.4.** Consider DAG D in Figure 4b and let X = \{X_1, X_2\}, and Y = \{Y\}. Then Forb(X, Y, D) = \{V_4, Y\}. For a set Z to satisfy the generalized adjustment criterion relative to (X, Y) in G, Z cannot contain nodes in \{V_4, Y\}, or \{X_1, X_2\} and Z must block all proper non-causal paths from X to Y in D.

However, \(X_2 ← V_4 → Y\) is a proper non-causal path from X to Y in D that cannot be blocked by any set Z that satisfies \(Z \cap \{X_1, X_2, V_4, Y\} = \emptyset\). Hence, there is no adjustment set relative to (X, Y) in D. But as we have seen in Example 3.10, the causal effect of X on Y is identifiable in D and furthermore, both X_1 and X_2 are causes of Y in D.

12
5 DISCUSSION

We introduced a causal identification formula that allows complete identification of causal effects in MPDAGs. Furthermore, we generalized the truncated identification formula to MPDAGs and gave a comparison of our graphical criterion to the current state of the art method for causal identification in MPDAGs.

Since the causal identification formula comes in the familiar form of the g-formula of Robins (1986) for DAGs, our results can be used to generalize applications of the g-formula to MPDAGs. For example, Murphy (2003), Collins et al. (2004), and Collins et al. (2007) give criteria for estimating the optimal dynamic treatment regime from longitudinal data that are based on the g-formula. This idea can further be combined with recent work of Rahmadi et al. (2017) and Rahmadi et al. (2018) that establishes an approach for estimating the MPDAG using data from longitudinal studies.

Future work could consider extending the causal identification formula and the truncated identification formula to PAGs and developing a complete identification formula for conditional causal effects in MPDAGs and PAGs.

A Preliminaries

Subsequences And Subpaths. A subsequence of a path p is obtained by deleting some nodes from p without changing the order of the remaining nodes. For a path p = (X_1, X_2, . . . , X_m), the subpath from X_i to X_k (1 ≤ i ≤ k ≤ m) is the path p(X_i, X_k) = (X_i, X_{i+1}, . . . , X_k).

Concatenation. We denote concatenation of paths by ⊕, so that for a path p = (X_1, X_2, . . . , X_m), p = p(X_1, X_r) ⊕ p(X_r, X_m), for 1 ≤ r ≤ m.

D-separation. If X and Y are d-separated given Z in a DAG D, we write X ⊥_D Y|Z.

Possible Descendants. If there is a possibly causal path from X to Y, then Y is a possible descendant of X. We use the convention that every node is a possible descendant of itself. The set of possible descendants of X in G is PossDe(X, G). For a set of nodes X ⊆ V, we let PossDe(X, G) = ∪_{V ∈ X} PossDe(X, G).

Bayesian And Causal Bayesian Networks. If a density f over V is consistent with DAG D = (V, E), then (D, f) form a Bayesian network. Let F be a set of density functions made up of all interventional densities f(v’|do(x)) for any X ⊆ V and V’ = V \ X that are consistent with D (F also includes all observational densities consistent with D), then (D, F) form a causal Bayesian network.

Rules Of The Do-calculus (Pearl, 2009). Let X, Y, Z and W be pairwise disjoint (possibly empty) sets of nodes in a DAG D = (V, E) Let D_X denote the graph obtained by deleting all edges into X from D. Similarly, let D_X denote the graph obtained by deleting all edges out of X in D and let D_{XZ} denote the graph obtained by deleting all edges into X and all edges out of Z in D. Let (D, F) be a causal Bayesian network, the following rules hold for densities in F.

Rule 1 (Insertion/deletion of observations). If Y ⊥_{D_X} Z|X \cup W, then

\[ f(y|do(x), w) = f(y|do(x), z, w). \] (7)
Rule 2. If $Y \perp_{\mathcal{D}_{\mathcal{X}}} Z|X \cup W$, then
\[ f(y|do(x), do(z), w) = f(y|do(x), z, w). \] (8)

Rule 3. If $Y \perp_{\mathcal{D}_{\mathcal{X}}} Z|X \cup W$, then
\[ f(y|do(x), w) = f(y|do(x), do(z), w), \] (9)
where $Z(W) = Z \setminus \text{An}(W, \mathcal{D}_{\mathcal{X}})$.

A.1 Existing Results

Theorem A.1 (Wright’s rule Wright, 1921). Let $X = AX + \epsilon$, where $A \in \mathbb{R}^{k \times k}$, $X = (X_1, \ldots, X_k)^T$ and $\epsilon = (\epsilon_1, \ldots, \epsilon_k)^T$ is a vector of mutually independent errors with means zero. Moreover, let $\text{Var}(X) = I$. Let $\mathcal{D} = (X, E)$, be the corresponding DAG such that $X_i \rightarrow X_j$ in $\mathcal{D}$ if and only if $A_{ji} \neq 0$. A nonzero entry $A_{ji}$ is called the edge coefficient of $X_i \rightarrow X_j$. For two distinct nodes $X_i, X_j \in X$, let $p_1, \ldots, p_r$ be all paths between $X_i$ and $X_j$ in $\mathcal{D}$ that do not contain a collider. Then $\text{Cov}(X_i, X_j) = \sum_{s=1}^{r} \pi_s$, where $\pi_s$ is the product of all edge coefficients along path $p_s, s \in \{1, \ldots, r\}$.

Theorem A.2 (c.f. Theorem 3.2.4 Mardia et al., 1980). Let $X = (X_1^T, X_2^T)^T$ be a $p$-dimensional multivariate Gaussian random vector with mean vector $\mu = (\mu_1^T, \mu_2^T)^T$ and covariance matrix $\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$, so that $X_1$ is a $q$-dimensional multivariate Gaussian random vector with mean vector $\mu_1$ and covariance matrix $\Sigma_{11}$ and $X_2$ is a $(p-q)$-dimensional multivariate Gaussian random vector with mean vector $\mu_2$ and covariance matrix $\Sigma_{22}$. Then $E[X_2|X_1 = x_1] = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(x_1 - \mu_1)$.

Lemma A.3 (c.f. Lemma C.1 of Perković et al., 2017, Lemma 8 of Perković et al., 2018). Let $X$ and $Y$ be disjoint node sets in a MPDAG $\mathcal{G}$. Suppose that there is a proper possibly causal path from $X$ to $Y$ that starts with an undirected edge in $\mathcal{G}$, then there is one such path $q = (X, V_1, \ldots, Y), X \in X, Y \in Y$ in $\mathcal{G}$ and DAGs $\mathcal{D}^1, \mathcal{D}^2$ in $[\mathcal{G}]$ such that the path in $\mathcal{D}^1$ consisting of the same sequence of nodes as $q$ is of the form $X \rightarrow V_1 \rightarrow \cdots \rightarrow Y$ and in $\mathcal{D}^2$ the path consisting of the same sequence of nodes as $q$ is of the form $X \leftarrow V_1 \rightarrow \cdots \rightarrow Y$.

