Finding Invariant Predictors Efficiently via Causal Structure (Supplementary Material)

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A PROOFS OF LEMMAS AND THEOREMS

A.1 PROOF OF THEOREM 3.2

Theorem A.1. *There exists a hedge for $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{W})$ according to the generalized hedge condition if and only if $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{W})$ is unidentifiable in G.*

Proof. Let $\mathbf{Z} \subseteq \mathbf{W}$ be the maximal set such that $P(Y|do(\mathbf{X}), \mathbf{W}) = P(Y|do(\mathbf{X}, \mathbf{Z}), \mathbf{W} \setminus \mathbf{Z})$. By Theorem 21 in [4], $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{W})$ is identifiable in G if and only if $P(Y, \mathbf{X} \setminus \mathbf{Z}|do(\mathbf{X}, \mathbf{Z}))$ is identifiable in G. By Theorem 3.2, there exists a hedge for $P(Y, \mathbf{W} \setminus \mathbf{Z}|do(\mathbf{X}, \mathbf{Z}))$ if and only if $p(y, \mathbf{W} \backslash \mathbf{Z}|do(\mathbf{X}, \mathbf{Z}))$ is unidentifiable in G. Therefore, we can apply the definition of hedge for $P(Y, \mathbf{W} \setminus \mathbf{Z}|do(\mathbf{X}, \mathbf{Z}))$ to formulate definition 3.1 such that there exists a hedge for $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{W})$ according to definition 3.1 if and only if $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{W})$ is unidentifiable in G. □

A.2 PROOF OF LEMMA 3.5

Lemma A.2. *Let $\mathbf{Y} = \{Y\}$.The output of **Find-MACS-on-set**$(G, \mathbf{Y})$ is the MACS of Y. The MACS of Y is a Y-rooted C-tree.*

Proof. The line **3** of the Algorithm 2 in Section B.2, first gets an induced subgraph of G over $An(Y)$. That implies every variable in the resulting graph has a directed path to Y and Y does not have any child in it. Then, in step 4, it recursively calls on **Find-MACS-on-set** with $G_{An(Y)}$. Then, every variable in $G_{An(Y)}$ must be in $An(Y)$. The execution of the algorithm will then move to step 6 to get an induced subgraph of $G_{An(Y)}$ over $C(Y)$.

If there is no bidirected path from any variable to Y, then the algorithm will return Y, which is a Y-rooted C-tree. Suppose otherwise that there is a bidirected path from some variables to Y, then we have two cases: Case i.) The variables $\mathbf{M}$ have bidirected paths to Y, but $De(\mathbf{M}) \cap An(Y) \setminus \mathbf{M}$ are not in $C(Y)$ such that $G_{C(Y)}$ is not a Y-rooted C-tree. Case ii.) The variables $\mathbf{M}$ have bidirected paths to Y and $De(\mathbf{M}) \cap An(Y) \setminus \mathbf{M}$ are in $C(Y)$ such that $G_{C(Y)}$ is a Y-rooted C-tree. For case i, when the algorithm recursively call on itself at Step 7. Since $De(\mathbf{M}) \cap An(Y) \backslash \mathbf{M}$ are not in $C(Y)$, $\mathbf{M} \notin An(Y)$ in $G_{C(Y)}$. Then it will return Y as G. For case ii, the result trivially follows. □

A.3 PROOF OF THEOREM 3.6

Theorem A.3. *For some $W \in Ch(S)$, if there exists a hedge for $P(Y|do(W))$, then for any $\mathbf{H}, \mathbf{J} \subseteq \mathbf{V}$, we have $(Y \not\perp\!\!\!\perp S|\mathbf{J})_{G_{\overline{H}}}$ or $P(Y|do(\mathbf{H}), \mathbf{J})$ is unidentifiable in G.*

Proof. Suppose there exists a Y-rooted C-tree F in G such that there exists a hedge for $P(Y|do(W))$ for some $W \in Ch(S)$. We will show that for any $\mathbf{H}, \mathbf{J} \subseteq \mathbf{V}$, we have $(Y \not\perp\!\!\!\perp S|\mathbf{J})_{G_{\overline{H}}}$ or $P(Y|do(\mathbf{H}), \mathbf{J})$ is unidentifiable in G

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First, suppose $\mathbf{H}$ does not contain any member in c-forest F. We will show that there exists an inducing path from S to Y such that $(Y \not\perp\!\!\!\perp S|\mathbf{J})_{G_{\overline{\mathbf{H}}}}$. Since every member in $F \setminus Y$ must have only one child and Y does not any children in G_F, every member in F is in $An(Y)$. By definition of hedge, $W \in F$. As F is a C-component by the definition of C-tree and $W \in Ch(S)$ and $W \in F$, for a member S_W of S that is $Pa(W)$, we can have a path from S_W to Y through the directed path from W to Y in F along which every variable on that path is a collider. Therefore, there exists an inducing path from S_W to F. By theorem 4.2 in [1], S_W cannot be d-separated from Y in G if and only if there exists an inducing path from S_W to Y in G. Therefore, $(Y \not\perp\!\!\!\perp \mathbf{S}|\mathbf{J})_{G_{\overline{H}}}$ for any $\mathbf{J} \subseteq \mathbf{V}$. Next, suppose $\mathbf{H}$ contains some members of F. By lemma A.17, that $P(Y|do(\mathbf{H}), \mathbf{J})$ is unidentifiable in G for any $\mathbf{J} \subseteq \mathbf{V}$. □

A.4 PROOF OF THEOREM 3.7

Theorem A.4. *If the selection variable S is a parent of MACS T_Y, then there is no graph surgery estimator in G.*

Proof. Let S be a parent of T_Y, where T_Y is the MACS of Y in G. By Lemma 3.5, T_Y is a Y-rooted C-tree. Since $S \in Pa(T_Y)$, there exists some members $W \in Ch(S)$ that are in T_Y such that there exists a hedge for $P(Y|do(W))$ by the following construction: let $F = T_Y, F' = \{Y\}$ to be two $\mathbf{R}$-rooted C-forest, where $\mathbf{R} = \{Y\}$. By Theorem 3.6, the result follows implying that there is no graph surgery estimator in G. □

A.5 PROOF OF THEOREM 3.8

Theorem A.5. *Let T_Y be the MACS of Y in G, $\mathcal{H} := \{H : H \in Ch(Y), Pa(T_H) \not\ni S\}$ and $T_J := \bigcup_{H\in\mathbf{K}} T_H$ for any $\mathbf{K} \subseteq \mathcal{H}$, where T_H is the MACS with respect to the variable H. Let $\mathbf{D} = Pa(T_Y \cup T_J)$. If S is not a parent of T_Y, then $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ is identifiable in G and $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$.*

Proof. Let T_Y be the MACS of Y in G. Let $\mathcal{H} := \{H : H \in Ch(Y), Pa(T_H) \not\ni S\}$, $T_J := \bigcup_{H\in\mathbf{K}} T_H$ for some $\mathbf{K} \subseteq \mathcal{H}$. Let $\mathbf{D} = Pa(T_Y \cup T_J)$. Recall that by the conditions of the theorem, S is not a parent of T_Y.

Consider any $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$. We first prove the following claim.

Claim: $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W}) \neq P(Y|do(\mathbf{D}, \mathbf{Z}), (\mathbf{K} \cup \mathbf{W}) \setminus \mathbf{Z})$ **for any** $\mathbf{Z} \subset \mathbf{K} \cup \mathbf{W}, \mathbf{Z} \neq \emptyset$**.**

Proof. For the sake of contradiction, suppose there exists a non-empty subset $\mathbf{Z}$ where the equality holds. Under the extended faithfulness assumption, this would only be true if do-calculus Rule 2 is applicable through the following graphical condition:

$$(Y \perp\!\!\!\perp \mathbf{Z}|\mathbf{K} \cup \mathbf{W} \setminus Z)_{G_{\underline{\mathbf{Z}},\overline{\mathbf{D}}}} \tag{1}$$

Now observe that any node U in $T_Y \cup T_J$ must belong to a T_H for some $H \in \mathbf{K}$ or T_Y. By definition of T_H (or T_Y), there must be a bidirected path from U to H (or Y) that only goes through nodes in T_H (or T_Y). By definition of T_H (or T_Y), any node along this bidirected path must be an ancestor of H (or Y). Therefore, there is a d-connecting path from U to H (or Y) that starts with an arrow into U. Note that further conditioning cannot break this path since the path only consists of colliders. Finally, for the case where U belongs to a T_H, as the conditioning set contains H, we can concatenate this path with the edge $Y \to H$ to obtain a d-connecting path to Y, since H is a collider along this concatenated path. This contradicts with the d-separation statement above. □

For the sake of contradiction, suppose for some $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$, either $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ is unidentifiable in G or $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$.

