# Supplement to Identifying causal effects in maximally oriented partially directed acyclic graphs 

Emilija Perković<br>Department of Statistics<br>University of Washington<br>Seattle, WA 98195-4322

## 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 $p=\left\langle X_{1}, X_{2}, \ldots, X_{m}\right\rangle$, the subpath from $X_{i}$ to $X_{k}(1 \leq i \leq k \leq m)$ is the path $p\left(X_{i}, X_{k}\right)=$ $\left\langle X_{i}, X_{i+1}, \ldots, X_{k}\right\rangle$.

Concatenation. We denote concatenation of paths by $\oplus$, so that for a path $p=\left\langle X_{1}, X_{2}, \ldots, X_{m}\right\rangle, p=$ $p\left(X_{1}, X_{r}\right) \oplus p\left(X_{r}, X_{m}\right)$, for $1 \leq r \leq m$.
D-separation. If $\mathbf{X}$ and $\mathbf{Y}$ are d-separated given $\mathbf{Z}$ in a DAG $\mathcal{D}$, we write $\mathbf{X} \perp_{\mathcal{D}} \mathbf{Y} \mid \mathbf{Z}$.

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 $\mathcal{G}$ is $\operatorname{PossDe}(X, \mathcal{G})$. For a set of nodes $\mathbf{X} \subseteq \mathbf{V}$, we let $\left.\operatorname{PossDe}(\mathbf{X}, \mathcal{G})=\cup_{X \in \mathbf{X}}\right) \operatorname{PossDe}(X, \mathcal{G})$.

Bayesian And Causal Bayesian Networks. If a density $f$ over $\mathbf{V}$ is consistent with DAG $\mathcal{D}=(\mathbf{V}, \mathbf{E})$, then $(\mathcal{D}, f)$ form a Bayesian network. Let $\mathbf{F}$ be a set of density functions made up of all interventional densities $f\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$ for any $\mathbf{X} \subset \mathbf{V}$ and $\mathbf{V}^{\prime}=\mathbf{V} \backslash \mathbf{X}$ that are consistent with $\mathcal{D}$ ( $\mathbf{F}$ also includes all observational densities consistent with $\mathcal{D}$ ), then $(\mathcal{D}, \mathbf{F})$ form a causal Bayesian network.

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

Rule 1 (Insertion/deletion of observations). If $\mathbf{Y} \perp_{\mathcal{D}_{\overline{\mathbf{x}}}}$ $\mathbf{Z} \mid \mathbf{X} \cup \mathbf{W}$, then

$$
\begin{equation*}
f(\mathbf{y} \mid d o(\mathbf{x}), \mathbf{w})=f(\mathbf{y} \mid \operatorname{do}(\mathbf{x}), \mathbf{z}, \mathbf{w}) \tag{1}
\end{equation*}
$$

Rule 2. If $\mathbf{Y} \perp_{\mathcal{D}_{\overline{\mathbf{x}} \underline{z}}} \mathbf{Z} \mid \mathbf{X} \cup \mathbf{W}$, then

$$
\begin{equation*}
f(\mathbf{y} \mid d o(\mathbf{x}), d o(\mathbf{z}), \mathbf{w})=f(\mathbf{y} \mid d o(\mathbf{x}), \mathbf{z}, \mathbf{w}) \tag{2}
\end{equation*}
$$

Rule 3. If $\mathbf{Y} \perp_{\mathcal{D}_{\overline{\mathbf{X Z}(\mathbf{W})}}} \mathbf{Z} \mid \mathbf{X} \cup \mathbf{W}$, then

$$
\begin{equation*}
f(\mathbf{y} \mid d o(\mathbf{x}), \mathbf{w})=f(\mathbf{y} \mid \operatorname{do}(\mathbf{x}), d o(\mathbf{z}), \mathbf{w}) \tag{3}
\end{equation*}
$$

where $\mathbf{Z}(\mathbf{W})=\mathbf{Z} \backslash \operatorname{An}\left(\mathbf{W}, \mathcal{D}_{\overline{\mathbf{X}}}\right)$.

## A. 1 EXISTING RESULTS

Theorem A. 1 (Wright's rule Wright, 1921). Let $\mathbf{X}=$ $\mathbf{A X}+\epsilon$, where $\mathbf{A} \in \mathbb{R}^{k \times k}, \mathbf{X}=\left(X_{1}, \ldots, X_{k}\right)^{T}$ and $\epsilon=$ $\left(\epsilon_{1}, \ldots, \epsilon_{k}\right)^{T}$ is a vector of mutually independent errors with means zero. Moreover, let $\operatorname{Var}(\mathbf{X})=\mathbf{I}$. Let $\mathcal{D}=$ $(\mathbf{X}, \mathbf{E})$, be the corresponding DAG such that $X_{i} \rightarrow X_{j}$ in $\mathcal{D}$ if and only if $A_{j i} \neq 0$. A nonzero entry $A_{j i}$ is called the edge coefficient of $X_{i} \rightarrow X_{j}$. For two distinct nodes $X_{i}, X_{j} \in \mathbf{X}$, 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 $\operatorname{Cov}\left(X_{i}, X_{j}\right)=\sum_{s=1}^{r} \pi_{s}$, 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 $\mathbf{X}=\left(\mathbf{X}_{\mathbf{1}}{ }^{T}, \mathbf{X}_{\mathbf{2}}{ }^{T}\right)^{T}$ be a p-dimensional multivariate Gaussian random vector with mean vector $\mu=$ $\left(\mu_{\mathbf{1}}^{T}, \mu_{\mathbf{2}}{ }^{T}\right)^{T}$ and covariance matrix $\boldsymbol{\Sigma}=\left[\begin{array}{ll}\boldsymbol{\Sigma}_{\mathbf{1 1}} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{\mathbf{2 1}} & \boldsymbol{\Sigma}_{22}\end{array}\right]$, so that $\mathbf{X}_{\mathbf{1}}$ is a $q$-dimensional multivariate Gaussian random vector with mean vector $\mu_{1}$ and covariance matrix $\boldsymbol{\Sigma}_{11}$ and $\mathbf{X}_{\mathbf{2}}$ is a $(p-q)$-dimensional multivariate Gaussian random vector with mean vector $\mu_{2}$ and covariance matrix $\boldsymbol{\Sigma}_{22}$. Then $E\left[\mathbf{X}_{\mathbf{2}} \mid \mathbf{X}_{\mathbf{1}}=\mathbf{x}_{\mathbf{1}}\right]=\mu_{\mathbf{2}}+$ $\boldsymbol{\Sigma}_{21} \boldsymbol{\Sigma}_{11}^{-1}\left(\mathrm{x}_{\mathbf{1}}-\mu_{\mathbf{1}}\right)$.