Lemma A.4 (Lemma 3.2 of Perković et al., 2017). Let $p^*$ be a path from $X$ to $Y$ in a MPDAG $\mathcal{G}$. If $p^*$ is non-causal in $\mathcal{G}$, then for every DAG $\mathcal{D}$ in $[\mathcal{G}]$ the corresponding path to $p^*$ in $\mathcal{D}$ is non-causal. Conversely, if $p$ is a causal path in at least one DAG $\mathcal{D}$ in $[\mathcal{G}]$, then the corresponding path to $p$ in $\mathcal{G}$ is possibly causal.

Lemma A.5 (Lemma 3.5 of Perković et al., 2017). Let $p = (V_1, \ldots, V_k)$ be a definite status path in a MPDAG $\mathcal{G}$. Then $p$ is possibly causal if and only if there is no $V_i \leftarrow V_{i+1}$, for $i \in \{1, \ldots, k-1\}$ in $\mathcal{G}$.

Lemma A.6 (Lemma 3.6 of Perković et al., 2017). Let $X$ and $Y$ be distinct nodes in a MPDAG $\mathcal{G}$. If $p$ is a possibly causal path from $X$ to $Y$ in $\mathcal{G}$, then a subsequence $p^*$ of $p$ forms a possibly causal unshielded path from $X$ to $Y$ in $\mathcal{G}$.

Lemma A.7 (c.f. Lemma 1 of Jaber et al., 2018b). Let $\mathcal{G} = (V, E)$ be a CPDAG or DAG and let $B = (B_1, \ldots, B_k), k \geq 1$, be the output of $\text{PTO}(\mathcal{G})$ (Algorithm 2). Then for each $i, j \in \{1, \ldots, k\}, B_i$ and $B_j$ are buckets in $V$ and if $i < j$, then $B_i < B_j$.
Algorithm 2: PTO algorithm (Jaber et al., 2018b)

\[\text{input : DAG or CPDAG } \mathcal{G} = (V, E).\]
\[\text{output: An ordered list } \mathbf{B} = (\mathbf{B}_1, \ldots, \mathbf{B}_k), k \geq 1 \text{ of the bucket decomposition of } V \text{ in } \mathcal{G}.\]

1. Let \( \mathcal{G}_{\text{undir}} \) be the undirected subgraph of \( \mathcal{G} \);
2. Let \( \text{ConComp} \) be the bucket decomposition of \( V \) in \( \mathcal{G}_{\text{undir}} \);
3. Let \( \mathbf{B} \) be an empty list;
4. while \( \text{ConComp} \neq \emptyset \) do
   5. Let \( C \in \text{ConComp} \);
   6. Let \( \overline{C} \) be the set of nodes in \( \text{ConComp} \) that are not in \( C \);
   7. if all edges between \( C \) and \( \overline{C} \) are into \( C \) in \( \mathcal{G} \) then
      8. Add \( C \) to the beginning of \( \mathbf{B} \);
   9. end
10. end
11. return \( \mathbf{B} \);

Lemma A.8 (c.f. Lemma E.6 of Henckel et al., 2019). Let \( X \) and \( Y \) be disjoint node sets in a maximal PDAG \( \mathcal{G} \) and suppose that there is no proper possibly causal path from \( X \) to \( Y \) that starts with an undirected edge in \( \mathcal{G} \). Let \( \mathcal{D} \) be a DAG in \( [\mathcal{G}] \). Then \( \text{Forb}(X, Y, \mathcal{G}) \subseteq \text{De}(X, \mathcal{G}) \).

B Proofs for Section 3.1

Proof of Proposition 3.2. This proof follows a similar reasoning as the proof of Theorem 2 of Shpitser and Pearl (2006) and proof of Theorem 57 of Perković et al. (2018).

By Lemma A.3, there is a proper possibly causal definite status path \( q = \langle X, V_1, \ldots, Y \rangle \), \( k \geq 1 \), \( X \in X \), \( Y \in Y \) in \( \mathcal{G} \) and DAGs \( \mathcal{D}^1 \) and \( \mathcal{D}^2 \) in \( [\mathcal{G}] \) such that \( X \rightarrow V_1 \rightarrow \cdots \rightarrow Y \) is in \( \mathcal{D}^1 \) and \( X \leftarrow V_1 \rightarrow \cdots \rightarrow Y \) is in \( \mathcal{D}^2 \) (the special case when \( k = 1 \) is \( X \leftarrow Y \)).

Consider a multivariate Gaussian density over \( V \) with mean vector zero, constructed using a linear structural causal model (SCM) with Gaussian noise. In particular, each random variable \( A \in V \) is a linear combination of its parents in \( \mathcal{D}^1 \) and a designated Gaussian noise variable \( \epsilon_A \) with zero mean and a fixed variance. The Gaussian noise variables \( \{\epsilon_A : A \in V\} \), are mutually independent.

We define the SCM such that all edge coefficients except for the ones on \( q_1 \) are 0, and all edge coefficients on \( q_1 \) are in (0, 1) and small enough so that we can choose the residual variances so that the variance of every random variable in \( V \) is 1.

The density \( f \) of \( V \) generated in this way is consistent with \( \mathcal{D}^1 \) and thus, \( f \) is also consistent with \( \mathcal{G} \) and \( \mathcal{D}^2 \) (Lauritzen et al., 1990). Moreover, \( f \) is consistent with DAG \( \mathcal{D}^{11} \) that is obtained from \( \mathcal{D}^1 \) by removing all edges except for the ones on \( q_1 \). Analogously, \( f \) is also consistent with DAG \( \mathcal{D}^{21} \) that is obtained from \( \mathcal{D}^2 \) by removing all edges except for the ones on \( q_2 \). Hence, let \( f_1(v) = f(v) \) and let \( f_2(v) = f(v) \).

Let \( f_1(v'|\text{do}(x)) \) be an interventional density consistent with \( \mathcal{D}^{11} \). Similarly let \( f_2(v'|\text{do}(x)) \) be an interventional density consistent with \( \mathcal{D}^{21} \). Then \( f_1(v'|\text{do}(x)) \) and \( f_1(v'|\text{do}(x)) \) are also interventional densities consistent with \( \mathcal{D}^1 \) and \( \mathcal{D}^2 \), respectively. Now, \( f_1(y|\text{do}(x)) \) is a
marginal interventional density of $Y$ that can be calculated from the density $f_1(v'|\text{do}(x))$ and the analogous is true for $f_2(y|\text{do}(x))$ and $f_2(v'|\text{do}(x))$.