Suppose $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ ***is unidentifiable in*** G.

By Theorem 3.2, there must exists a hedge for $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$. The claim above implies that the maximal set $\mathbf{Z}$ such that $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ = $P(Y|do(\mathbf{D}, \mathbf{Z}), \mathbf{K} \cup \mathbf{W} \setminus \mathbf{Z})$ is an empty set by rule 2 of do-calculus.

Since $\mathbf{Z} = \emptyset$, by Definition 3.1, there exists a hedge for $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ only if there exists two $\mathbf{R}$-rooted C-forests F, F' such that $F \cap \mathbf{D} \neq \emptyset$ and $F' \cap \mathbf{D} = \emptyset$ for some $\mathbf{R} \subset An(Y \cup \mathbf{K} \cup \mathbf{W})_{G_{\overline{\mathbf{D}}}}$. Consider any such $\mathbf{R}, F, F'$. Since $F' \cap \mathbf{D} = \emptyset$ and F' is a $\mathbf{R}$-rooted C-forest, it must be the case that $\mathbf{D} \cap \mathbf{R} = \emptyset$. Since $\mathbf{D} \cap \mathbf{R} = \emptyset$ and intervening on $\mathbf{D}$ removes the incoming edges of $\mathbf{D}$, any member of $An(Y \cup \mathbf{K} \cup \mathbf{W})$ will be in $T_Y \cup T_J$ such that $\mathbf{R} \subseteq T_Y \cup T_J$. But this is a contradiction due to the following:

Suppose $\mathbf{R} \subseteq T_Y \cup T_J$. Since $\mathbf{D} \cap \mathbf{R} = \emptyset$ and $F \cap \mathbf{D} \neq \emptyset$, that implies some members of $\mathbf{D}$ must have a directed path to some members in $\mathbf{R}$. If that is the case, then that member of $\mathbf{D}$ must also be in $T_Y \cup T_H$, where T_Y is a Y-rooted C-tree and T_H is a H-rooted C-tree for some $H \in Ch(Y)$, which is also in T_J. But this is a contradiction as any member of $\mathbf{D}$ cannot be in $T_Y \cup T_J$ by the definition of $\mathbf{D}$. Thus, $\mathbf{R} \not\subseteq (T_Y \cup T_J)$.

Therefore, there is no hedge for $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$. By Theorem 3.2, $P(Y|do(\mathbf{D}), \mathbf{K}, \mathbf{W})$ is identifiable in G.

Suppose $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$.

Next, we will show $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$. Given that S is not a parent of T_Y, we will consider two cases separately: $i.) S \in An(Y)$; $ii.) S \notin An(Y)$

$\underline{S \in An(Y)}$: Suppose there exists a d-connecting path from S to Y by conditioning on $\mathbf{W} \cup \mathbf{K}$ and intervening on $\mathbf{D}$ for some $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$. First, there is no directed path from S to Y in $G_{\overline{\mathbf{D}}}$ since S is not a parent of T_Y by the conditions of the theorem and we intervene on $\mathbf{D}$, which is a superset of $Pa(T_Y)$ and $Y \in T_Y$. For some $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$, conditioning on $\mathbf{W}$ must have opened paths with colliders that are in $An(\mathbf{W})$. However, since any member of $\mathbf{W}$ is in $T_Y \cup T_J$ and any incoming edges of $Pa(T_Y \cup T_J)$ are removed in $G_{\overline{\mathbf{D}}}$ and S is not a parent of any member of T_J by definition of T_J, there cannot be a d-connecting path from S to Y in $G_{\overline{\mathbf{D}}}$. Therefore, a contradiction. We have $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq (T_Y \cup T_J) \setminus (Y \cup \mathbf{K})$ when $S \in An(Y)$.

$\underline{S \notin An(Y)}$: we will show $i.)$ there is no d-connecting path from S to Y ends with a member of $Ch(Y)$ and $ii.)$ there is no d-connecting path from S to Y ends with a bidirected neighbor of Y.

Show that there is no d-connecting path from S ***to*** Y ***that ends with a member of*** $Ch(Y)$. Any child of Y where parents of its MACS do not contain S will be in $T_J = \bigcup_{H \in \mathbf{K}} T_H$ for some $\mathbf{K} \subseteq \mathcal{H}$ and we intervene on $Pa(T_Y \cup T_J)$ so that there is no path from S to any such child of Y. Suppose the d-connecting path from S to Y ends with some other members of $Ch(Y)$. However, for any such path, we must have conditioned on the descendants of those children of Y to open the path from S to Y through some descendants of Y, but any child of Y that is in $\mathbf{K}$, its parents are also intervened such that any path from S to Y through those children are blocked. For any other children that are not in $\mathbf{K}$ either form a collider or their descendants form a collider to block any other active paths from S to Y. Therefore, there is no d-connecting path from S to Y that ends with a member of $Ch(Y)$.

Show that there is no d-connecting path from S ***to*** Y ***ends with a bidirected neighbor of*** Y. Suppose further that bidirected neighbor of Y is a child of Y. From above, we have proved there is no d-connecting path from S to Y ends with a member of $Ch(Y)$. Suppose that bidirected neighbor of Y is not a child of Y and there exists some d-connecting paths from S to Y that ends with those bidirected neighbor of Y, for the case where there is no any descendant of those bidirected neighbors of Y is in $\mathbf{W}$, any path from S to Y along that bidirected neighbor of Y is blocked as there exists a collider along any such path and that bidirected neighbor is not in T_J. Therefore, there is no d-connecting path from S to Y. For the case where there exists some descendants of those bidirected neighbors $\mathbf{X}$ of Y is in $\mathbf{W}$, but any parent of those descendants must be in $\mathbf{D}$ such that all the incoming edges of any such parent are removed so that any d-connecting path from S to any of those parents will be blocked. Any d-connecting path from S to the members along the upstream path of those parents to $\mathbf{X}$ will be blocked by a collider along the path by concatenating the path $Y \to X$ or $M \to L$ for some descendants M, L of $\mathbf{X}$, where $M \neq L$.

Therefore, we have $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{K})_{G_{\overline{\mathbf{D}}}}$. □

A.6 PROOF OF THEOREM 3.10

Theorem A.6. *Let T_Y be the MACS of Y in G, T_H be the MACS of a child H of Y in G. Define $T_{\mathbf{C}} := \bigcup_{H \in Ch(Y)} T_H$, $\mathcal{Z} := \{Z : Z \in (C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})$ s.t. $Pa(T_{Y \cup Z}) \not\ni S\}$ and $T_B := \bigcup_{Z \in \mathbf{M}} T_{Y \cup Z}$ for any $\mathbf{M} \subseteq \mathcal{Z}$ where $T_{Y \cup Z}$ is the MACS for the set $(Y \cup Z)$. Let $\mathbf{D} = Pa(T_B)$. If S is not a parent of T_Y, then $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$ is identifiable in G and $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq (T_B) \setminus (Y \cup \mathbf{M})$.*

Proof. Let T_Y be the MACS of Y in G, T_H be the MACS of a child H of Y in G. Define $T_{\mathbf{C}} := \bigcup_{H \in Ch(Y)} T_H$. Let $\mathcal{Z} := \{Z : Z \in (C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})$ s.t. $Pa(T_{Y \cup Z}) \not\ni S\}$, $T_B := \bigcup_{Z \in \mathbf{M}} T_Z$ for some $\mathbf{M} \subseteq \mathcal{Z}$. Let $\mathbf{D} = Pa(T_B)$. Recall that by the conditions of the theorem, S is not a parent of T_Y.

Consider any $\mathbf{W} \subseteq (T_B) \setminus (Y \cup \mathbf{M})$. We first prove the following claim.