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Algorithm 2: PTO algorithm (Jaber et al., 2018)
input : DAG or CPDAG \(\mathcal{G}=(\mathbf{V}, \mathbf{E})\).
output : An ordered list \(\mathbf{B}=\left(\mathbf{B}_{\mathbf{1}}, \ldots, \mathbf{B}_{\mathbf{k}}\right), k \geq 1\)
                of the bucket decomposition of \(\mathbf{V}\) in \(\mathcal{G}\).
1 Let ConComp be the bucket decomposition of \(\mathbf{V}\)
    in \(\mathcal{G}\);
Let \(\mathbf{B}\) be an empty list;
while ConComp \(\neq \emptyset\) do
        Let \(\mathbf{C} \in \mathbf{C o n C o m p}\);
        Let \(\overline{\mathbf{C}}\) be the set of nodes in ConComp that
        are not in \(\mathbf{C}\);
        if all edges between \(\mathbf{C}\) and \(\overline{\mathbf{C}}\) are into \(\mathbf{C}\) in \(\mathcal{G}\)
        then
            Add \(\mathbf{C}\) to the beginning of \(\mathbf{B}\);
        end
end
return B;
```

Lemma A. 3 (c.f. Lemma C. 1 of Perković et al., 2017, Lemma 8 of Perković et al., 2018). Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in a MPDAG $\mathcal{G}$. Suppose that there is a proper possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ that starts with an undirected edge in $\mathcal{G}$, then there is one such path $q=\left\langle X, V_{1}, \ldots, Y\right\rangle, X \in \mathbf{X}, Y \in \mathbf{Y}$ 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 $p=\left\langle V_{1}, \ldots, V_{k}\right\rangle$ 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 $\mathbf{A .} 7$ (c.f. Lemma 1 of Jaber et al., 2018). Let $\mathcal{G}=(\mathbf{V}, \mathbf{E})$ be a CPDAG or $D A G$ and let $\mathbf{B}=$ $\left(\mathbf{B}_{\mathbf{1}}, \ldots, \mathbf{B}_{\mathbf{k}}\right), k \geq 1$, be the output of $\operatorname{PTO}(\mathcal{G})$ (Algorithm 2). Then for each $i, j \in\{1, \ldots k\}, \mathbf{B}_{\mathbf{i}}$ and $\mathbf{B}_{\mathbf{j}}$ are buckets in $\mathbf{V}$ and if $i<j$, then $\mathbf{B}_{\mathbf{i}}<\mathbf{B}_{\mathbf{j}}$.
Lemma A. 8 (c.f. Lemma E. 6 of Henckel et al., 2019).

Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in an MPDAG $\mathcal{G}$ and suppose that there is no proper possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ that starts with an undirected edge in $\mathcal{G}$. Let $\mathcal{D}$ be a $D A G$ in $[\mathcal{G}]$. Then $\operatorname{Forb}(\mathbf{X}, \mathbf{Y}, \mathcal{G}) \subseteq \operatorname{De}(\mathbf{X}, \mathcal{G})$.

## B PROOFS FOR SECTION 3.1 OF THE MAIN TEXT

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 path $q=\left\langle X, V_{1}, \ldots, Y\right\rangle, k \geq 1, X \in \mathbf{X}, Y \in \mathbf{Y}$ 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 $A \in \mathbf{V}$ 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 $\left\{\epsilon_{A}: A \in \mathbf{V}\right\}$, 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 $\mathbf{V}$ is 1 .

The density $f$ of $\mathbf{V}$ 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 $f_{1}(\mathbf{v})=f(\mathbf{v})$ and let $f_{2}(\mathbf{v})=f(\mathbf{v})$.
Let $f_{1}\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$ be an interventional density consistent with $\mathcal{D}^{11}$. Similarly let $f_{2}\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$ be an interventional density consistent with $\mathcal{D}^{21}$. Then $f_{1}\left(\mathbf{v}^{\prime} \mid \operatorname{do}(\mathbf{x})\right)$ and $f_{1}\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$ are also interventional densities consistent with $\mathcal{D}^{1}$ and $\mathcal{D}^{2}$, respectively. Now, $f_{1}(\mathbf{y} \mid d o(\mathbf{x}))$ is a marginal interventional density of $\mathbf{Y}$ that can be calculated from the density $f_{1}\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$ and the analagous is true for $f_{2}(\mathbf{y} \mid d o(\mathbf{x}))$ and $f_{2}\left(\mathbf{v}^{\prime} \mid d o(\mathbf{x})\right)$.

In order to show that $f_{1}(\mathbf{y} \mid d o(\mathbf{x})) \neq f_{2}(\mathbf{y} \mid d o(\mathbf{x}))$, it suffices to show that $f_{1}(y \mid d o(\mathbf{x}=1)) \neq f_{2}(y \mid d o(\mathbf{x}=\mathbf{1}))$ for at least one $Y \in \mathbf{Y}$ when all $\mathbf{X}$ variables are set to 1 by a do-intervention. In order for $f_{1}(y \mid d o(\mathbf{x}=1)) \neq$
$f_{2}(y \mid d o(\mathbf{x}=\mathbf{1}))$ to hold, it is enough to show that the expectation of $Y$ is not the same under these two densities. Hence, let $E_{1}[Y \mid d o(\mathbf{X}=\mathbf{1})]$ denote the expectation of $Y$, under $f_{1}(y \mid d o(\mathbf{X}=\mathbf{1}))$ and let $E_{2}[Y \mid d o(\mathbf{X}=\mathbf{1})]$ denote the expectation of $\mathbf{Y}$, under $f_{2}(y \mid d o(\mathbf{X}=\mathbf{1}))$.

Since $Y$ is d-separated from $\mathbf{X}$ in $\mathcal{D}_{\frac{\mathbf{X}}{21}}^{21}$ we can use Rule 3 of the do-calculus (see equation (3)) to conclude that $E_{2}[Y \mid d o(\mathbf{X}=\mathbf{1})]=E[Y]=0$. Similarly, since $Y$ is d-separated from $\mathbf{X}$ in $\mathcal{D}_{\mathbf{X}}^{11}$, we can use Rule 2 of the do-calculus (see equation (2)) to conclude that $E_{1}[Y \mid$ $d o(\mathbf{X}=\mathbf{1})]=E[Y \mid X=1]$. By Theorems A. 2 and A.1, $E[Y \mid X=1]=\operatorname{Cov}(X, Y)=a$, where $a$ is the product of all edge coefficients on $q_{1}$. Since $a \neq 0$, $E_{1}[Y \mid d o(\mathbf{X}=\mathbf{1})] \neq E_{2}[Y \mid \operatorname{do}(\mathbf{X}=\mathbf{1})]$.