In order to show that $f_1(y|\text{do}(x)) \neq f_2(y|\text{do}(x))$, it suffices to show that $f_1(y|\text{do}(x) = 1) \neq f_2(y|\text{do}(x) = 1)$ for at least one $Y \in Y$ when all $X$ variables are set to 1 by a do-intervention. In order for $f_1(y|\text{do}(x) = 1) \neq f_2(y|\text{do}(x) = 1)$ to hold, it is enough to show that the expectation of $Y$ is not the same under these two densities. Hence, let $E_i[Y | \text{do}(X = 1)]$ denote the expectation of $Y$, under $f_1(y|\text{do}(X = 1))$ and let $E_2[Y | \text{do}(X = 1)]$ denote the expectation of $Y$, under $f_2(y|\text{do}(X = 1))$.

Since $Y$ is d-separated from $X$ in $D^{|X|}_2$, we can use Rule 3 of the do-calculus (see equation (9)) to conclude that $E_2[Y | \text{do}(X = 1)] = E[Y] = 0$. Similarly, since $Y$ is d-separated from $X$ in $D^{|X|}_1$, we can use Rule 2 of the do-calculus (see equation (8)) to conclude that $E_1[Y | \text{do}(X = 1)] = E[Y|X = 1]$. By Theorems A.2 and A.1, $E[Y | X = 1] = \text{Cov}(X,Y) = a$, where $a$ is the product of all edge coefficients on $q_1$. Since $a \neq 0$, $E_1[Y | \text{do}(X = 1)] \neq E_2[Y | \text{do}(X = 1)]$. 

C Proofs for Section 3.2

Proof of Lemma 3.4. Lemma C.1 and Lemma A.7 together imply that Algorithm 2 can be applied to a MPDAG $\mathcal{G}$ and also that the output of PTO($\mathcal{G}$) is the same as that of PTO($V, \mathcal{G}$). Furthermore, PTO($\mathcal{G}$) = PTO($V, \mathcal{G}$) = $\{B_1, \ldots, B_r\}$, where for all $i, j \in \{1, \ldots, r\}$, $B_i$ and $B_j$ are buckets in $V$ in $\mathcal{G}$, and if $i < j$, then $B_i < B_j$ with respect to $\mathcal{G}$.

The statement of the lemma then follows directly from the definition of buckets (Definition 3.3), since for each $l \in \{1, \ldots, k\}$, there exists $s \in \{1, \ldots, r\}$ such that $B_l = D \cap B_s$ and $(B_1, \ldots, B_k)$ is exactly the output of PTO($V, \mathcal{G}$).

Lemma C.1. Let $B$ be a bucket in $V$ in MPDAG $\mathcal{G} = (V, E)$ and let $X \in V$, $X \notin B$. If there is a causal path from $X$ to $B$ in $\mathcal{G}$, then for every node $B \in B$ there is a causal path from $X$ to $B$ in $\mathcal{G}$.

Proof of Lemma C.1. Let $p$ be a shortest causal path from $X$ to $B$ in $\mathcal{G}$. Then $p$ is of the form $X \to \ldots \to A \to B$, possibly $X = A$ and $A \notin B$.

Let $B' \in B$, $B' \neq B$ and let $q = (B = W_1, \ldots, W_r = B')$, $r > 1$ be a shortest undirected path from $B$ to $B'$ in $\mathcal{G}$. It is enough to show that there is an edge $A \to B'$ in $\mathcal{G}$.

Since $A \to B-W_2$, by the properties of MPDAGs (Meek, 1995, see Figure 1 in the main text), $A \to W_2$ or $A \to W_2$ is in $\mathcal{G}$. Since $A \notin B$, $A \to W_2$ is in $\mathcal{G}$. If $r = 2$, we are done. Otherwise, $A \to W_2 \cdots W_k$ is in $\mathcal{G}$ and we can apply the same reasoning as above iteratively until we obtain $A \to W_k$ is in $\mathcal{G}$.

D Proofs for Section 3.3

Lemma D.1. Let $X$ and $Y$ be disjoint node sets in $V$ in MPDAG $\mathcal{G} = (V, E)$ and suppose that there is no proper possibly causal path from $X$ to $Y$ that starts with an undirected edge in $\mathcal{G}$. Further, let $(B_1, \ldots, B_k) = \text{PCO}(\text{An}(Y, \mathcal{G} \setminus V, X), \mathcal{G})$, $k \geq 1$.

(i) For $i \in \{1, \ldots, k\}$, there is no proper possibly causal path from $X$ to $B_i$ that starts with an undirected edge in $\mathcal{G}$.
(ii) For \( i \in \{2, \ldots, k\} \), let \( \mathbf{P}_i = (\bigcup_{j=i}^{i-1} \mathbf{B}_i) \cap \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). Then for every DAG \( \mathcal{D} \) in \( \mathcal{G} \) and every interventional density \( f \) consistent with \( \mathcal{D} \) we have

\[
f(b_i | b_{i-1}, \ldots, b_1, \text{do}(x)) = f(b_i | \text{pa}(b_i), \text{do}(x)).
\]

(iii) For \( i \in \{2, \ldots, k\} \), let \( \mathbf{P}_i = (\bigcup_{j=i}^{i-1} \mathbf{B}_i) \cap \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). For \( i \in \{1, \ldots, k\} \), let \( \mathbf{X}_{\mathbf{P}_i} = \mathbf{X} \cap \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). Then for every DAG \( \mathcal{D} \) in \( \mathcal{G} \) and every interventional density \( f \) consistent with \( \mathcal{D} \) we have

\[
f(b_i | b_{i-1}, \ldots, b_1, \text{do}(x)) = f(b_i | \text{pa}(b_i), \text{do}(x_{\mathbf{P}_i})).
\]

Additionally, \( f(b_1 | \text{do}(x)) = f(b_1 | \text{do}(x_{\mathbf{P}_1})) \).

(iv) For \( i \in \{2, \ldots, k\} \), let \( \mathbf{P}_i = (\bigcup_{j=i}^{i-1} \mathbf{B}_i) \cap \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). For \( i \in \{1, \ldots, k\} \), let \( \mathbf{X}_{\mathbf{P}_i} = \mathbf{X} \cap \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). Then for every DAG \( \mathcal{D} \) in \( \mathcal{G} \) and every interventional density \( f \) consistent with \( \mathcal{D} \) we have

\[
f(b_i | b_{i-1}, \ldots, b_1, \text{do}(x)) = f(b_i | \text{pa}(b_i), \text{do}(x_{\mathbf{P}_i})),
\]

for values \( \text{pa}(b_i; \mathcal{G}) \) of \( \text{Pa}(\mathbf{B}_i; \mathcal{G}) \) that are in agreement with \( \mathbf{x} \).