Claim: $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W}) \neq P(Y|do(\mathbf{D}, \mathbf{Q}), (\mathbf{M} \cup \mathbf{W}) \setminus \mathbf{Q})$ **for any** $\mathbf{Q} \subset \mathbf{M} \cup \mathbf{W}, \mathbf{Q} \neq \emptyset$**.**

Proof. For the sake of contradiction, suppose there exists a non-empty subset $\mathbf{Q}$ where the equality holds. Under the extended faithfulness assumption, this would only be true if do-calculus Rule 2 is applicable through the following graphical condition:

$$(Y \perp\!\!\!\perp \mathbf{Q}|\mathbf{M} \cup \mathbf{W} \setminus Q)_{G_{\underline{\mathbf{Q}},\overline{\mathbf{D}}}} \tag{2}$$

Now observe that any node U in T_B must belong to a $T_{Y \cup Z}$ for some $Z \in \mathbf{M}$. By definition of $T_{Y \cup Z}$, there must be a bidirected path from U to Z and Y that only goes through nodes in $T_{Y \cup Z}$. By definition of $T_{Y \cup Z}$, any node along this bidirected path must be an ancestor of Z or Y. Therefore, there is a d-connecting path from U to Z or Y that starts with an arrow into U. Note that further conditioning cannot break this path since the path only consists of colliders. Finally, for the case where there is a d-connecting path from U to Z , as the conditioning set contains Z, we can concatenate this path with the edge $Y \leftrightarrow Z$ to obtain a d-connecting path to Y, since Z is a collider along this concatenated path. This contradicts with the d-separation statement above. □

For the sake of contradiction, suppose for some $\mathbf{W} \subseteq (T_B) \setminus (Y \cup \mathbf{M})$, either $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$ is unidentifiable in G or $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$.

Suppose $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$ ***is unidentifiable in*** G.

By Theorem 3.2, there must exists a hedge for $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$. The claim above implies that the maximal set $\mathbf{Q}$ such that $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W}) = P(Y|do(\mathbf{D}, \mathbf{Q}), \mathbf{M} \cup \mathbf{W} \setminus \mathbf{Q})$ is an empty set by rule 2 of do-calculus.

Since $\mathbf{Q} = \emptyset$, by Definition 3.1, there exists a hedge for $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$ only if there exists two $\mathbf{R}$-rooted C-forests F, F' such that $F \cap \mathbf{D} \neq \emptyset$ and $F' \cap \mathbf{D} = \emptyset$ for some $\mathbf{R} \subset An(Y \cup \mathbf{M} \cup \mathbf{W})_{G_{\overline{\mathbf{D}}}}$. Consider any such $\mathbf{R}, F, F'$. Since $F' \cap \mathbf{D} = \emptyset$ and F' is a $\mathbf{R}$-rooted C-forest, it must be the case that $\mathbf{D} \cap \mathbf{R} = \emptyset$. Since $\mathbf{D} \cap \mathbf{R} = \emptyset$ and intervening on $\mathbf{D}$ removes the incoming edges of $\mathbf{D}$, any member of $An(Y \cup \mathbf{M} \cup \mathbf{W})$ will be in T_B such that $\mathbf{R} \subseteq T_B$. But this is a contradiction due to the following:

Suppose $\mathbf{R} \subseteq T_B$. Since $\mathbf{D} \cap \mathbf{R} = \emptyset$ and $F \cap \mathbf{D} \neq \emptyset$, that implies some members of $\mathbf{D}$ must have a directed path to some members in $\mathbf{R}$. If that is the case, then some members of $\mathbf{D}$ must also be in $T_{Y \cup Z}$, which is also in T_B. But this is a contradiction as any member of $\mathbf{D}$ cannot be in T_B by the definition of $\mathbf{D}$. Thus, $\mathbf{R} \not\subseteq T_B$.

Therefore, there is no hedge for $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$. By Theorem 3.2, $P(Y|do(\mathbf{D}), \mathbf{M}, \mathbf{W})$ is identifiable in G.

Suppose $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$.

Next, we will show $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq (T_B) \setminus (Y \cup \mathbf{M})$. Given that S is not a parent of T_Y, we will consider two cases separately: $i.)S \in An(Y)$; $ii.)S \notin An(Y)$

<u>$S \in An(Y)$</u>: Suppose there exists a d-connecting path from S to Y by conditioning on $\mathbf{W} \cup \mathbf{M}$ and intervening on $\mathbf{D}$ for some $\mathbf{W} \subseteq T_B \setminus (Y \cup \mathbf{M})$. First, there is no directed path from S to Y in $G_{\overline{\mathbf{D}}}$ since S is not a parent of T_Y by the conditions of the theorem and we intervene on $\mathbf{D}$, which is a superset of $Pa(T_Y)$ and $Y \in T_Y$ since $T_Y \subset T_B$. For some $\mathbf{W} \subseteq T_B \setminus (Y \cup \mathbf{M})$, conditioning on $\mathbf{W}$ must have opened paths with colliders that are in $An(\mathbf{W})$. However, since any member of $\mathbf{W}$ is in T_B and any incoming edges of $Pa(T_B)$ are removed in $G_{\overline{\mathbf{D}}}$ and S is not a parent of any member of $T_{Y \cup Z}$ by definition of T_B, there cannot be a d-connecting path from S to Y in $G_{\overline{\mathbf{D}}}$. Therefore, a contradiction. We have $(Y \not\perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$ for any $\mathbf{W} \subseteq T_B \setminus (Y \cup \mathbf{M})$ when $S \in An(Y)$.

<u>$S \notin An(Y)$</u>: we will show $i.)$ there is no d-connecting path from S to Y ends with a member of $Ch(Y)$ and $ii.)$ there is no d-connecting path from S to Y ends with a bidirected neighbor of Y.

Show that there is no d-connecting path from S ***to*** Y ***that ends with a member of*** $Ch(Y)$. For the case where there is no descendant of any children of Y are in $\mathbf{W}$. Since $\mathbf{W}$ does not contain any child of Y, any d-connecting path from S to any child J of Y, we can concatenate this path with the edge $Y \to J$ to obtain a blocked path to Y as J is a collider along this concatenated path. Suppose there exists some descendants of some children of Y that are in $\mathbf{W}$. Note that for any member in $\mathbf{W}$, its parents are in $\mathbf{D}$ such that all incoming edges of those parents are removed and there cannot be a d-connecting path from S to Y by concatenating the path $Y \to J$ for any child J of Y as any J is not in $\mathbf{W}$ nor such path can be opened by conditioning on $\mathbf{W}$.

Show that there is no d-connecting path from S ***to*** Y ***ends with a bidirected neighbor of*** Y. Suppose further that bidirected neighbor of Y is a child of Y. From above, we have proved there is no d-connecting path from S to Y ends with a member of $Ch(Y)$. Any bidirected neighbor of Y where it is not a child of Y and the parents of its MACS do not contain S will be in $T_B = \bigcup_{Z \in \mathbf{M}} T_{Y \cup Z}$ for some $\mathbf{M} \subseteq \mathcal{Z}$ and we intervene on $Pa(T_B)$ so that there is no path from S to any such bidirected neighbor of Y. Suppose the d-connecting path from S to Y ends with some other members of bidirected neighbors that is not child of Y. Since those bidirected neighbors $\mathbf{A}$ are not in $\mathbf{W}$, there exists some descendants of $\mathbf{A}$ are in $\mathbf{W}$. However, for any such descendant, its parent must be in $\mathbf{D}$ such that all the incoming edges of that parent are removed. That implies any such path is blocked. Since no member of $\mathbf{A}$ are in $\mathbf{W}$, any d-connecting path will be blocked by concatenating $Y \to A$ and having a collider $A \in \mathbf{A}$ along that concatenated path. Thus, there is no d-connecting path from S to Y ends with a bidirected neighbor of Y.

Therefore, we have $(Y \perp\!\!\!\perp S|\mathbf{W}, \mathbf{M})_{G_{\overline{\mathbf{D}}}}$. □

A.7 PROOF OF THEOREM 3.11

We will first prove the following lemma.

Lemma A.7. *If $S \notin An(Y)$ and **ID4IP** (Algorithm 3) returns **FAIL**, then there is no parent of Y in G.*

Proof. For the sake of contradiction, assume there exists some parents of Y in G. Given as the conditions of the lemma, we know that $S \notin An(Y)$ and **ID4IP** returns **FAIL**. Since $S \notin An(Y)$, **ID4IP** will only return **FAIL** at line **13** since line **6** requires that $S \in An(Y)$. $P(Y|do(Pa(T_Y)), T_Y \setminus Y)$ will be a graph surgery estimator by Corollary 3.9. This is a contradiction because **ID4IP** returns **FAIL** at line **13** due to $P_{set} = \emptyset$. Therefore, if $S \notin An(Y)$ and **ID4IP** returns **FAIL**, there is no parent of Y in G. □

Theorem A.8. *If there exists a graph surgery estimator, **ID4IP** outputs a graph surgery estimator.*

Claim: Given $S \in An(Y)$, if there exists a graph surgery estimator, **ID4IP** (Algorithm 3) outputs a graph surgery estimator.