## C PROOFS FOR SECTION 3.2 OF THE MAIN TEXT

Lemma C.1. Let $\mathbf{D}$ be any subset of $\mathbf{V}$ in MPDAG $\mathcal{G}=$ $(\mathbf{V}, \mathbf{E})$. Then the call to algorithm $\operatorname{PCO}(\mathbf{D}, \mathcal{G})$ will complete. Meaning that, at each iteration of the while loop in $\operatorname{PCO}(\mathbf{D}, \mathcal{G})$ (Algorithm 1), there is a bucket $\mathbf{C}$ among the remaining buckets in ConComp (the bucket decomposition of $\mathbf{V}$ ) such that all edges between $\mathbf{C}$ and ConComp $\backslash \mathbf{C}$ are into $\mathbf{C}$ in $\mathcal{G}$.

Proof of Lemma C.1. Let $\mathbf{C}_{\mathbf{1}}, \ldots, \mathbf{C}_{\mathbf{k}}$ be the buckets in ConComp at some iteration of the while loop in the call to $\operatorname{PCO}(\mathbf{D}, \mathcal{G})$. Suppose for contradiction that there is no bucket $\mathbf{C}_{\mathbf{i}}, i \in\{1, \ldots, k\}$ such that all edges between $\mathbf{C}_{\mathbf{i}}$ and $\cup_{j=1}^{k} \mathbf{C}_{\mathbf{j}} \backslash \mathbf{C}_{\mathbf{i}}$ are into $\mathbf{C}_{\mathbf{i}}$. We will show that this leads to the conclusion that $\mathcal{G}$ is not acyclic (a contradiction).

Consider a directed graph $\mathcal{G}_{1}$ constructed so that each bucket in ConComp represents one node in $\mathcal{G}_{1}$. Meaning, a bucket $\mathbf{C}_{\mathbf{i}}, i \in\{1, \ldots, k\}$ is represented by a node $C_{i}$ in $\mathcal{G}_{1}$. Also, let $C_{i} \rightarrow C_{j}, i, j \in\{1, \ldots, k\}$, be in $\mathcal{G}_{1}$ if $A \rightarrow B$ is in $\mathcal{G}$ and $A \in C_{i}, B \in C_{j}$.

Since there is no bucket $\mathbf{C}_{\mathbf{i}}$ in ConComp such that all edges between $\mathbf{C}_{\mathbf{i}}$ and $\cup_{j=1}^{k} \mathbf{C}_{\mathbf{j}} \backslash \mathbf{C}_{\mathbf{i}}$ are into $\mathbf{C}_{\mathbf{i}}$, there is either a directed cycle in $\mathcal{G}_{1}$, or $C_{l} \rightarrow C_{r}$ and $C_{r} \rightarrow C_{l}$ is in $\mathcal{G}_{1}$ for some $l, r \in\{1, \ldots, k\}$. For simplicity, we will refer to both previously mentioned cases as directed cycles.
Let us choose one such directed cycle in $\mathcal{G}_{1}$, that is, let $C_{r_{1}} \rightarrow \cdots \rightarrow C_{r_{m}} \rightarrow C_{r_{1}}, 2 \leq m \leq k, r_{1}, \ldots, r_{m} \in$ $\{1, \ldots, k\}$, be in $\mathcal{G}_{1}$. Let $A_{i} \in \mathbf{C}_{\mathbf{r}_{\mathbf{i}}}$ and $B_{i+1} \in \mathbf{C}_{\mathbf{r}_{\mathbf{i}+1}}$, for all $i \in\{1, \ldots, m-1\}$, such that $A_{i} \rightarrow B_{i+1}$ is in $\mathcal{G}$. Additionally, let $A_{m} \in \mathbf{C}_{\mathbf{r}_{\mathrm{m}}}$, and $B_{1} \in \mathbf{C}_{\mathbf{r}_{1}}$ such that $A_{m} \rightarrow B_{1}$ is in $\mathcal{G}$.

Since $A_{1} \rightarrow B_{2}$ is in $\mathcal{G}$ and $B_{2}$ and $A_{2}$ are in the same
bucket $\mathbf{C}_{\mathbf{r}_{2}}$ in $\mathcal{G}$, by Lemma C.2, $A_{1} \rightarrow A_{2}$. The same reasoning can be applied to conclude that $A_{i} \rightarrow A_{i+1}$, for all $i \in\{1, \ldots, m-1\}$ and also that $A_{m} \rightarrow A_{1}$ is in $\mathcal{G}$. Thus, $A_{1} \rightarrow A_{2} \rightarrow \cdots \rightarrow A_{m} \rightarrow A_{1}$, a directed cycle is in $\mathcal{G}$, a contradiction.

Proof of Lemma 3.5. Lemma C. 2 and Lemma A. 7 together imply that Algorithm 2 can be applied to a MPDAG $\mathcal{G}$ and also that the output of $\operatorname{PTO}(\mathcal{G})$ is the same as that of $\operatorname{PCO}(\mathbf{V}, \mathcal{G})$. Furthermore, $\operatorname{PTO}(\mathcal{G})=$ $\operatorname{PCO}(\mathbf{V}, \mathcal{G})=\left(\overline{\mathbf{B}_{\mathbf{1}}}, \ldots, \overline{\mathbf{B}_{\mathbf{r}}}\right) r \geq k$, where for all $i, j \in$ $\{1, \ldots, r\}, \overline{\mathbf{B}_{\mathbf{i}}}$ and $\overline{\mathbf{B}_{\mathbf{j}}}$ are buckets in $\mathbf{V}$ in $\mathcal{G}$, and if $i<j$, then $\overline{\mathbf{B}_{\mathbf{i}}}<\overline{\mathbf{B}_{\mathbf{j}}}$ with respect to $\mathcal{G}$.
The statement of the lemma then follows directly from the definition of buckets (Definition 3.3) and Corollary 3.4, since for each $l \in\{1, \ldots, k\}$, there exists $s \in$ $\{1, \ldots, r\}$ such that $\mathbf{B}_{\mathbf{l}}=\mathbf{D} \cap \overline{\mathbf{B}_{\mathbf{s}}}$ and $\left(\mathbf{B}_{\mathbf{1}}, \ldots, \mathbf{B}_{\mathbf{k}}\right)$ is exactly the output of $\operatorname{PCO}(\mathbf{V}, \mathcal{G})$.

Lemma C.2. Let $\mathbf{B}$ be a bucket in $\mathbf{V}$ in MPDAG $\mathcal{G}=$ $(\mathbf{V}, \mathbf{E})$ and let $X \in \mathbf{V}, X \notin \mathbf{B}$. If there is a causal path from $X$ to $\mathbf{B}$ in $\mathcal{G}$, then for every node $B \in \mathbf{B}$ there is a causal path from $X$ to $B$ in $\mathcal{G}$.

Proof of Lemma C.2. Let $p$ be a shortest causal path from $X$ to $\mathbf{B}$ in $\mathcal{G}$. Then $p$ is of the form $X \rightarrow \ldots A \rightarrow$ $B$, possibly $X=A$ and $A \notin \mathbf{B}$.

Let $B^{\prime} \in \mathbf{B}, B^{\prime} \neq B$ and let $q=\left\langle B=W_{1}, \ldots, W_{r}=\right.$ $\left.B^{\prime}\right\rangle, r>1$ be a shortest undirected path from $B$ to $B^{\prime}$ in $\mathcal{G}$. It is enough to show that there is an edge $A \rightarrow B^{\prime}$ is in $\mathcal{G}$.

Since $A \rightarrow B-W_{2}$, by the properties of MPDAGs (Meek, 1995, see Figure 2 in the main text), $A \rightarrow W_{2}$ or $A-W_{2}$ is in $\mathcal{G}$. Since $A \notin \mathbf{B}, A \rightarrow W_{2}$ is in $\mathcal{G}$. If $r=2$, we are done. Otherwise, $A \rightarrow W_{2}-W_{3}-\cdots-W_{k}$ is in $\mathcal{G}$ and and we can apply the same reasoning as above iteratively until we obtain $A \rightarrow W_{k}$ is in $\mathcal{G}$.