**Proof of Lemma D.1.** (i): Suppose for a contradiction that there is a proper possibly causal path from \( \mathbf{X} \) to \( \mathbf{B}_i \) that starts with an undirected edge in \( \mathcal{G} \). Let \( p = \langle X, \ldots, B \rangle \), \( X \in \mathbf{X}, B \in \mathbf{B}_i \), be a shortest such path in \( \mathcal{G} \). Then \( p \) is unshielded in \( \mathcal{G} \) (Lemma A.6).

Since \( B \in \text{An}(Y, \mathcal{G} \setminus X) \) there is a causal path \( q \) from \( B \) to \( Y \) in \( \mathcal{G} \) that does not contain a node in \( X \). No node other than \( B \) is both on \( q \) and \( p \) (otherwise, by definition \( p \) is not possibly causal from \( X \) to \( B \)). Hence, by Lemma D.2, \( p \parallel q \) is a proper possibly causal path from \( X \) to \( Y \) that starts with an undirected edge in \( \mathcal{G} \), which is a contradiction.

(ii): Let \( \mathbf{N}_i = (\bigcup_{j=i}^{i-1} \mathbf{B}_j) \setminus \text{Pa}(\mathbf{B}_i; \mathcal{G}) \). If \( \mathbf{B}_i \perp_{\mathcal{D}_{\mathcal{G}}} \mathbf{N}_i \perp (\mathbf{X} \cup \mathbf{P}_i) \), then by Rule 1 of the do calculus: \( f(b_i | b_{i-1}, \ldots, b_1, \text{do}(x)) = f(b_i | \text{pa}(b_i), \text{do}(x)) \) (see equation (7)).

Suppose for a contradiction that there is a path from \( \mathbf{B}_i \) to \( \mathbf{N}_i \) that is \( \mathcal{D} \)-connecting given \( \mathbf{X} \cup \mathbf{P}_i \) in \( \mathcal{D}_{\mathcal{G}} \). Let \( p = \langle B_i, \ldots, N \rangle \), \( B_i \in \mathbf{B}_i \), \( N \in \mathbf{N}_i \) be a shortest such path. Let \( \mathcal{D}_{\mathcal{G}} \) be the path in \( \mathcal{G} \) that consists of the same sequence of nodes as \( p \) in \( \mathcal{D}_{\mathcal{G}} \).

First suppose that \( p \) is of the form \( B_i \rightarrow \ldots \rightarrow N \). Since \( B_i \in \mathbf{B}_i \) and \( \mathbf{N}_i \subseteq (\bigcup_{j=i}^{i-1} \mathbf{B}_j) \), \( p \) is not causal from \( B_i \) to \( N \) (Lemma 3.4). Hence, let \( C \) be the closest collider to \( B_i \) on \( p \), that is, \( p \) has the form \( B_i \rightarrow \cdots \rightarrow C \leftarrow \ldots \). Since \( p \) is \( \mathcal{D} \)-connecting given \( \mathbf{X} \cup \mathbf{P}_i \) in \( \mathcal{D}_{\mathcal{G}} \), \( C \) must be an ancestor of \( \mathbf{P}_i \) in \( \mathcal{D}_{\mathcal{G}} \). However, then there is a causal path from \( B_i \in \mathbf{B}_i \) to \( \mathbf{P}_i \subseteq (\bigcup_{j=i}^{i-1} \mathbf{B}_j) \) which contradicts Lemma 3.4.

Next, suppose that \( p \) is of the form \( B_i \leftarrow A \ldots N \), \( A \notin \mathbf{B}_i \). Since \( \text{Pa}(\mathbf{B}_i; \mathcal{G}) \subseteq (\mathbf{X} \cup \mathbf{P}_i) \) and since \( p \) is \( \mathcal{D} \)-connecting given \( (\mathbf{X} \cup \mathbf{P}_i) \), \( B_i \leftarrow A \) is in \( \mathcal{G} \) and \( A \notin (\mathbf{X} \cup \mathbf{P}_i) \).

Note that \( p^* \) cannot be unshielded, since that would imply that \( N \in \mathbf{B}_i \) and contradict Lemma 3.4. Hence, let \( B \) be the closest node to \( B_i \) on \( p^* \) such that \( p^*(B, N) \) starts with a directed edge (possibly \( B = A \)). Then \( p^* \) is either of the form \( B_i \leftarrow A \cdots \leftarrow L \leftarrow B \rightarrow R \ldots N \) or of the form \( B_i \leftarrow A \ldots \leftarrow L \rightarrow B \leftarrow R \ldots N \).

Suppose first that \( p^* \) is of the form \( B_i \leftarrow A \cdots \leftarrow L \rightarrow B \rightarrow R \ldots N \). Then \( B \notin (\mathbf{X} \cup \mathbf{B}_i \cup \mathbf{P}_i) \) otherwise, \( p \) is either blocked by \( \mathbf{X} \cup \mathbf{P}_i \), or a shorter path could have been chosen.

Let \( (\mathbf{B}_{i_1}, \ldots, \mathbf{B}_{i_r}) = \text{PCO}(V, \mathcal{G}), r \geq k \). Let \( l \in \{i, \ldots, r\} \) such that \( B_{i_l} \cap \mathbf{B}_i \neq \emptyset \), then \( B_{i_l} \in \mathbf{B}_i \) and \( N \in (\bigcup_{j=i}^{i-1} \mathbf{B}_j) \). Now consider subpath \( p(B, N) \). By Lemma 3.4, \( p(B, N) \) cannot be causal from \( B \) to \( N \). Hence, there is a collider on \( p(B, N) \) and we can derive the contradiction using the same reasoning as above.
Suppose next that \( p^* \) is of the form \( B_1 - A - \cdots - L - B \leftarrow R \ldots N. \) Then either \( R \rightarrow L \) or \( R - L \) is in \( \mathcal{G} \) (Meek, 1995, see Figure 3 in the main text). Then \( \langle L, R \rangle \) is also an edge in \( \mathcal{D}_X \) otherwise, \( L \) or \( R \) is in \( X \) and a non-collider on \( p \), so \( p \) would be blocked by \( X \cup P_i \).

Hence, \( q = p(B_i, L) \uplus (L, R) \uplus p(R, N) \) is a shorter path than \( p \) in \( \mathcal{D}_X \). If \( L \) and \( R \) have the same collider/non-collider status on \( q \) on \( p \), then \( q \) is also \( d \)-connecting given \( X \cup P_i \), which would contradict our choice of \( p \). Hence, the collider/non-collider status of \( L \) or \( R \), is different on \( p \) and \( q \). We now discuss the cases for the change of collider/non-collider status of \( L \) and \( R \) and derive a contradiction in each.