We will first prove the above claim

Proof. As given by the condition, $S \in An(Y)$ and there exists a graph surgery estimator. By Theorem 3.7, $S \notin Pa(T_Y)$, where T_Y is the MACS of Y. S has no incoming edges by problem set up so S cannot be in T_Y. Also, since there is a directed path from S to Y and S is not a parent of T_Y, $S \in An(M)$ for some $M \in Pa(T_Y)$. By Corollary 3.9, **ID4IP** will output a graph surgery estimator at line **7** of the algorithm. □

Next, we will prove the theorem.

Proof. With the claim above, we only need to consider the case where $S \notin An(Y)$. Suppose $S \notin An(Y)$. Note that since $S \notin An(Y)$, this **FAIL** is returned by line **13** of the algorithm.

We will prove it by using contraposition. Suppose **ID4IP** returns **FAIL**, for the sake of contradiction, suppose also there exists a graph surgery estimator $P(Y|do(\mathbf{Q}), \mathbf{W})$ for some $\mathbf{Q} \subseteq \mathbf{V}$ and some $\mathbf{W} \subseteq \mathbf{V} \setminus \mathbf{Q}$.

We will consider the following cases where $i.)$ $\mathbf{Q} = \emptyset, \mathbf{W} \neq \emptyset$; $ii.)$ $\mathbf{Q} \neq \emptyset, \mathbf{W} = \emptyset$; $iii.)$ $\mathbf{Q} \neq \emptyset, \mathbf{W} \neq \emptyset$

i.)$\mathbf{Q} = \emptyset, \mathbf{W} \neq \emptyset$. Given $\mathbf{Q} = \emptyset, \mathbf{W} \neq \emptyset$, it must be the case that there exists some $W \in \mathbf{W}$ that has a d-connecting path to Y. By Lemma A.7, Y has no parents in G. It implies that any such path must end at a child of Y or a bidirected neighbor of Y. If such path ends at a child of Y, for any such child K of Y, there exists an inducing path from S to K since $S \in Pa(T_K)$ and T_K is a K-rooted C-tree. It implies that there exists no subset in $\mathbf{V}$ such that Y and S can be d-separated by Theorem 4.2 in [1]. Since $\mathbf{Q} = \emptyset$, we have $(Y \not\perp\!\!\!\perp S|\mathbf{W})_G$, which is a contradiction. Similarly, if such path ends at a bidirected neighbor of Y that is not a child of Y, for any such bidirected neighbor Z of Y, $S \in Pa(T_{Y \cup Z})$, which implies $(Y \not\perp\!\!\!\perp S|\mathbf{W})_G$. It is because **ID4IP** returns **FAIL** implies that S is a parent of the MACS of $\{Y, Z\}$ for any bidirected neighbor Z of Y that is not a child of Y. Observe that any node U in $T_{Y \cup Z}$ for any Z, U has a bidirected path to Z. By the definition of $T_{Y \cup Z}$, any node along this bidirected path must be an ancestor of Z. Therefore, there is a d-connecting path from U to Z that starts with an arrow into U. Note that further conditioning cannot break this path since the path only consists of colliders. As $\mathbf{W} \neq \emptyset$, if Z is not in $\mathbf{W}$, then any such member will be d-separated from Y by concatenating any d-connecting path from U to Z with $Y \leftrightarrow Z$ such that $P(Y|\mathbf{W}) = P(Y)$. If Z is in $\mathbf{W}$, then $(Y \not\perp\!\!\!\perp S|\mathbf{W})_G$. Therefore, we have reached a contradiction for the case when $\mathbf{Q} = \emptyset, \mathbf{W} \neq \emptyset$.

ii.)$\mathbf{Q} \neq \emptyset, \mathbf{W} = \emptyset$. By Lemma A.7, there is no parent of Y in G. Any member of Q must be non-ancestors of Y. Then, either Y has a directed path to some $Q \in \mathbf{Q}$ or there is no directed path to any $Q \in \mathbf{Q}$ such that $(Y \perp\!\!\!\perp \mathbf{Q})_{G_{\overline{\mathbf{Q}}}}$. By rule 3 of do-calculus, that implies $P(Y|do(\mathbf{Q})) = P(Y)$, which is a contradiction.

iii.)$\mathbf{Q} \neq \emptyset, \mathbf{W} \neq \emptyset$. We consider the case where $P(Y|do(\mathbf{Q}), \mathbf{W}) \neq P(Y|\mathbf{W})$ and $P(Y|do(\mathbf{Q}), \mathbf{W}) \neq P(Y|do(\mathbf{Q}))$ as we have reached contradiction for those cases. Since there is no parent of Y in G by Lemma A.7, both $\mathbf{Q}$ and $\mathbf{W}$ must be non-ancestors of Y. Also, since **ID4IP** returns **FAIL**, there is no children H of Y where $S \notin Pa(T_H)$ and there is also no bidirected neigbhor Z of $\mathbf{Y}$ such that $S \notin Pa(T_{Y \cup Z})$.

If S is not connected with Y and **ID4IP** return **FAIL**, then there will be no children or bidirected neighbors of Y. It is because S is disconnected with Y implies $S \notin Pa(T_H)$ and $S \notin Pa(T_{Y \cup Z})$ for any child and bidirected neighbor of Y. To see this, suppose there exist some children of Y and bidirected neighbor of Y in G, **ID4IP** will not return **FAIL** as any of those children and bidirected neighbors will be in either T_H or $T_{Y \cup Z}$ for some children of Y, H and bidirected neighbors Z of Y. We can have predictors return at line **8** and **10** of Algorithm 3. Thus, it is a contradiction. Since there are no children of Y and bidirected neighbors of Y and no parents of Y, any variable in $\mathbf{V}$ will be d-separated from Y in G so that any query will be equal to $P(Y)$ such that there is no graph surgery estimator.

Suppose S is connected with Y. Since $S \notin An(Y)$, for S to be connected with Y, any path from S to Y must have a collider. Let $\mathbf{J}$ be the largest set such that $P(Y|do(\mathbf{Q}), \mathbf{W}) = P(Y|do(\mathbf{Q} \cup \mathbf{J}), \mathbf{W} \setminus \mathbf{J})$ by rule 2 of do-calculus. In addition, let $\mathbf{M}$ be the largest set such that $P(Y|do(\mathbf{Q} \cup \mathbf{J}), \mathbf{W} \setminus \mathbf{J}) = P(Y|do((\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}), \mathbf{W} \setminus \mathbf{J})$ by rule 3 of do-calculus. If $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M} = \emptyset$, then we reach the same contradiction as (**i.**). Suppose $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M} \neq \emptyset$, it must be the case that any member in $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ is d-connected with Y when conditioning on $\mathbf{W} \setminus \mathbf{J}$ in $G_{\overline{(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}}}$ as implied by rule 3 of do-calculus.

Any such d-connecting path from a member A of $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ to Y must begin with an outgoing edge of some members N in $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ in $G_{\overline{(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}}}$. Since Y does not have any parents, this d-connecting path must end at some children of Y or some bidirected neighbors of Y that are in $\mathbf{W} \setminus \mathbf{J}$. However, for any such child H or bidirected neighbor Z of Y, it must be that $S \in Pa(T_H)$ and $S \in Pa(T_{Y \cup Z})$ as implied by the condition that **ID4IP** returns **FAIL**.

For the case where the d-connecting path ends at H, without loss of generality, we consider the following three cases: $i.$ N is in T_H or $ii.$ $N \in An(T_H) \setminus T_H$ or $iii.$ $N \in De(T_H) \setminus T_H$. Note that the case $N \in T_H$ subsumes the case when H is also a bidirected neighbor of Y.

$\underline{i. N \in T_H}$: If N is in T_H, then $P(Y|do(\mathbf{Q}), \mathbf{W})$ is unidentifiable in G by the following construction of hedge condition: for a query $P(Y|do((\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}), \mathbf{W} \setminus \mathbf{J})$, we can let $\mathbf{R} = \{H\}$, which is a proper subset of $An(Y \cup (\mathbf{W} \setminus \mathbf{J}))$. Also, we can let $F' = \{H\}$ and $F = T_H$ as T_H is a H-rooted C-tree. The result then follows Theorem 3.2.