## D PROOFS FOR SECTION 3.3 OF THE MAIN TEXT

The proof of Theorem 3.6 is given in the main text. Here we provide proofs for the supporting results.
Lemma D.1. Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in $\mathbf{V}$ in MPDAG $\mathcal{G}=(\mathbf{V}, \mathbf{E})$ and suppose that there is no proper possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ that starts with an undirected edge in $\mathcal{G}$. Further, let $\left(\mathbf{B}_{\mathbf{1}}, \ldots \mathbf{B}_{\mathbf{k}}\right)=$ $\operatorname{PCO}\left(\operatorname{An}\left(\mathbf{Y}, \mathcal{G}_{\mathbf{V} \backslash \mathbf{x}}\right), \mathcal{G}\right), k \geq 1$.
(i) For $i \in\{1, \ldots, k\}$, there is no proper possibly causal path from $\mathbf{X}$ to $\mathbf{B}_{\mathbf{i}}$ that starts with an undirected edge in $\mathcal{G}$.
(ii) For $i \in\{2, \ldots, k\}$, let $\mathbf{P}_{\mathbf{i}}=\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{i}}\right) \cap \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. Then for every $D A G \mathcal{D}$ in $[\mathcal{G}]$ and every interventional density $f$ consistent with $\mathcal{D}$ we have

$$
f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{b}_{\mathbf{i}-\mathbf{1}}, \ldots, \mathbf{b}_{\mathbf{1}}, d o(\mathbf{x})\right)=f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o(\mathbf{x})\right)
$$

(iii) For $i \in\{2, \ldots, k\}$, let $\mathbf{P}_{\mathbf{i}}=\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{i}}\right) \cap \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. For $i \in\{1, \ldots, k\}$, let $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}=\mathbf{X} \cap \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. Then for every $D A G \mathcal{D}$ in $[\mathcal{G}]$ and every interventional density $f$ consistent with $\mathcal{D}$ we have

$$
f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o(\mathbf{x})\right)=f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o\left(\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}\right)\right)
$$

Additionally, $f\left(\mathbf{b}_{\mathbf{1}} \mid \operatorname{do}(\mathbf{x})\right)=f\left(\mathbf{b}_{\mathbf{1}} \mid \operatorname{do}\left(\mathbf{x}_{\mathbf{p}_{\mathbf{1}}}\right)\right)$.
(iv) For $i \in\{2, \ldots, k\}$, let $\mathbf{P}_{\mathbf{i}}=\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{i}}\right) \cap \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. For $i \in\{1, \ldots, k\}$, let $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}=\mathbf{X} \cap \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. Then for every $D A G \mathcal{D}$ in $[\mathcal{G}]$ and every interventional density $f$ consistent with $\mathcal{D}$ we have

$$
f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o\left(\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}\right)\right)=f\left(\mathbf{b}_{\mathbf{i}} \mid \operatorname{pa}\left(\mathbf{b}_{\mathbf{i}}, \mathcal{G}\right)\right)
$$

for values $\mathrm{pa}\left(\mathbf{b}_{\mathbf{i}}, \mathcal{G}\right)$ of $\mathrm{Pa}\left(\mathbf{b}_{\mathbf{i}}, \mathcal{G}\right)$ 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 $\mathbf{B}_{\mathbf{i}}$ that starts with an undirected edge in $\mathcal{G}$. Let $p=$ $\langle X, \ldots, B\rangle, X \in \mathbf{X}, B \in \mathbf{B}_{\mathbf{i}}$, be a shortest such path in $\mathcal{G}$. Then $p$ is unshielded in $\mathcal{G}$ (Lemma A.6).

Since $B \in \operatorname{An}\left(\mathbf{Y}, \mathcal{G}_{\mathbf{V} \backslash \mathbf{X}}\right)$ there is a causal path $q$ from $B$ to $\mathbf{Y}$ in $\mathcal{G}$ that does not contain a node in $\mathbf{X}$. 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, $p \oplus q$ is a proper possibly causal path from $\mathbf{X}$ to $\mathbf{Y}$ that starts with an undirected edge in $\mathcal{G}$, which is a contradiction.
(ii): Let $\mathbf{N}_{\mathbf{i}}=\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right) \backslash \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. If $\mathbf{B}_{\mathbf{i}} \quad \perp_{\mathcal{D}_{\overline{\mathbf{X}}}} \mathbf{N}_{\mathbf{i}} \mid\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right)$, then by Rule 1 of the do calculus: $f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{b}_{\mathbf{i}-\mathbf{1}}, \ldots, \mathbf{b}_{\mathbf{1}}, d o(\mathbf{x})\right)=f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o(\mathbf{x})\right)$ (see equation (1)).

Suppose for a contradiction that there is a path from $\mathbf{B}_{\mathbf{i}}$ to $\mathbf{N}_{\mathbf{i}}$ that is d-connecting given $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}_{\overline{\mathbf{x}}}$. Let $p=\left\langle B_{i}, \ldots, N\right\rangle, B_{i} \in \mathbf{B}_{\mathbf{i}}, N \in \mathbf{N}_{\mathbf{i}}$ be a shortest such path. Let $p^{*}$ be the path in $\mathcal{G}$ that consists of the same sequence of nodes as $p$ in $\mathcal{D}_{\overline{\mathbf{X}}}$.
First suppose that $p$ is of the form $B_{i} \rightarrow \ldots N$. Since $B_{i} \in \mathbf{B}_{\mathbf{i}}$ and $\mathbf{N}_{\mathbf{i}} \subseteq\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right), p$ is not causal from $B_{i}$ to $N$ (Lemma 3.5). Hence, let $C$ be the closest collider to $B_{i}$ on $p$, that is, $p$ has the form $B_{i} \rightarrow \cdots \rightarrow C \leftarrow \ldots N$. Since $p$ is d-connecting given $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}_{\overline{\mathbf{X}}}, C$ must be an ancestor of $\mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$. However, then there is a causal path from $B_{i} \in \mathbf{B}_{\mathbf{i}}$ to $\mathbf{P}_{\mathbf{i}} \subseteq\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right)$ which contradicts Lemma 3.5.