Suppose that \( L \) is a collider on \( q \), and a non-collider on \( p \). This implies that \( W \rightarrow L \rightarrow B \leftarrow R \) is a subpath of \( p \) and \( L \leftarrow R \) is in \( \mathcal{D}_X \). Even though \( L \) is not a collider on \( p \), \( B \) is a collider on \( p \) and \( L \in \text{An}(B, \mathcal{D}_X) \). Since \( p \) is \( d \)-connecting given \( X \cup P_i \), \( \text{De}(B, \mathcal{D}_X) \cap (X \cup P_i) \neq \emptyset \). However, then also \( \text{De}(L, \mathcal{D}_X) \cap (X \cup P_i) \neq \emptyset \) and \( q \) is also \( d \)-connecting given \( X \cup P_i \) and a shorter path between \( B_i \) and \( N_i \) than \( p \), which is a contradiction.

The contradiction can be derived in exactly the same way as above in the case when \( R \) is a collider on \( q \), and a non-collider on \( p \). Since \( B \leftarrow R \) is in \( \mathcal{D}_X \), \( R \) cannot be anything but a non-collider on \( q \), so the only case left to consider is if \( L \) is a non-collider on \( q \) and a collider on \( p \).

For \( L \) to be a non-collider on \( q \) and a collider on \( p \), \( W \rightarrow L \leftarrow B \leftarrow R \) must be a subpath of \( p \) and \( L \rightarrow R \) should be in \( \mathcal{D}_X \). But then there is a cycle in \( \mathcal{D}_X \), which is a contradiction.

(iii): We will show that \( f(b_i | p_i, do(x)) = f(b_i | p_i, do(x_{ni})) \). The simpler case, \( f(b_1 | do(x)) = f(b_1 | do(x_{ni})) \) follows from the same proof, when \( B_1 \) is replaced by \( B_1 \) and \( P_i \) is removed.

Let \( X_{ni} = X \setminus \text{Pa}(B_1, \mathcal{G}) \) and let \( X_{ni} = X_{ni} \setminus \text{An}(P_i, \mathcal{D}_{X_{ni}}) \). That is \( X \in X_{ni} \) if \( X \in X_{ni} \) and if there is no causal path from \( X \) to \( P_i \) in \( \mathcal{D} \) that does not contain a node in \( X_{ni} \).

Note that \( \text{Pa}(B_i, \mathcal{G}) = X_{ni} \cup P_i \). By Rule 3 of the do-calculus, for \( f(b_i | p_i, do(x)) = f(b_i | p_i, do(x_{ni})) \) to hold, it is enough to show that \( B_i \perp \! \! \! \perp X_{ni} \setminus \text{Pa}(B_i, \mathcal{G}) \) (see equation (9))

Suppose for a contradiction that there is a \( d \)-connecting path from \( B_i \) to \( X_{ni} \) in \( \mathcal{D}_{X_{ni}} \). Let \( p = \langle B_i, \ldots, X \rangle \), \( B_i \in B_1 \), \( X \in X_{ni} \), be a shortest such path in \( \mathcal{D}_{X_{ni}} \). Let \( p^* \) be the path in \( \mathcal{G} \) that consists of the same sequence of nodes as \( p \) in \( \mathcal{D}_{X_{ni}} \). This proof follows a very similar line of reasoning to the proof of (ii) above.

Let \( \{B_1, \ldots, B_r\} \) be \( \mathcal{P}(O, \mathcal{G}) \), \( r \geq k \). Let \( l \in \{i, \ldots, r\} \) such that \( B_i \cap B_i' \neq \emptyset \), then \( B_i \in B_i' \) and \( \text{Pa}(B_i, \mathcal{G}) \subseteq (\cup_{j=1}^{i-1} B_j) \).

Suppose that \( p \) is of the form \( B_1 \rightarrow \ldots \cdot X \). If \( X \in X_{ni} \), then \( p \) is not a causal path since \( p \) is a path in \( \mathcal{D}_{X_{ni}} \). Otherwise, \( X \in \text{An}(P_i, \mathcal{D}_{X_{ni}}) \) and so any causal path from \( B_i \) to \( X \) would need to contain a node in \( X_{ni} \) and hence, would be blocked by \( \text{Pa}(B_i, \mathcal{G}) \). Thus, \( p \) is not a causal path from \( B_i \) to \( X \).

Hence, let \( C \) be the closest collider to \( B_i \) on \( p \), that is, \( p \) has the form \( B_1 \rightarrow \cdots \leftarrow C \rightarrow \ldots \cdot X \). Since \( p \) is \( d \)-connecting given \( \text{Pa}(B_i, \mathcal{G}) \), \( C \) is be an ancestor of \( \text{Pa}(B_i, \mathcal{G}) \) in \( \mathcal{D}_{X_{ni}} \).

However, this would imply that \( p \) is not a causal path from \( B_i \in B_i' \) to \( \text{Pa}(B_i, \mathcal{G}) \subseteq (\cup_{j=1}^{i-1} B_j) \) in \( \mathcal{D}_{X_{ni}} \), which contradicts Lemma 3.4.

Next, suppose that \( p \) is of the form \( B_i \leftarrow A \ldots X \), \( A \notin B_i \). Since \( p \) is \( d \)-connecting given \( \text{Pa}(B_i, \mathcal{G}) \), \( A \notin \text{Pa}(B_i, \mathcal{G}) \). Hence, \( B_i \rightarrow A \) is in \( \mathcal{G} \).

Then \( A \in B_i' \). Note that by (i) above, \( X \cap B_i' = \emptyset \), so \( p^* \) is not an undirected path in \( \mathcal{G} \).
Hence, let \( B \) be the closest node to \( B_i \) on \( p^* \) such that \( p^*(B, X) \) starts with a directed edge (possibly \( B = A \)). Then \( p^* \) is either of the form \( B_i - A - \cdots - L - B \rightarrow R \ldots X \) or of the form \( B_i - A - \cdots - L - B \leftarrow R \ldots X \).

Suppose first that \( p^* \) is of \( B_i - A - \cdots - L - B \rightarrow R \ldots X \). Then \( B \in B_i^t \) and so \( B \notin X \). Since \( p \) is d-connecting given \( Pa(B_i, G) \), \( B \notin Pa(B_i, G) \) and additionally, \( B \notin B_i \) otherwise, a shorter path could have been chosen.

Now consider subpath \( p(B, X) \). There is at least one collider on \( p(B, X) \). Since \( B_i, B_j \in B_i^t \), the same reasoning as above can be used to derive a contradiction in this case.

Suppose next that \( p^* \) is of the form \( B_i - A - \cdots - L - B \leftarrow R \ldots X \). Then either \( R \rightarrow L \) or \( R - L \) is in \( G \) (Meek, 1995, see Figure 3 in the main text). We first show that in either case, edge \( \langle L, R \rangle \) is also in \( \overline{D_{X_{pi}X_{ni}}} \).

Since \( L \in B_i \) and since \( X \cap B_j = \emptyset \), \( L \notin X \). Hence, if \( R \rightarrow L \) is in \( G \), \( R \rightarrow L \) is in \( \overline{D_{X_{pi}X_{ni}}} \). If \( R - L \) is in \( G \), then \( R \in B_i \) and since \( X \cap B_j = \emptyset \), \( R \notin X \), so \( \langle L, R \rangle \) is in \( \overline{D_{X_{pi}X_{ni}}} \).