For the next two cases, we will make use of this observation: observe that for any node U in T_H. By the definition of T_H, there must be a bidirected path from U to H that only goes through nodes in T_H and any node along this bidirected path must be an ancestor of H. Therefore, there is a d-connecting path from U to H that starts with an arrow into U. Note that further conditioning cannot break this path since the path only consists of colliders.

$\underline{ii. N \in An(T_H) \setminus T_H}$: If N is in the $An(T_H) \setminus T_H$ and $H \in \mathbf{W} \setminus \mathbf{J}$, then $(Y \not\perp\!\!\!\perp S|\mathbf{W} \setminus \mathbf{J})_{G_{\overline{\mathbf{Q} \cup \mathbf{J} \setminus \mathbf{M}}}}$. It is because $S \in Pa(T_H)$ such that we can construct a d-connecting path from S to Y by concatenating $Y \rightarrow H$ with the bidirected path as outlined in the observation. Note that no member in $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ can be in T_H due to unidentifiability of the query as shown previously. Therefore, we have a contradiction. If $H \notin \mathbf{W} \setminus \mathbf{J}$, then any such path is blocked by H, which contradicts the fact that $(\mathbf{Q} \cup \mathbf{J} \setminus \mathbf{M})$ is non-empty by rule 3 of do-calculus.

$\underline{iii. N \in De(T_H) \setminus T_H}$: If $N \in De(T_H) \setminus T_H$ and $H \in \mathbf{W} \setminus \mathbf{J}$, then we can obtain a d-connecting path from S to Y by concatenating $Y \rightarrow H$ with the bidirected path as outlined in the observation, which is a contradiction. If $N \in De(T_H) \setminus T_H$ and $H \notin \mathbf{W} \setminus \mathbf{J}$, then the such path is blocked by H, which contradict to the fact that $(\mathbf{Q} \cup \mathbf{J} \setminus \mathbf{M})$ is non-empty by rule 3 of do-calculus.

For the case where the d-connecting path ends at a bidirected neighbor Z of Y that is not a child of Y, without loss of generality, we also consider three cases: $i.N$ is in $T_{Y \cup Z}$ or $ii.N \in An(T_{Y \cup Z}) \setminus T_{Y \cup Z}$ or $iii.N \in De(T_{Y \cup Z})$.

$\underline{i. N \in T_{Y \cup Z}}$: If N is in $T_{Y \cup Z}$, we can construct two $\mathbf{R}$-rooted C-forests $F = T_{Y \cup Z}, F' = \{Y, Z\}$ such that $F \cap N \neq \emptyset, F' \cap N = \emptyset$, where $\mathbf{R} = \{Y, Z\}$, which is the proper subset of $An(Y \cup (\mathbf{W} \setminus \mathbf{J}))$ such that there exists a hedge for $P(Y|do((\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}), \mathbf{W} \setminus \mathbf{J})$ by the characterization of generalized hedge condition. By Theorem 3.2, $P(Y|do((\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}), \mathbf{W} \setminus \mathbf{J})$ is unidentifiable in G, which is a contradiction.

For the next two cases, we will make use of this observation: observe that any node U in $T_{Y \cup Z}$, there must be a bidirected path from U to Z and Y that only goes through nodes in $T_{Y \cup Z}$. By definition of $T_{Y \cup Z}$, any node along this bidirected path must be an ancestor of Z or Y. Therefore, there is a d-connecting path from U to Z or Y that starts with an arrow into U. Note that further conditioning cannot break this path since the path only consists of colliders.

$\underline{ii.N \in An(T_{Y \cup Z}) \setminus T_{Y \cup Z}}$: If N is in $An(T_{Y \cup Z}) \setminus T_{Y \cup Z}$ and $Z \in \mathbf{W} \setminus \mathbf{J}$, then $(Y \not\perp\!\!\!\perp S | \mathbf{W} \setminus \mathbf{J})_{G_{\overline{\mathbf{Q} \cup \mathbf{J} \setminus \mathbf{M}}}}$. It is because $S \in Pa(T_{Y \cup Z})$ such that we can construct a d-connecting path from S to Y by concatenating $Y \leftrightarrow Z$ with the bidirected path as outlined in the observation. Also, no member in $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ can be in $T_{Y \cup Z}$ due to unidentifiability of the query as shown previously. If $Z \notin \mathbf{W} \setminus \mathbf{J}$, then any such path is blocked by Z, which contradicts the fact that $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ is non-empty by rule 3 of do-calculus

$\underline{iii.N \in De(T_{Y \cup Z}) \setminus T_{Y \cup Z}}$: If $N \in De(T_{Y \cup Z}) \setminus T_{Y \cup Z}$ and $Z \in \mathbf{W} \setminus \mathbf{J}$, then we can obtain a d-connecting path from S to Y by concatenating $Y \leftrightarrow Z$ with the bidirected path as outlined in the observation. If $N \in De(T_{Y \cup Z}) \setminus T_{Y \cup Z}$ and $Z \notin \mathbf{W} \setminus \mathbf{J}$, then such path is blocked by Z, which contradict to the fact that $(\mathbf{Q} \cup \mathbf{J}) \setminus \mathbf{M}$ is non-empty by rule 3 of do-calculus.

Therefore, we reach a contradiction to the case where $\mathbf{Q} \neq \emptyset$ and $\mathbf{W} \neq \emptyset$.

Thus, there exists no graph surgery estimator. By contraposition, if there exists a graph surgery estimator, **ID4IP** (Algorithm 3) outputs a graph surgery estimator. □

A.8 PROOF OF THEOREM 3.12

Theorem A.9. ***(Soundness of Algorithm 3:ID4IP)*** *When* ***Algorithm 3:ID4IP*** *returns an estimator, it is a graph surgery estimator with respect to the given target and the selection variable in G.*

Proof. For line **5- 6** in Algorithm 3, the soundness follows Theorem 3.7 where we describe how selection variable being a parent of T_y implies there is no graph surgery estimator. Then, the soundness of line **7** will follow Corollary 3.9 which shows how **ID4IP** can get graph surgery estimators by utilizing the parents of the MACS of Y.

In addition, Theorem 3.8 ensures the correctness of line **8** which utilizes the parents of the MACS of some children of the target that are not selection variables. For line **10**, the soundness follows Theorem 3.10 which shows how **ID4IP** can find graph surgery estimators if any by utilizing the parents of the MACS of the bidirected neighbors of Y. Lastly, line **13** follows Theorem 3.11 which guarantees **ID4IP** to find at least one graph surgery estimator or show that there is no graph surgery estimator. □

A.9 PROOF OF THEOREM 4.1

In this proof, we will make use of the following theorems for the proof.

Theorem A.10. ***(Bayes-ball Complexity)*** *[2] Given a causal graph $G = (\mathbf{V}, \mathbf{E})$, the time complexity of Bayes-ball algorithm is $O(|\mathbf{V}| + |\mathbf{E_V}|)$, where $\mathbf{E_V}$ are the edges incident to the nodes marked during the algorithm. In the worst case, it is linear time in the size of the graph.*

Theorem A.11. *[5]* ***Find-MACS-on-set****$(G, \mathbf{Y})$ outputs the MACS of $\mathbf{Y}$ in polynomial time in the size of graph.*

Proof. Let $|Ch(S)| = C$. the Graph Surgery Estimator algorithm first finds all supersets of $Ch(S)$. Getting all supersets of $Ch(S)$ takes the complexity of $O(2^{|\mathbf{V}|-C})$. Then, for each superset $\mathbf{M}$, the Graph Surgery Estimator algorithm finds the power set of $\mathbf{V} \setminus (\mathbf{M} \cup Y)$, which takes $O(2^{|\mathbf{V}| \setminus (\mathbf{M} \cup Y)})$. Asymptotically, the complexity of finding power set for each superset becomes $O(2^{|\mathbf{V}|-(C+1)})$ as $Ch(S)$ is the smallest superset of $Ch(S)$. Then, for each member $\mathbf{Q}$ of each power set, two major operations attribute to the complexity of the algorithm are:

1. Using a for-loop to search through each member in $\mathbf{Q}$. Then, it checks for d-separation condition within each loop, resulting in the complexity of $O(|\mathbf{Q}| \times (|\mathbf{V} + \mathbf{E_V}|))$ with the use of Bayes-ball algorithm [2].
2. Calling **ID** algorithm for checking the identifiability of the returned unconditional query, which takes the complexity of $O(B)$