Next, suppose that $p$ is of the form $B_{i} \leftarrow A \ldots N$, $A \notin \mathbf{B}_{\mathbf{i}}$. Since $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right) \subseteq\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right)$ and since $p$ is d-connecting given $\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right), B_{i}-A$ is in $\mathcal{G}$ and $A \notin\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right)$.
Note that $p^{*}$ cannot be undirected, since that would imply that $N \in \mathbf{B}_{\mathbf{i}}$ and contradict Lemma 3.5. 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 $B_{i}-A-\cdots-L-B \rightarrow R \ldots N$ or of the form $B_{i}-A-\cdots-L-B \leftarrow R \ldots N$.

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

Let $\left(\mathbf{B}_{\mathbf{1}}^{\prime}, \ldots \mathbf{B}_{\mathbf{r}}^{\prime}\right)=\operatorname{PCO}(\mathbf{V}, \mathcal{G}), r \geq k$. Let $l \in$ $\{i, \ldots, r\}$ such that $\mathbf{B}_{\mathbf{1}}^{\prime} \cap \mathbf{B}_{\mathbf{i}} \neq \emptyset$, then $B_{i}, B \in \mathbf{B}_{\mathbf{1}}^{\prime}$ and $N \in\left(\cup_{j=1}^{l-1} \mathbf{B}_{\mathbf{j}}^{\prime}\right)$. Now consider subpath $p(B, N)$. By Lemma 3.5, $p(B, N)$ 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 $B_{i}-A-\cdots-L-$ $B \leftarrow R \ldots N$. Then either $R \rightarrow L$ or $R-L$ is in $\mathcal{G}$ (Meek, 1995, see Figure 4 in the main text). Then $\langle L, R\rangle$ is also an edge in $\mathcal{D}_{\overline{\mathbf{X}}}$ otherwise, $L$ or $R$ is in $\mathbf{X}$ and a non-collider on $p$, so $p$ would be blocked by $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}$.
Hence, $q=p\left(B_{i}, L\right) \oplus\langle L, R\rangle \oplus p(R, N)$ is a shorter path than $p$ in $\mathcal{D}_{\overline{\mathbf{X}}}$. If $L$ and $R$ have the same collider/noncollider status on $q$ on $p$, then $q$ is also d-connecting given $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}$, 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 $\mathcal{D}_{\overline{\mathbf{X}}}$. Even though $L$ is not a collider on $p, B$ is a collider on $p$ and $L \in \operatorname{An}\left(B, \mathcal{D}_{\overline{\mathbf{X}}}\right)$. Since $p$ is d-connecting given $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}, \operatorname{De}\left(B, \mathcal{D}_{\overline{\mathbf{X}}}\right) \cap\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right) \neq \emptyset$. However, then also $\operatorname{De}\left(L, \mathcal{D}_{\overline{\mathbf{X}}}\right) \cap\left(\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}\right) \neq \emptyset$ and $q$ is also d-connecting given $\mathbf{X} \cup \mathbf{P}_{\mathbf{i}}$ and a shorter path between $\mathbf{B}_{\mathbf{i}}$ and $\mathbf{N}_{\mathbf{i}}$ 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 noncollider on $p$. Since $B \leftarrow R$ is in $\mathcal{D}_{\overline{\mathbf{X}}}, R$ 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 $\mathcal{D}_{\overline{\mathbf{X}}}$. But then there is a cycle in $\mathcal{D}_{\overline{\mathbf{X}}}$, which is a contradiction.
(iii): We will show that $f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o(\mathbf{x})\right)=$ $f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o\left(\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}\right)\right)$. The simpler case, $f\left(\mathbf{b}_{\mathbf{1}} \mid d o(\mathbf{x})\right)=$ $f\left(\mathbf{b}_{\mathbf{1}} \mid\left(\mathbf{x}_{\mathbf{p}_{1}}\right)\right.$ follows from the same proof, when $\mathbf{B}_{\mathbf{i}}$ is replaced by $\mathbf{B}_{\mathbf{1}}$ and $\mathbf{P}_{\mathbf{i}}$ is removed.
Let $\mathbf{X}_{\mathbf{n}_{\mathbf{i}}}=\mathbf{X} \backslash \operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$ and let $\mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}=\mathbf{X}_{\mathbf{n}_{\mathbf{i}}} \backslash$ $\operatorname{An}\left(\mathbf{P}_{\mathbf{i}}, \mathcal{D}_{\overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}}\right)$. That is $X \in \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}$ if $X \in \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}$ and if there is no causal path from $X$ to $\mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}$ that does not contain a node in $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$.
Note that $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)=\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \cup \mathbf{P}_{\mathbf{i}}$. By Rule 3 of the do-calculus, for $f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o(\mathbf{x})\right)=f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o\left(\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}\right)\right)$ to hold, it is enough to show that $\mathbf{B}_{\mathbf{i}} \quad \perp_{\mathcal{D}} \overline{\mathbf{x}_{\mathbf{p}_{\mathbf{i}} \mathbf{x}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}}$ $\mathbf{X}_{\mathbf{n}_{\mathbf{i}}} \mid \mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$ (see equation (3)).