Hence, \( q = p(B_i, L) \oplus \langle L, R \rangle \oplus p(R, X) \) is a shorter path than \( p \) in \( \overline{D_{X_{pi}X_{ni}}} \). If \( L \) and \( R \) have the same collider/non-collider status on \( q \) on \( p \), then \( q \) is also d-connecting given \( Pa(B_i, G) \), which would contradict our choice of \( p \). Hence, the collider/non-collider status of \( L \) or \( R \), is different on \( p \) and \( q \). We now discuss the cases for the change of collider/non-collider status of \( L \) and \( R \) and derive a contradiction in each.

Suppose that \( L \) is a collider on \( q \), and a non-collider on \( p \). This implies that \( W \rightarrow L \rightarrow B \leftarrow R \rightarrow R \) is a subpath of \( p \) and \( L \leftarrow R \) are in \( \overline{D_{X_{pi}X_{ni}}} \). Even though \( L \) is not a collider on \( p \), \( B \) is a collider on \( p \) and \( L \in An(B, \overline{D_{X_{pi}X_{ni}}} \). Since \( p \) is d-connecting given \( Pa(B_i, G) \), \( De(B, \overline{D_{X_{pi}X_{ni}}} \cap Pa(B_i, G) \neq \emptyset \). However, then also \( De(L, \overline{D_{X_{pi}X_{ni}}} \cap Pa(B_i, G) \neq \emptyset \) and \( q \) is also d-connecting given \( Pa(B_i, G) \) and a shorter path between \( B_i \) and \( X_{ni} \) than \( p \), which is a contradiction.

The contradiction can be derived in exactly the same way as above in the case when \( R \) is a collider on \( q \), and a non-collider on \( p \). Since \( B \leftarrow R \) is in \( \overline{D_{X_{pi}X_{ni}}} \), \( R \) cannot be anything but a non-collider on \( q \), so the only case left to consider is if \( L \) is a non-collider on \( q \) and a collider on \( p \).

For \( L \) to be a non-collider on \( q \) and a collider on \( p \), \( W \rightarrow L \leftarrow B \leftarrow R \) must be a subpath of \( p \) and \( L \rightarrow R \) should be in \( \overline{D_{X_{pi}X_{ni}}} \). But then there is a cycle in \( \overline{D_{X_{pi}X_{ni}}} \) which is a contradiction.

(iv): If \( B_i \perp_{\overline{D_{X_{pi}}} X_{pi}}^d P_1 \), then \( f(b_i|p_i, do(x_{pi})) = f(b_i|pa(b_i, G)) \) by Rule 2 of the do calculus (equation (8)).

Suppose for a contradiction that there is a d-connecting path from \( B_i \) to \( X_{pi} \) in \( \overline{D_{X_{pi}X_{ni}}} \). Let \( p = \langle B_i, \ldots, X \rangle \), \( B_i \in B_i \), \( X \in X_{pi} \), be a shortest such path in \( \overline{D_{X_{pi}X_{ni}}} \). Let \( p^* \) be the path in \( G \) that consists of the same sequence of nodes as \( p \) in \( \overline{D_{X_{pi}}} \). This proof follows a very similar line of reasoning to the proof of (ii) above.

Let \( \langle B_1', \ldots, B_r' \rangle = FC0(V, G) \), \( r \geq k \). Let \( l \in \{i, \ldots, r\} \) such that \( B_j' \cap B_i \neq \emptyset \), then \( B_i \in B_i' \) and by (i) above, \( X_{pi} \subseteq (\cup_{j=1}^{r-1} B_j') \).

Suppose that \( p \) is of the form \( B_i \rightarrow \cdots \rightarrow X \). Since \( B_i \in B_i' \) and \( X_{pi} \subseteq (\cup_{j=1}^{r-1} B_j') \), by Lemma 3.4, there is at least one collider on \( p \). Hence, let \( C \) be the closest collider to \( B_i \) on \( p \), that is, \( p \) has the form \( B_i \rightarrow \cdots \rightarrow C \leftarrow \cdots \rightarrow X \). Since \( p \) is d-connecting given \( P_i \) in \( \overline{D_{X_{pi}}} \),
C is be an ancestor of $P_1$ in $D_{X_{pi}}$. However, this would imply that there is a causal path from $B_i \in B_i$ to $P_1 \subseteq (\cup_{j=1}^{t-1} B_j)$ in $D_{X_{pi}}$, which contradicts Lemma 3.4.

Next, suppose that $p$ is of the form $B_i \leftarrow A \ldots X, A \notin B_i$. Since $p$ is a path in $D_{X_{pi}}, A \notin X_{pi}$. Additionally, since $p$ is $d$-connecting given $P_1, A \notin P_1$. Hence, $B_i - A$ is in $G$.

Then $A \in B_i^t$ and since $X \subseteq (\cup_{j=1}^{t-1} B_j), p^*(A, X)$ is not an undirected path in $G$. Hence, let $B$ be the closest node to $B_i$ on $p^*$ such that $p^*(B, X)$ starts with a directed edge (possibly $B = A$). Then $p^*$ is either of the form $B_i - A - \ldots - L - B \rightarrow R \ldots X$ or of the form $B_i - A - \ldots - L - B \leftarrow R \ldots X$.

Suppose first that $p^*$ is of $B_i - A - \ldots - L - B \rightarrow R \ldots X$. Then $B \in B_i^t$ and since $X_{pi} \subseteq (\cup_{j=1}^{t-1} B_j), B \notin X_{pi}$. Since $p$ is $d$-connecting given $P_1, B \notin P_1$ and additionally, $B \notin B_i$ otherwise, a shorter path could have been chosen.

Now consider subpath $p(B, X)$. Since $B, B_i \in B_i^t$, the same reasoning as above can be used to derive a contradiction in this case.

Suppose next that $p^*$ is of the form $B_i - A - \ldots - L - B \leftarrow R \ldots X$. Then each $R \rightarrow L$ or $R - L$ is in $G$ (Meek, 1995, see Figure 3 in the main text). Since $R \rightarrow B$ is in $D_{X_{pi}}, R \notin X_{pi}$. Hence, $q = p(B_i, L) \oplus (L, R) \oplus p(R, X)$ is a shorter path than $p$ in $D_{X_{pi}}$. If $L$ and $R$ have the same collider/non-collider status on $q$ on $p$, then $q$ is also $d$-connecting given $P_1$, which would contradict our choice of $p$. Hence, the collider/non-collider status of $L$ or $R$, is different on $p$ and $q$. We now discuss the cases for the change of collider/non-collider status of $L$ and $R$ and derive a contradiction in each.