□

Theorem A.12. ***(GSE Complexity)*** *Let $|Ch(S)| = C$, $\mathbf{M} = Ch(S)$, $\mathbf{Q} = \mathbf{V} \setminus (\mathbf{M} \cup Y)$. Given a causal graph $G = (\mathbf{V}, \mathbf{E})$ and disjoint variables $\mathbf{X}, \mathbf{Y} \subset V$, the time complexity of Graph Surgery Estimator (GSE) (Algorithm 5 in Section B.4) is: $O(2^{2(|\mathbf{V}|-C)-1} \times B)$, where B represents the time complexity of **ID** algorithm.*

Proof. From Theorem A.11 and A.10, we can derive the the complexity of the Graph Surgery Estimator as $O(2^{|\mathbf{V}|-C+|\mathbf{V}\setminus(\mathbf{M}\cup Y)|} \times |\mathbf{Q}| \times (|\mathbf{V}| + |\mathbf{E_V}|) \times B)$, which we can simplify to $O(2^{2(|\mathbf{V}|-C)-1} \times B)$. □

A.10 PROOF OF THEOREM 4.3

Theorem A.13. ***(ID4IP Complexity)*** *Given a causal graph $G = (\mathbf{V}, E)$ and disjoint variables $\mathbf{X}, \mathbf{Y} \subseteq \mathbf{V}$, the complexity of **ID4IP** (Algorithm 3) is $O(|(C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})| + |Ch(Y)| + 1)K + (|T_Y| - 1 + |T_J| + |T_J^{'}| - |\mathcal{H}^{'}| - |\mathcal{H}|)B)$, where K represents the time complexity of **Find-MACS-on-set** and B represents the time complexity of **ID** algorithm, T_Y be the MACS of Y in G, T_H be the MACS of a child H of Y in G, and $T_{\mathbf{C}} := \bigcup_{H \in Ch(Y)} T_H$.*

Proof. By Theorem 4.2, **Find-MACS-on-set** outputs the MACS of a set in polynomial time in the size of the graph. We let $O(K)$ be the complexity of **Find-MACS-on-set** so that line **4** takes $O(K)$. Let $O(B)$ be the time complexity of **ID** algorithm. At line **7** of **ID4IP**, it takes $O(|T_Y| - 1)$ to search through the sets $\mathbf{W}$ and each time it calls on **ID** algorithm so that each **Greedy-Eval** takes $O((|T_Y| - 1)B)$. The line **8** takes $O(|Ch(Y)|K + (|T_J| - |\mathcal{H}|)B)$ because we call on **Find-MACS-on-set** $|Ch(Y)|$ many times and each time **Find-MACS-on-set** takes $O(K)$. Now we have, $\mathcal{H} := \{H : H \in Ch(Y), Pa(T_H) \not\ni S\}$ and $T_J := \bigcup_{H \in \mathbf{K}} T_H$ for any $\mathbf{K} \subseteq \mathcal{H}$, where T_H is the MACS with respect to the variable H. Therefore, after finding the MACS of each child of Y, we use **Greedy-Eval**, which calls on **ID** algorithm $|T_J| - |\mathcal{H}|$ times.

Line **10**, similar to line **8**, it finds the MACS of each bidirected neighbor of Y that is not child nor parent of Y, which results in $O(|(C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})|K)$. Here, we have, $\mathcal{H}' := \{H' : H' \in (C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}}), Pa(T_{H'}) \not\ni S\}$ and $T_J' := \bigcup_{H' \in \mathbf{K}} T_{H'}$ for any $\mathbf{K} \subseteq \mathcal{H}'$, where $T_{H'}$ is the MACS with respect to the variable H'. Then, we will use **Greedy-Eval**, which calls on **ID** algorithm $|T_J^{'}| - |\mathcal{H}^{'}|$ times, where $T_J^{'} \neq T_J$ and $\mathcal{H}^{'} \neq \mathcal{H}$. Therefore, line **10** takes $O(|(C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})|K + (|T_J^{'}| - |\mathcal{H}^{'}|)B)$. Therefore, **ID4IP** takes $O(K + (|T_Y| - 1)B + |Ch(Y)|K + (|T_J| - |\mathcal{H}|)B + |(C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})|K + (|T_J^{'}| - |\mathcal{H}^{'}|)B)$, which can be simplified to $O(|(C(Y) \cap Nbr(Y)) \setminus (T_Y \cup T_{\mathbf{C}})| + |Ch(Y)| + 1)K + (|T_Y| - 1 + |T_J| + |T_J^{'}| - |\mathcal{H}^{'}| - |\mathcal{H}|)B)$ □

A.11 PROOF OF LEMMA A.14

Lemma A.14. *If there is no hedge for $P(\mathbf{Y}|do(\mathbf{X}))$, then $P(\mathbf{Y}|do(\mathbf{X}))$ is identifiable in G.*

Proof. Suppose there is no hedge for $P(\mathbf{Y}|\text{do}(\mathbf{X}))$. Therefore, for any $\mathbf{R} \subseteq An(Y)_{G_{\overline{\mathbf{X}}}}$, there does not exist two $\mathbf{R}$-rooted C forests $F' \subset F \subseteq V$ such that $F \cap \mathbf{X} \neq \emptyset$ and $F' \cap \mathbf{X} = \emptyset$. Equivalently, it must be the case that for any $\mathbf{R} \subseteq An(Y)_{G_{\overline{\mathbf{X}}}}$ and $\mathbf{R}$-rooted C forests $F' \subset F \subseteq V$, either $F \cap \mathbf{X} = \emptyset$ or $F' \cap \mathbf{X} \neq \emptyset$.

We consider two cases: $i.$) there is no bidirected path from $\mathbf{X}$ to any of its children $ii.$) there is a bidirected path from $\mathbf{X}$ to some of its children.

Suppose there is no bidirected path from any of the nodes in $\mathbf{X}$ to any of their children in $G_{An(\mathbf{Y})}$. By Theorem 4 of [7], the query $P(\mathbf{Y}|\text{do}(\mathbf{X}))$ is then identifiable.

Suppose there is a bidirected path from some of the nodes in $\mathbf{X}$ to some of their children in $G_{An(\mathbf{Y})}$. For case ii, suppose there is a bidirected path from $\mathbf{X}$ to some of its children in $G_{An(\mathbf{Y})}$. For any $\mathbf{R} \subseteq An(\mathbf{Y})_{G_{\overline{\mathbf{X}}}}$, either there is $\mathbf{R}$-rooted C-forest F' such that $F' \cap \mathbf{X} = \emptyset$ but $F \cap \mathbf{X} \neq \emptyset$ or there is a $\mathbf{R}$-rooted C-forest F such that $F \cap \mathbf{X} \neq \emptyset$ but $F' \cap \mathbf{X} \neq \emptyset$ for any $\mathbf{R}$-rooted C-forest F'. Given these conditions, we will show that by soundness of **ID** algorithm [4] , we will have $p(\mathbf{y}|do(\mathbf{x}))$ being identifiable in G.

We will briefly describe the **ID** algorithm (Algorithm 3) here. At step 6, the **ID** algorithm takes the induced subgraph of G over $An(\mathbf{Y})$, then it partitions $G_{An(\mathbf{Y})}$ into various induced subgraphs of $G_{An(\mathbf{Y})}$ over all possible C-components at step 13 of the algorithm. Since there is a hedge for $p(\mathbf{y}|do(\mathbf{x}))$ if and only if the **ID** algorithm returns at step 18 of the algorithm by the soundness of **ID** algorithm, we will proceed by showing we will never run into step 18 of the algorithm given the conditions described in the previous paragraph.

When **ID** algorithm returns FAIL, the graph G at step 17 may not necessarily refer to the original causal graph G that has been passed into **ID**, but rather a subgraph of G after taking step 13 of the algorithm along with the other potential recursive steps 6 through 11. We use $G' \subseteq G$ in the rest of the argument for the sake of clarity.