Suppose for a contradiction that there is a d-connecting path from $\mathbf{B}_{\mathbf{i}}$ to $\mathbf{X}_{\mathbf{n}_{\mathbf{i}}}$ in $\mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. Let $p=\left\langle B_{i}, \ldots, X\right\rangle$, $B_{i} \in \mathbf{B}_{\mathbf{i}}, X \in \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}$, be a shortest such path in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{P}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. Let $p^{*}$ be the path in $\mathcal{G}$ that consists of the same sequence of nodes as $p$ in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{P}_{\mathbf{i}}} \mathbf{X}_{\mathrm{n}_{\mathbf{i}}}^{\prime}}$. This proof follows a very similar line of reasoning to the proof of (ii) above.
Let $\left(\mathbf{B}_{\mathbf{1}}^{\prime}, \ldots \mathbf{B}_{\mathbf{r}}^{\prime}\right)=\operatorname{PCO}(\mathbf{V}, \mathcal{G}), r \geq k$. Let $l \in$ $\{i, \ldots, r\}$ such that $\mathbf{B}_{\mathbf{1}}^{\prime} \cap \mathbf{B}_{\mathbf{i}} \neq \emptyset$, then $B_{i} \in \mathbf{B}_{\mathbf{1}}^{\prime}$ and $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right) \subseteq\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right)$.
Suppose that $p$ is of the form $B_{i} \rightarrow \ldots X$. If $X \in \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}$, then $p$ is not a causal path since $p$ is a path in $\mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. Otherwise, $X \in \operatorname{An}\left(\mathbf{P}_{\mathbf{i}}, \mathcal{D}_{\overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}}\right)$ and so any causal path from $B_{i}$ to $X$ would need to contain a node in $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$ and hence, would be blocked by $\operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. 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 $B_{i} \rightarrow \cdots \rightarrow C \leftarrow \ldots X$. Since $p$ is d-connecting given $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right), C$ is be an ancestor of $\operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$ in $\mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. However, this would imply that there is a causal path from $B_{i} \in \mathbf{B}_{1}^{\prime}$ to $\operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right) \subseteq$ $\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right)$ in $\mathcal{D}_{\mathbf{x}_{\mathbf{P}_{\mathbf{i}}}}$, which contradicts Lemma 3.5.

Next, suppose that $p$ is of the form $B_{i} \leftarrow A \ldots X$, $A \notin \mathbf{B}_{\mathbf{i}}$. Since $p$ is d-connecting given $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$, $A \notin \operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$. Hence, $B_{i}-A$ is in $\mathcal{G}$.
Then $A \in \mathbf{B}_{1}^{\prime}$. Note that by (i) above, $\mathbf{X} \cap \mathbf{B}_{1}^{\prime}=\emptyset$, 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 $B \in \mathbf{B}_{1}$ and so $B \notin \mathbf{X}$. Since $p$ is dconnecting given $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right), B \notin \mathrm{~Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$ and additionally, $B \notin \mathbf{B}_{\mathbf{i}}$ 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 $B, B_{i} \in \mathbf{B}_{\mathbf{1}}^{\prime}$, 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 $\mathcal{G}$ (Meek, 1995, see Figure 4 in the main text). We first show that in either case, edge $\langle L, R\rangle$ is also in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{p}_{\mathbf{i}}} \mathbf{X}_{\mathrm{n}_{\mathrm{i}}}^{\prime}}$.

Since $L \in \mathbf{B}_{1}^{\prime}$ and since $\mathbf{X} \cap \mathbf{B}_{1}^{\prime}=\emptyset, L \notin \mathbf{X}$. Hence, if $R \rightarrow L$ is in $\mathcal{G}, R \rightarrow L$ is in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{p}_{\mathbf{i}}} \mathbf{X}_{\mathrm{n}_{\mathrm{i}}}^{\prime}}$. If $R-L$ is in $\mathcal{G}$, then $R \in \mathbf{B}_{1}^{\prime}$ and since $\mathbf{X} \cap \mathbf{B}_{1}^{\prime}=\emptyset, R \notin \mathbf{X}$, so $\langle L, R\rangle$ is in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{p}_{\mathrm{i}}} \mathbf{X}_{\mathrm{n}_{\mathrm{i}}}^{\prime}}$.
Hence, $q=p\left(B_{i}, L\right) \oplus\langle L, R\rangle \oplus p(R, X)$ is a shorter path than $p$ in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{P}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. If $L$ and $R$ have the same collider/non-collider status on $q$ on $p$, then $q$ is also dconnecting given $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$, 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 $L \leftarrow R$ are in $\mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}$. Even though $L$ is not a collider on $p, B$ is a collider on $p$ and $L \in \operatorname{An}\left(B, \mathcal{D}_{\overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}}\right)$. Since $p$ is d-connecting given $\operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right), \operatorname{De}\left(B, \mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}\right) \cap \operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right) \neq \emptyset$. However, then also $\operatorname{De}\left(L, \mathcal{D} \overline{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}\right) \cap \operatorname{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right) \neq \emptyset$ and $q$ is also d-connecting given $\mathrm{Pa}\left(\mathbf{B}_{\mathbf{i}}, \mathcal{G}\right)$ and a shorter path between $\mathbf{B}_{\mathbf{i}}$ and $\mathbf{X}_{\mathbf{n}_{\mathbf{i}}}$ 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 noncollider on $p$. Since $B \leftarrow R$ is in $\mathcal{D}_{\overline{\mathbf{X}_{\mathbf{P}_{\mathbf{i}}} \mathbf{X}_{\mathbf{n}_{\mathbf{i}}}^{\prime}}}, R$ 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 $\mathcal{D} \overline{\mathbf{X}_{\mathrm{P}_{\mathrm{i}}} \mathbf{X}_{\mathrm{n}_{\mathrm{i}}}^{\prime}}$. . But then there is a cycle in $\mathcal{D} \overline{\mathbf{X}_{\mathrm{p}_{\mathrm{i}}} \mathbf{X}_{\mathrm{n}_{\mathrm{i}}}^{\prime}}$, which is a contradiction.