Suppose that $L$ is a collider on $q$, and a non-collider on $p$. This implies that $W \rightarrow L \rightarrow B \leftarrow R$ is the shortest path between $B_i$ and $X_{pi}$, which is a contradiction.

The contradiction can be derived in exactly the same way as above in the case when $R$ is a collider on $q$, and a non-collider on $p$. Since $B \leftarrow R$ is in $D_{X_{pi}}, R$ cannot be anything but a non-collider on $q$, so the only case left to consider is if $L$ is a non-collider on $q$ and a collider on $p$.

For $L$ to be a non-collider on $q$ and a collider on $p$, $W \rightarrow L \leftarrow B \leftarrow R$ must be a subpath of $p$ and $L \rightarrow R$ should be in $D_{X_{pi}}$. But then there is a cycle in $D_{X_{pi}}$, which is a contradiction.

\textbf{Lemma D.2.} Let $X, Y$ and $Z$ be distinct nodes in MPDAG $G = (V, E)$. Suppose that there is an unshielded possibly causal path $p$ from $X$ to $Y$ and a causal path $q$ from $Y$ to $Z$ in $G$ such that the only node that $p$ and $q$ have in common is $Y$. Then $p \oplus q$ is a possibly causal path from $X$ to $Z$.

\textbf{Proof of Lemma D.2.} Suppose for a contradiction that there is an edge $V_q \rightarrow V_p$, where $V_q$ is a node on $q$ and $V_p$ is a node on $p$ (additionally, $V_p \neq Y \neq V_q$). Then $p(V_p, Y)$ cannot be a causal path from $V_p$ to $Y$ since otherwise there is a cycle in $G$. So $p(V_p, Y)$ takes the form $V_p \rightarrow V_{p+1} \ldots Y$.

Let $D$ be a DAG in $[G]$, that contains $V_p \rightarrow V_{p+1}$. Since $p(V_p, Y)$ is an unshielded possibly causal path in $G$, it corresponds to $V_p \rightarrow \cdots \rightarrow Y$ in $D$. Then $V_q \rightarrow V_p \rightarrow \cdots \rightarrow Y$ and $q(Y, V_q)$ form a cycle in $D$, a contradiction. \qed
E Proofs for Section 4

Proof of Proposition 4.2. If the causal effect of $X$ on $Y$ is not identifiable in $G$, by Theorem 3.5, there is a proper possibly causal path from $X$ to $Y$ that starts with an undirected edge in $G$. Then by Theorem 4.1, there is no adjustment set relative to $(X, Y)$ in $G$.

Hence, suppose that there is no proper possibly causal path from $X$ to $Y$ that starts with an undirected edge in $G$ and consider $Pa(X, G)$. By Theorem 4.1, it is enough to show that $Pa(X, G)$ satisfies the generalized adjustment criterion relative to $(X, Y)$.

If $G$ is a DAG, $Pa(X, G)$ is an adjustment set relative to $(X, Y)$ by Theorem 3.3.2 of Pearl (2009). Hence, suppose that $G$ is not a DAG.

Since $G$ is acyclic, $Pa(X, G) \cap De(X, G) = \emptyset$. Additionally, by Lemma A.8, $Forb(X, Y, G) \subseteq De(X, G)$. Hence, $Pa(X, G)$ satisfies $Pa(X, G) \cap Forb(X, Y, G) = \emptyset$, that is, condition 2 in Theorem 4.1 relative to $(X, Y)$ in $G$.

Consider a non-causal definite status path $p$ from $X$ to $Y$. If $p$ is of the form $X \leftarrow \ldots Y$ in $G$, then $p$ is blocked by $Pa(X, G)$. If $p$ is of the form $X \rightarrow \ldots Y$, then $p$ contains at least one collider $C \in De(X, G)$ and since $Pa(X, G) \cap De(X, G) = \emptyset$, $p$ is blocked by $Pa(X, G)$.

Lastly, suppose that $p$ is of the form $X \ldots Y$. Since $p$ is a non-causal path from $X$ to $Y$ and since $p$ is of definite status in $G$, by Lemma A.5, there is at least one edge pointing towards $X$ on $p$. Let $D$ be the closest node to $X$ on $p$ such that $p(D, Y)$ is of the form $D \leftarrow \ldots Y$ in $G$. Then by Lemma A.5, $p(X, D)$ is a possibly causal path from $X$ to $D$ so let $p'$ be an unshielded subsequence of $p(X, D)$ that forms a possibly causal path from $X$ to $D$ in $G$ (Lemma A.6). Additionally, $p$ is of definite status, so $D$ must be a collider on $p$.

In order for $p$ to be blocked by $Pa(X, G)$ it is enough to show that $De(D, G) \cap Pa(X, G) = \emptyset$. Suppose for a contradiction that $E \in De(D, G) \cap Pa(X, G)$. Let $q$ be a directed path from $D$ to $E$ in $G$. Then $p'$ and $q$ satisfy Lemma D.2 in $G$, so $p' \oplus q$ is a possibly causal path from $X$ to $E$. By definition of a possibly causal path in MPDAGs, this contradicts that $E \in Pa(X, G)$. □

References

Andersson, S. A., Madigan, D., and Perlman, M. D. (1997). A characterization of Markov equivalence classes for acyclic digraphs. Annals of Statistics, 25:505–541.

Chickering, D. M. (2002). Learning equivalence classes of Bayesian-network structures. Journal of Machine Learning Research, 2:445–498.

Collins, L. M., Murphy, S. A., and Bierman, K. L. (2004). A conceptual framework for adaptive preventive interventions. Prevention Science, 5(3):185–196.

Collins, L. M., Murphy, S. A., and Strecher, V. (2007). The multiphase optimization strategy (MOST) and the sequential multiple assignment randomized trial (SMART): new methods for more potent ehealth interventions. American Journal of Preventive Medicine, 32(5):S112–S118.

Eigenmann, M., Nandy, P., and Maathuis, M. H. (2017). Structure learning of linear Gaussian structural equation models with weak edges. In Proceedings of UAI 2017.
Galles, D. and Pearl, J. (1995). Testing identifiability of causal effects. In Proceedings of UAI 1995, pages 185–195.

Hauser, A. and Bühlmann, P. (2012). Characterization and greedy learning of interventional Markov equivalence classes of directed acyclic graphs. Journal of Machine Learning Research, 13:2409–2464.

Heuckel, L., Perković, E., and Maathuis, M. H. (2019). Graphical criteria for efficient total effect estimation via adjustment in causal linear models. arXiv:1907.02435.

Hernán, M. A. and Robins, J. M. (2019). Causal inference. Boca Raton: Chapman & Hall/CRC, forthcoming.

Hoyer, P. O., Hyvarinen, A., Scheines, R., Spirtes, P. L., Ramsey, J., Lacerda, G., and Shimizu, S. (2008). Causal discovery of linear acyclic models with arbitrary distributions. In Proceedings of UAI 2008, pages 282–289.