For the sake of contradiction, assume there exists a C-component in some subgraphs of $G' \subseteq G$ such that $C(G' \backslash \mathbf{X}) = \{S\}$ and $C(G') = \{G'\}$. By definition, we can construct a $\mathbf{R}$-rooted C-forest F' as S such that $F' \cap \mathbf{X} = \emptyset$. Now, given $C(G') = \{G'\}$ and by definition of hedge, $\mathbf{X} \notin \mathbf{R}$, we can also construct another $\mathbf{R}$-rooted C-forest F such that $F \cap \mathbf{X} \neq \emptyset$. Then, there exists a hedge for $P(\mathbf{Y}|do(\mathbf{X}))$, which is a contradiction. Therefore, we will never run into step 5 of the **ID** algorithm. Then, **ID** will return an identifiable query. Therefore, we have that $P(\mathbf{Y}|do(\mathbf{X}))$ is identifiable in G. □

A.12 PROOF OF THEOREM A.15

Theorem A.15. *There exists a hedge for $P(\mathbf{Y}|do(\mathbf{X}))$ if and only if $P(\mathbf{Y}|do(\mathbf{X}))$ is unidentifiable in G*

Proof. By Lemma A.14 and Theorem 4 in [3], the result follows. □

A.13 PROOF OF THEOREM A.16

Theorem A.16. *$P(Y|do(\mathbf{X}))$ is identifiable if and only if there is no hedge for $P(Y|do(\mathbf{X}'))$ where $\mathbf{X}'$ is the smallest subset of $\mathbf{X}$ such that $P(Y|do(\mathbf{X}')) = P(Y|do(\mathbf{X}))$.*

Proof. ($\Leftarrow$) Suppose there is no hedge for $P(Y|do(\mathbf{X}'))$, where $\mathbf{X}'$ is the smallest subset of $\mathbf{X}$ such that $P(Y|do(\mathbf{X}')) = p(y|do(\mathbf{x}))$. Since $P(Y|do(\mathbf{X}')) = P(Y|do(\mathbf{X}))$, there also exists no hedge for $P(Y|do(\mathbf{X}))$. By Lemma A.14, we have that $P(Y|do(\mathbf{X}))$ is identifiable in G.
($\Rightarrow$) Suppose there exists a hedge for $P(Y|do(\mathbf{X}'))$, where $\mathbf{X}'$ is the smallest subset of $\mathbf{X}$ such that $P(Y|do(\mathbf{X}')) = P(Y|do(\mathbf{X}))$. Then, by Theorem 4 in [3], we have that $P(Y|do(\mathbf{X}'))$ is unidentifiable so that $P(Y|do(\mathbf{X}))$ is also unidentifiable. By contraposition, $p(y|do(\mathbf{x}))$ is identifiable implies there is no hedge for $P(Y|do(\mathbf{X}'))$, where $\mathbf{X}'$ is the smallest subset of $\mathbf{X}$ such that $P(Y|do(\mathbf{X}')) = P(Y|do(\mathbf{X}))$ □

A.14 PROOF OF LEMMA A.17

Lemma A.17. *Let F be a Y-rooted C-tree in $G = (\mathbf{V}, \mathbf{E})$. For any $K \in F \setminus \{Y\}$ such that $K \subseteq \mathbf{J} \subseteq \mathbf{V} \setminus \{Y\}$ and for any $\mathbf{W} \subseteq \mathbf{V} \setminus (\mathbf{J} \cup Y)$, $P(Y|do(\mathbf{J}), \mathbf{W})$ is unidentifiable in G.*

Proof. We will show that there exists a hedge for $p(y|do(\mathbf{j}), \mathbf{w})$ according to the definition 3.1. By Theorem 20 in [4], there exists a unique maximal set $\mathbf{Z}$ such that $P(Y|do(\mathbf{J}), \mathbf{W}) = P(Y|do(\mathbf{J}, \mathbf{Z}), \mathbf{W} \backslash \mathbf{Z})$. Since $K \in F \backslash \{Y\}$ and $K \subseteq \mathbf{J}$, we have that $F \cap (\mathbf{J} \cup \mathbf{Z}) \neq \emptyset$. Next, we let $F' = \{Y\}$ such that $F' \cap (\mathbf{J} \cup \mathbf{Z}) = \emptyset$. By definition 3.1, there exists a hedge for $P(Y|do(\mathbf{J}), \mathbf{W})$. By Theorem 3.2, $P(Y|do(\mathbf{J}), \mathbf{W})$ is unidentifiable in G. □

B ALGORITHMS

In this section, we provide the pseudo-codes of the algorithms that we call as sub-routines from the algorithms in the main paper.

B.1 COMPUTELOSS

Input: A set of targets $\mathbf{Y}$, an intervention set $\mathbf{X}$
Output: the value of $P(\mathbf{Y}|do(\mathbf{X}))$
$P = \mathbf{ID}(\mathbf{Y}, \mathbf{X}, G)$ {Algorithm 3}
$P_s = P / \sum_Y P$
$L =$ Compute validation loss $l(P_s)$
Return L

Algorithm 1: computeLoss($\mathbf{Y}, \mathbf{X}$)

B.2 FIND-MACS-ON-SET

Input: A causal graph G , an AC-component $\mathbf{Y}$ in G
Output: $T_{\mathbf{Y}}$, a subgraph of G, the maximal ancestral confounded set for $\mathbf{Y}$ in G.
if $\exists X \notin An(\mathbf{Y})_G$ **then**
  Return Find-MACS-on-set$(G_{An(\mathbf{Y})}, \mathbf{Y})$
if $\exists Y \in \mathbf{Y}, \exists X \notin C(Y)_G$ **then**
  Return Find-MACS-on-set$(G_{C(Y)}, \mathbf{Y})$
else
  Return G

Algorithm 2: Find-MACS-on-set$(G, \mathbf{Y})$[5]

B.3 ID ALGORITHM

Input: a set of target variables $\mathbf{Y}$, a set of random variables for intervention $\mathbf{X}$, a probability distribution P, a causal graph G
Output: Expression for $P(Y|do(\mathbf{X}))$ in terms of P or **FAIL**(F, F')
if $\mathbf{X} = \emptyset$ **then**
  Return $\sum_{\mathbf{V} \setminus \mathbf{Y}} P(\mathbf{v})$
if $\mathbf{V} \setminus An(\mathbf{Y})_G \neq \emptyset$ **then**
  Return ID$(\mathbf{Y}, \mathbf{X} \cap An(\mathbf{Y})_G, \sum_{\mathbf{V} \setminus An(\mathbf{Y})_G} P, G_{An(\mathbf{Y})})$
Let $\mathbf{W} = (\mathbf{V} \setminus \mathbf{X}) \setminus An(\mathbf{Y})_{G_{\overline{\mathbf{X}}}}$
if $\mathbf{W} \neq \emptyset$ **then**
  Return ID$(\mathbf{Y}, \mathbf{X} \cup \mathbf{W}, P, G)$
if $C(G \setminus \mathbf{X}) = \{S_1, \dots, S_k\}$ **then**
  Return $\sum_{\mathbf{V} \setminus (\mathbf{Y} \cup \mathbf{X})} \prod_i$ **ID**$(S_i, \mathbf{V} \setminus S_i, P, G)$
if $C(G \setminus \mathbf{X}) = \{S\}$ **then**
  if $C(G) = \{G\}$ **then**
    Return FAIL$(G, G \cap S)$
  if $S \in C(G)$ **then**
    Return $\sum_{S \setminus \mathbf{Y}} \prod_{\{i|V_i \in S\}} P(V_i|V_\pi^{i-1})$
  if $\exists S$ s.t. $S \subset S' \in C(G)$ **then**
    Return ID$(\mathbf{Y}, \mathbf{X} \cap S', \prod_{\{i|V_i \in S\}} P(V_i|V_\pi^{(i-1)} \setminus S), G_{S'})$

Algorithm 3: ID$(\mathbf{Y}, \mathbf{X}, P, G)$ [4]

B.4 GRAPH SURGERY ESTIMATOR ALGORITHM

In this section, we present the main algorithms in [6].