(iv):. If $\mathbf{B}_{\mathbf{i}} \perp_{\mathcal{D}_{\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}}} \mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \mid \mathbf{P}_{\mathbf{i}}$, then $f\left(\mathbf{b}_{\mathbf{i}} \mid \mathbf{p}_{\mathbf{i}}, d o\left(\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}\right)\right)=$ $f\left(\mathbf{b}_{\mathbf{i}} \mid p a\left(\mathbf{b}_{\mathbf{i}}, \mathcal{G}\right)\right)$ by Rule 2 of the do calculus (equation (2)).

Suppose for a contradiction that there is a d-connecting path from $\mathbf{B}_{\mathbf{i}}$ to $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$ in $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$. Let $p=\left\langle B_{i}, \ldots, X\right\rangle$, $B_{i} \in \mathbf{B}_{\mathbf{i}}, X \in \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$, be a shortest such path in $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$. Let
$p^{*}$ be the path in $\mathcal{G}$ that consists of the same sequence of nodes as $p$ in $\mathcal{D}_{\overline{\mathbf{X}}}$. This proof follows a very similar line of reasoning to the proof of (ii) above.
Let $\left(\mathbf{B}_{\mathbf{1}}^{\prime}, \ldots \mathbf{B}_{\mathbf{r}}^{\prime}\right)=\operatorname{PCO}(\mathbf{V}, \mathcal{G}), r \geq k$. Let $l \in$ $\{i, \ldots, r\}$ such that $\mathbf{B}_{\mathbf{1}}^{\prime} \cap \mathbf{B}_{\mathbf{i}} \neq \emptyset$, then $B_{i} \in \mathbf{B}_{\mathbf{1}}^{\prime}$ and by (i) above, $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \subseteq\left(\cup_{j=1}^{l-1} \mathbf{B}_{\mathbf{j}}^{\prime}\right)$.
Suppose that $p$ is of the form $B_{i} \rightarrow \ldots X$. Since $B_{i} \in$ $\mathbf{B}_{1}^{\prime}$ and $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \subseteq\left(\cup_{j=1}^{l-1} \mathbf{B}_{\mathbf{j}}^{\prime}\right)$, by Lemma 3.5, 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 $B_{i} \rightarrow \cdots \rightarrow C \leftarrow \ldots X$. Since $p$ is d-connecting given $\mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}_{\mathbf{x}_{\mathrm{P}_{\mathbf{i}}}}, C$ is be an ancestor of $\mathbf{P}_{\mathbf{i}}$ in $\mathcal{D}_{\mathbf{X}_{\mathbf{P}_{\mathbf{i}}}}$. However, this would imply that there is a causal path from $B_{i} \in \mathbf{B}_{\mathbf{i}}$ to $\mathbf{P}_{\mathbf{i}} \subseteq\left(\cup_{j=1}^{i-1} \mathbf{B}_{\mathbf{j}}\right)$ in $\mathcal{D}_{\mathbf{X}_{\mathrm{P}_{\mathrm{i}}}}$, which contradicts Lemma 3.5.

Next, suppose that $p$ is of the form $B_{i} \leftarrow A \ldots X, A \notin$ $\mathbf{B}_{\mathbf{i}}$. Since $p$ is a path in $\mathcal{D}_{\mathbf{X}_{\mathrm{p}_{\mathbf{i}}}}, A \notin \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$. Additionally, since $p$ is d-connecting given $\mathbf{P}_{\mathbf{i}}, A \notin \mathbf{P}_{\mathbf{i}}$. Hence, $B_{i}-A$ is in $\mathcal{G}$.

Then $A \in \mathbf{B}_{\mathbf{1}}^{\prime}$ and since $X \in\left(\cup_{j=1}^{l-1} \mathbf{B}_{\mathbf{j}}^{\prime}\right), p^{*}(A, X)$ 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 $B \in \mathbf{B}_{1}^{\prime}$ and since $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}} \subseteq\left(\cup_{j=1}^{l-1} \mathbf{B}_{\mathbf{j}}^{\prime}\right)$, $B \notin \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$. Since $p$ is d-connecting given $\mathbf{P}_{\mathbf{i}}, B \notin \mathbf{P}_{\mathbf{i}}$ and additionally, $B \notin \mathbf{B}_{\mathbf{i}}$ otherwise, a shorter path could have been chosen.

Now consider subpath $p(B, X)$. Since $B, B_{i} \in \mathbf{B}_{\mathbf{1}}^{\prime}$, 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 $\mathcal{G}$ (Meek, 1995, see Figure 4 in the main text). Since $R \rightarrow$ $B$ is in $\mathcal{D}_{\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}}, R \notin \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$. Since $L \in \mathbf{B}_{\mathbf{1}}^{\prime}, L \notin \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$, so $\langle L, R\rangle$ is also in $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$.

Hence, $q=p\left(B_{i}, L\right) \oplus\langle L, R\rangle \oplus p(R, X)$ is a shorter path than $p$ in $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$. If $L$ and $R$ have the same collider/noncollider status on $q$ on $p$, then $q$ is also d-connecting given $\mathbf{P}_{\mathbf{i}}$, 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 $L \leftarrow R$ are in $\mathcal{D}_{\underline{\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}}}$. Even though, $L$ is not a