Huang, Y. and Valtorta, M. (2006). Pearl’s calculus of intervention is complete. In Proceedings of UAI 2006.

Jaber, A., Zhang, J., and Bareinboim, E. (2018a). Causal identification under Markov equivalence. In Proceedings of UAI 2018.

Jaber, A., Zhang, J., and Bareinboim, E. (2018b). A graphical criterion for effect identification in equivalence classes of causal diagrams. In Proceedings of IJCAI 2018, pages 5024–5030.

Jaber, A., Zhang, J., and Bareinboim, E. (2019). Causal identification under Markov equivalence: Completeness results. In Proceedings of ICML 2019, volume 97, pages 2981–2989.

Kohler-Hausmann, I. (2018). Eddie Murphy and the dangers of counterfactual causal thinking about detecting racial discrimination. Northwestern University Law Review, 113.

Lauritzen, S. L., Dawid, A. P., Larsen, B. N., and Leimer, H.-G. (1990). Independence properties of directed Markov fields. Networks, 20(5):491–505.

Maathuis, M. H. and Colombo, D. (2015). A generalized back-door criterion. Annals of Statistics, 43:1060–1088.

Mardia, K. V., Kent, J. T., and Bibby, J. M. (1980). Multivariate analysis (probability and mathematical statistics). Academic Press London.

Meek, C. (1995). Causal inference and causal explanation with background knowledge. In Proceedings of UAI 1995, pages 403–410.

Murphy, S. A. (2003). Optimal dynamic treatment regimes. Journal of the Royal Statistical Society: Series B, 65(2):331–355.

Nandy, P., Maathuis, M. H., and Richardson, T. S. (2017). Estimating the effect of joint interventions from observational data in sparse high-dimensional settings. Annals of Statistics, 45(2):647–674.

Pearl, J. (1993). Comment: Graphical models, causality and intervention. Statistical Science, 8:266–269.
Pearl, J. (1995). Causal diagrams for empirical research. *Biometrika*, 82:669–688.

Pearl, J. (2009). *Causality: Models, Reasoning, and Inference*. Cambridge University Press, New York, NY, second edition.

Pearl, J. and Robins, J. M. (1995). Probabilistic evaluation of sequential plans from causal models with hidden variables. In *Proceedings of UAI 1995*, pages 444–453.

Perković, E., Kalisch, M., and Maathuis, M. H. (2017). Interpreting and using CPDAGs with background knowledge. In *Proceedings of UAI 2017*.

Perković, E., Textor, J., Kalisch, M., and Maathuis, M. H. (2015). A complete generalized adjustment criterion. In *Proceedings of UAI 2015*, pages 682–691.

Perković, E., Textor, J., Kalisch, M., and Maathuis, M. H. (2018). Complete graphical characterization and construction of adjustment sets in Markov equivalence classes of ancestral graphs. *Journal of Machine Learning Research*, 18.

Rahmadi, R., Groot, P., Heins, M., Knoop, H., Heskes, T., et al. (2017). Causality on cross-sectional data: stable specification search in constrained structural equation modeling. *Applied Soft Computing*, 52:687–698.

Rahmadi, R., Groot, P., van Rijn, M. H., van den Brand, J. A., Heins, M., Knoop, H., Heskes, T., Initiative, A. D. N., Group, M. S., and consortium, O. (2018). Causality on longitudinal data: Stable specification search in constrained structural equation modeling. *Statistical Methods in Medical Research*, 27(12):3814–3834.

Richardson, T. S., Evans, R. J., Robins, J. M., and Shpitser, I. (2017). Nested Markov properties for acyclic directed mixed graphs. arXiv preprint arXiv:1701.06686.

Richardson, T. S. and Spirtes, P. (2002). Ancestral graph Markov models. *Annals of Statistics*, 30:962–1030.

Robins, J. M. (1986). A new approach to causal inference in mortality studies with a sustained exposure period-application to control of the healthy worker survivor effect. *Mathematical Modelling*, 7:1393–1512.

Rothenhäusler, D., Ernest, J., and Bühlmann, P. (2018). Causal inference in partially linear structural equation models: identifiability and estimation. *Annals of Statistics*, 46:2904–2938.

Scheines, R., Spirtes, P., Glymour, C., Meek, C., and Richardson, T. (1998). The TETRAD project: constraint based aids to causal model specification. *Multivariate Behavioral Research*, 33(1):65–117.

Shpitser, I. and Pearl, J. (2006). Identification of joint interventional distributions in recursive semi-Markovian causal models. In *Proceedings of AAAI 2006*, pages 1219–1226.

Shpitser, I., VanderWeele, T., and Robins, J. M. (2010). On the validity of covariate adjustment for estimating causal effects. In *Proceedings of UAI 2010*, pages 527–536.

Spirtes, P., Glymour, C., and Scheines, R. (2000). *Causation, Prediction, and Search*. MIT Press, Cambridge, MA, second edition.
Taubman, S. L., Robins, J. M., Mittleman, M. A., and Hernán, M. A. (2009). Intervening on risk factors for coronary heart disease: an application of the parametric g-formula. *International Journal of Epidemiology*, 38(6):1599–1611.

Tian, J. and Pearl, J. (2002). A general identification condition for causal effects. In *Proceedings of AAAI 2002*, pages 567–573.

van der Zander, B., Liškiewicz, M., and Textor, J. (2014). Constructing separators and adjustment sets in ancestral graphs. In *Proceedings of UAI 2014*, pages 907–916.

VanderWeele, T. J. and Robinson, W. R. (2014). On causal interpretation of race in regressions adjusting for confounding and mediating variables. *Epidemiology*, 25(4).

Wang, Y., Solus, L., Yang, K. D., and Uhler, C. (2017). Permutation-based causal inference algorithms with interventions. In *Proceedings of NeurIPS 2017*.

Westreich, D., Cole, S. R., Young, J. G., Palella, F., Tien, P. C., Kingsley, L., Gange, S. J., and Hernán, M. A. (2012). The parametric g-formula to estimate the effect of highly active antiretroviral therapy on incident AIDS or death. *Statistics in Medicine*, 31(18):2000–2009.

Wright, S. (1921). Correlation and causation. *Journal of Agricultural Research*, 20(7):557–585.

Young, J. G., Cain, L. E., Robins, J. M., OReilly, E. J., and Hernán, M. A. (2011). Comparative effectiveness of dynamic treatment regimes: an application of the parametric g-formula. *Statistics in Biosciences*, 3(1):119.

Zhang, J. (2008a). Causal reasoning with ancestral graphs. *Journal of Machine Learning Research*, 9:1437–1474.

Zhang, J. (2008b). On the completeness of orientation rules for causal discovery in the presence of latent confounders and selection bias. *Artificial Intelligence*, 172:1873–1896.