Input: Acyclic Directed Mixed Graph (ADMG) $G = (\mathbf{V}, \mathbf{E})$, disjoint variable sets $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$
Output: Unconditional query $P(\mathbf{Y}|do(\mathbf{X}), \mathbf{Z})$
$\mathbf{X}' = \mathbf{X}$
$\mathbf{Y}' = \mathbf{Y}$
$\mathbf{Z}' = \mathbf{Z}$
while $\exists Z \in \mathbf{Z} s.t. (\mathbf{Y} \perp\!\!\!\perp Z|\mathbf{X}, \mathbf{Z} \setminus \{Z\})_{G_{\overline{\mathbf{X}}, \underline{Z}}}$ **do**
  $\mathbf{X}' = \mathbf{X}' \cup Z$
  $\mathbf{Z}' = \mathbf{Z}' \setminus \{Z\}$
$\mathbf{Y}' = \mathbf{Y} \cup \mathbf{Z}$
Return $\mathbf{X}'$, $\mathbf{Y}'$ of unconditional query $P(\mathbf{Y}'|do(\mathbf{X}'))$

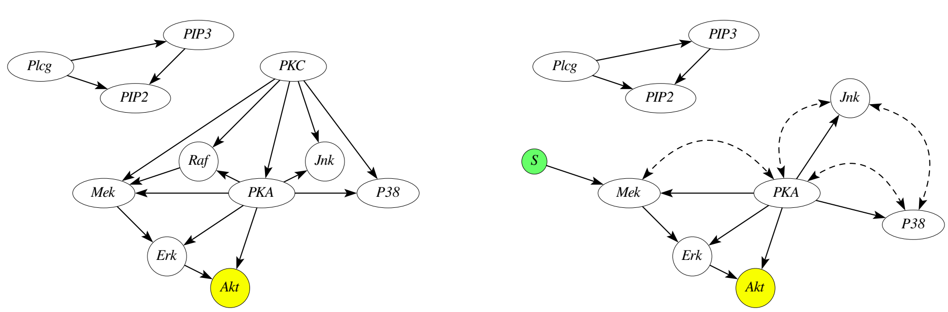
Algorithm 4: Unconditional Query: UQ$(\mathbf{X}, \mathbf{Y}, \mathbf{Z}; G)$[6]

Input: ADMG G, mutable variables $\mathbf{M}$, target T
Ouput: Expression for the surgery estimator or **FAIL** if there is no stable estimator.
$S_{ID} = \emptyset$
$Loss = \emptyset$
for $\mathbf{Z} \in \mathcal{P}(\mathbf{V} \setminus (\mathbf{M} \cup \{T\}))$ **do**
  if $T \notin \mathbf{M}$ **then**
    $\mathbf{X}, \mathbf{Y} = UQ(\mathbf{M}, \{T\}, \mathbf{Z}, \mathcal{G})$
    try
      $P = \mathbf{ID}(\mathbf{X}, \mathbf{Y}, G)$
      $P_s = P / \sum_Y P$
      Compute the validation loss $l(P_s)$
      S_{ID}.append(P_s); $Loss$.append$(l(P_s))$
    catch
      continue
  $\mathbf{X}, \mathbf{Y} = \mathbf{UQ}(\mathbf{M}, \{T\}, \mathbf{Z}; \mathbf{G}_{\overline{T}})$
  $\mathbf{X} = \mathbf{X} \cup \{T\}$
  $\mathbf{Y} = \mathbf{Y} \setminus \{T\}$
  if $\mathbf{Y} \cap (T \cup Ch(T)) = \emptyset$ **then**
    continue
  try
    $P = \mathbf{ID}(\mathbf{X}, \mathbf{Y}, G)$
    $P_s = P / \sum_Y P$
    Compute the validation loss $l(P_s)$
    S_{ID}.append(P_s); $Loss$.append$(l(P_s))$
  catch
    continue
if $S_{ID} = \emptyset$ **then**
  Return FAIL
Return $P_s \in S_{ID}$ with lowest corresponding $Loss$

Algorithm 5: Graph Surgery Estimator $(G, \mathbf{M}, Y)$[6]

C SEMI-SYNTHETIC CAUSAL GRAPHS

C.1 SACHS CAUSAL GRAPH

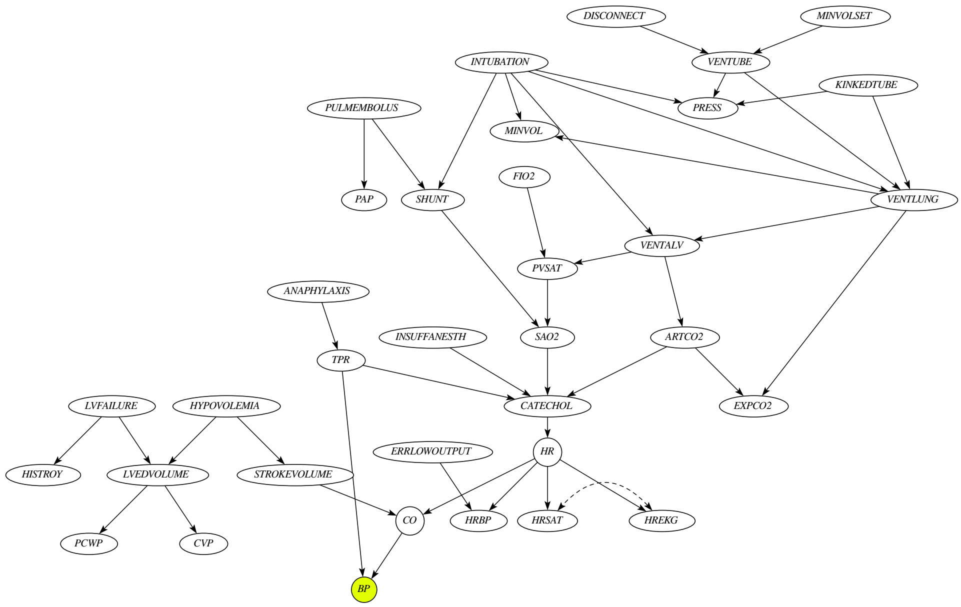


(a) Original Sachs causal graph with the target variable (yellow)

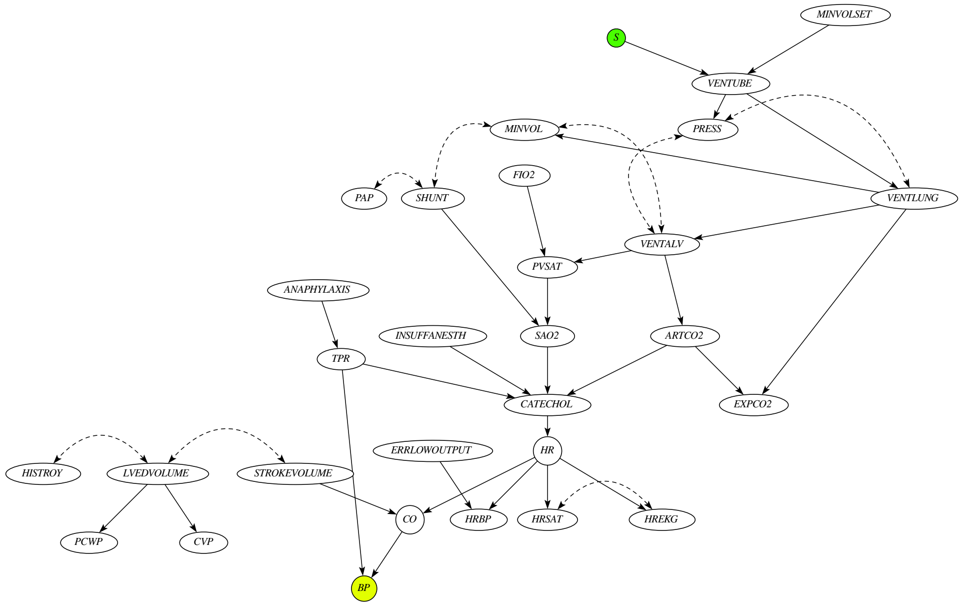
(b) Modified Sachs causal graph with the selection variable (green)

Figure 1: Semi-synthetic experimental results

C.2 ALARM CAUSAL GRAPH



(a) Original Alarm causal graph with the target variable (yellow)



(b) Modified Alarm causal graph with the selection variable (green)

Figure 2: Semi-synthetic causal graph: Alarm

REFERENCES

[1] Thomas Richardson and Peter Spirtes. Ancestral graph markov models. *The Annals of Statistics*, 30(4):962–1030, 2002.

[2] Ross D Shachter. Bayes-ball: The rational pastime (for determining irrelevance and requisite information in belief networks and influence diagrams). *arXiv preprint arXiv:1301.7412*, 2013.

[3] Ilya Shpitser and Judea Pearl. *Identification of joint interventional distributions in recursive semi-Markovian causal models*. eScholarship, University of California, 2006.

[4] Ilya Shpitser and Judea Pearl. Complete identification methods for the causal hierarchy. *Journal of Machine Learning Research*, 9:1941–1979, 2008.

[5] Ilya Shpitser and Judea Pearl. *Dormant independence*. AAAI Press, 2008.

[6] Adarsh Subbaswamy, Peter Schulam, and Suchi Saria. Preventing failures due to dataset shift: Learning predictive models that transport. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 3118–3127. PMLR, 2019.

[7] Jin Tian and Judea Pearl. *A general identification condition for causal effects*. eScholarship, University of California, 2002.