collider on $p, B$ is a collider on $p$ and $L \in \operatorname{An}\left(B, \mathcal{D} \mathbf{X}_{\mathbf{p}_{\mathbf{i}}}\right)$. Since $p$ is d-connecting given $\mathbf{P}_{\mathbf{i}}, \operatorname{De}\left(B, \mathcal{D}_{\mathbf{x}_{\mathbf{P}_{\mathbf{i}}}}\right) \cap \overline{\mathbf{P}_{\mathbf{i}}} \neq$ $\emptyset$. However, then also $\operatorname{De}\left(L, \mathcal{D}_{\mathbf{x}_{\mathbf{p}_{\mathbf{i}}}}\right) \cap \mathbf{P}_{\mathbf{i}} \neq \emptyset$ and $q$ is also d-connecting given $\mathbf{P}_{\mathbf{i}}$ and a shorter path between $\mathbf{B}_{\mathbf{i}}$ and $\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}$ 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 noncollider on $p$. Since $B \leftarrow R$ is in $\mathcal{D}_{\mathbf{X}_{\mathbf{P}_{\mathbf{i}}}}, R$ 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 $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$. But then there is a cycle in $\mathcal{D}_{\mathbf{X}_{\mathbf{p}_{\mathbf{i}}}}$, which is a contradiction.

Lemma D.2. Let $X, Y$ and $Z$ be distinct nodes in MPDAG $\mathcal{G}=(\mathbf{V}, \mathbf{E})$. Suppose that there is an unshielded possibly causal path p from $X$ to $Y$ and a causal path $q$ from $Y$ to $Z$ in $\mathcal{G}$ 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 $Z$.

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 $p\left(V_{p}, Y\right)$ cannot be a causal path from $V_{p}$ to $Y$ since otherwise there is a cycle in $\mathcal{G}$. So $p\left(V_{p}, Y\right)$ takes the form $V_{p}-V_{p+1} \ldots Y$.
Let $\mathcal{D}$ be a DAG in $[\mathcal{G}]$, that contains $V_{p} \rightarrow V_{p+1}$. Since $p\left(V_{p}, Y\right)$ is an unshielded possibly causal path in $\mathcal{G}$, it corresponds to $V_{p} \rightarrow \cdots \rightarrow Y$ in $\mathcal{D}$. Then $V_{q} \rightarrow V_{p} \rightarrow$ $\cdots \rightarrow Y$ and $q\left(Y, V_{q}\right)$ form a cycle in $\mathcal{D}$, a contradiction.

Proof of Corollary 3.7. The first statement in Corollary 3.7 follows from the proof of Theorem 3.6 when replacing $\mathbf{Y}$ with $\mathbf{V}$ and $\mathbf{X}$ with empty set.

For the second statement in Corollary 3.7, note that since there are no undirected edges $X-V$ in $\mathcal{G}$, where $X \in \mathbf{X}$ and $V \in \mathbf{V}^{\prime}$, some of the buckets $\mathbf{V}_{\mathbf{i}}, i \in\{1, \ldots, k\}$ in the bucket decomposition of $\mathbf{V}$ will contain only nodes in $\mathbf{X}$. Hence, obtaining the bucket decomposition of $\mathbf{V}^{\prime}=$ $\mathbf{V} \backslash \mathbf{X}$ is the same as leaving out buckets $\mathbf{V}_{\mathbf{i}}$ that contain only nodes in $\mathbf{X}$ from $\mathbf{V}_{\mathbf{1}}, \ldots, \mathbf{V}_{\mathbf{k}}$. The statement then follows from Theorem 3.6 when taking $\mathbf{Y}=\mathbf{V}^{\prime}$.

## E PROOFS FOR SECTION 4 OF THE MAIN TEXT

Proof of Proposition 4.2. If the causal effect of $X$ on $Y$ is not identifiable in $\mathcal{G}$, by Theorem 3.6, there is a proper possibly causal path from $X$ to $Y$ that starts with
an undirected edge in $\mathcal{G}$. Then by Theorem 4.1, there is no adjustment set relative to $(X, Y)$ in $\mathcal{G}$.

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

If $\mathcal{G}$ is a $\mathrm{DAG}, \operatorname{Pa}(X, \mathcal{G})$ is an adjustment set relative to ( $X, Y$ ) by Theorem 3.3.2 of Pearl (2009). Hence, suppose that $\mathcal{G}$ is not a DAG.
Since $\mathcal{G}$ is acyclic, $\operatorname{Pa}(X, \mathcal{G}) \cap \operatorname{De}(X, \mathcal{G})=\emptyset$. Additionally, by Lemma A.8, $\operatorname{Forb}(X, Y, \mathcal{G}) \subseteq \operatorname{De}(X, \mathcal{G})$. Hence, $\operatorname{Pa}(X, \mathcal{G})$ satisfies $\operatorname{Pa}(X, \mathcal{G}) \cap \operatorname{Forb}(X, Y, \mathcal{G})=$ $\emptyset$, that is, condition 2 in Theorem 4.1 relative to $(X, Y)$ in $\mathcal{G}$.
Consider a non-causal definite status path $p$ from $X$ to $Y$. If $p$ is of the form $X \leftarrow \ldots Y$ in $\mathcal{G}$, then $p$ is blocked by $\operatorname{Pa}(X, \mathcal{G})$. If $p$ is of the form $X \rightarrow \ldots Y$, then $p$ contains at least one collider $C \in \operatorname{De}(X, \mathcal{G})$ and since $\operatorname{Pa}(X, \mathcal{G}) \cap \operatorname{De}(X, \mathcal{G})=\emptyset, p$ is blocked by $\operatorname{Pa}(X, \mathcal{G})$.

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 $\mathcal{G}$, 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 $\mathcal{G}$. Then by Lemma A.5, $p(X, D)$ is a possibly causal path from $X$ to $D$ so let $p^{\prime}$ be an unshielded subsequence of $p(X, D)$ that forms a possibly causal path from $X$ to $D$ in $\mathcal{G}$ (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 $\mathrm{Pa}(X, \mathcal{G})$ it is enough to show that $\operatorname{De}(D, \mathcal{G}) \cap \operatorname{Pa}(X, \mathcal{G})=\emptyset$. Suppose for a contradiction that $E \in \operatorname{De}(D, \mathcal{G}) \cap \mathrm{Pa}(X, \mathcal{G})$. Let $q$ be a directed path from $D$ to $E$ in $\mathcal{G}$. Then $p^{\prime}$ and $q$ satisfy Lemma D. 2 in $\mathcal{G}$, so $p^{\prime} \oplus q$ is a possibly causal path from $X$ to $E$. By definition of a possibly causal path in MPDAGs, this contradicts that $E \in \mathrm{~Pa}(X, \mathcal{G})$.

Lemma E.1. Let $\mathbf{X}$ and $\mathbf{Y}$ be disjoint node sets in an $\operatorname{MPDAG} \mathcal{G}=(\mathbf{V}, \mathbf{E})$. 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

$$
f(\mathbf{y} \mid d o(\mathbf{x}))=f(\mathbf{y})
$$

Proof of Lemma E.1. Lemma E. 1 follows from Lemma A. 4 and Rule 3 of the do-calculus of Pearl (2009) (see equation (3)).

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