Graphical tools for selecting accurate and valid conditional instrumental sets

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Abstract

We consider the accurate estimation of total causal effects in the presence of unmeasured confounding using conditional instrumental sets. Specifically, we consider the two-stage least squares estimator in the setting of a linear structural equation model with correlated errors that is compatible with a known acyclic directed mixed graph. To set the stage for our results, we fully characterise the class of conditional instrumental sets that result in a consistent two-stage least squares estimator for our target total effect. We refer to members of this class as valid conditional instrumental sets. Equipped with this definition, we provide three graphical tools for selecting accurate and valid conditional instrumental sets: First, a graphical criterion that for certain pairs of valid conditional instrumental sets identifies which of the two corresponding estimators has the smaller asymptotic variance. Second, a forward algorithm that greedily adds covariates that reduce the asymptotic variance to a valid conditional instrumental set. Third, a valid conditional instrumental set for which the corresponding estimator has the smallest asymptotic variance we can ensure with a graphical criterion.

1 Introduction

Suppose we want to estimate the total causal effect of an exposure X on an outcome Y in the presence of latent confounding. This is often done with the two-stage least squares estimator. The two-stage least squares estimator is computed based on a tuple \( \{ Z, W \} \) of covariate sets, where we refer to \( Z \) as the instrumental set, to \( W \) as the conditioning set and to \( \{ Z, W \} \) as the conditional instrumental set. It is well-known that the two-stage least squares estimator is only consistent if we use certain tuples \( \{ Z, W \} \) and we call such tuples valid conditional instrumental sets relative to \( (X, Y) \). Determining valid conditional instrumental sets has received considerable research attention (e.g. Bowden and Turkington, 1990; Angrist et al., 1996; Hernán and Robins, 2006; Wooldridge, 2010). In the graphical framework, which we adopt in this paper, the most relevant results are by Brito and Pearl (2002) who have proposed a necessary graphical criterion for a conditional instrumental set to be valid.

Besides validity, there also exists another aspect to this problem that has received less attention: the choice of conditional instrumental set also affects the estimator’s statistical accuracy. While in some cases no valid conditional instrumental set may exist, in other cases multiple valid tuples may be available. In such cases, each valid tuple leads to a consistent estimator of the total effect but the respective estimators may differ in terms of their asymptotic variance. This raises the following question: can we identify tuples that lead to estimators that are not just consistent but also accurate. This is an important problem, as it is well-known that the two-stage least squares estimator can suffer from low accuracy (Kinal, 1980).

It is known that increasing the number of instruments, i.e., enlarging \( Z \), cannot harm the two-stage least squares estimator’s asymptotic variance but may improve it (e.g. Wooldridge, 2010). However, this may also increase the estimator’s finite sample bias (Bekker, 1994). A related result that does not suffer from this drawback is given by Kuroki and Cai (2004). They provide a graphical criterion that
can identify in some cases which of two tuples \( \{Z_1, W\} \) and \( \{Z_2, W\} \) is more accurate. However, this result is limited to singleton \( Z_1 \) and \( Z_2 \) with a fixed conditioning set \( W \). The selection of the conditioning set \( W \) has received even less attention. The only result we are aware of is by Vansteelandt and Didelez (2018), who establish that if a set \( W \) is independent of the instrumental set \( Z \) then using \( \{Z, W\} \) rather than \( \{Z, \emptyset\} \) cannot harm the accuracy but may improve it. We are not aware of any work that considers changes to the instrumental set \( Z \) and the conditioning set \( W \) simultaneously.

In this paper we aim to fill this gap in the setting of a linear structural equation model with correlated errors that is compatible with a known acyclic directed mixed graph. To set the stage for our results, we derive a necessary and sufficient graphical condition for a conditional instrumental set to be valid. We also derive a new formula for the asymptotic variance of the two-stage least squares estimator. This formula only holds for valid conditional instrumental sets but has a simpler dependence on the conditional instrumental set and the underlying graph.

Equipped with these two results, we provide three graphical tools to select more accurate valid conditional instrumental sets. The first result is a graphical criterion that for certain pairs of valid conditional instrumental sets identifies which of the two corresponding estimators has the smaller asymptotic variance. This criterion includes the results by Kuroki and Cai (2004) and Vansteelandt and Didelez (2018) as special cases. It is also the first criterion that can compare pairs of valid conditional instrumental sets, where both the instrumental set and the conditioning set are different. The second result is an algorithm that takes any valid conditional instrumental set and greedily adds covariates to it that decrease the asymptotic variance and preserve validity. As our third tool, we construct a conditional instrumental set that, given mild constraints, has the following two properties: i) it is valid and ii) its asymptotic variance is not dominated by that of any other conditional instrumental set for all linear structural equation models compatible with the acyclic directed mixed graph. The second property implies that this estimator has the smallest asymptotic variance we can ensure with only a graphical criterion; a property which we call graphical optimality.

Lastly, we provide a simulation study to quantify the gains that can be expected from applying our results in practice and apply our results to a real data example. All proofs are provided in the Supplement.

## 2 Preliminaries

We consider acyclic directed mixed graphs where nodes represent random variables, directed edges \((-\to)\) represent direct effects and bi-directed edges \(\leftrightarrow\) represent error correlations induced by latent variables. We now give the most important definitions. The remaining ones together with an illustrating example are given in Section A.2 of the Appendix.

**Linear structural equation model:** Consider an acyclic directed mixed graph \( G = (V, E) \), with nodes \( V = \{V_1, \ldots, V_p\} \) and edges \( E \), where the nodes represent random variables. The random vector \( V \) is generated from a linear structural equation model compatible with \( G \) if

\[
V \leftarrow A \epsilon + \epsilon
\]

such that the following three properties hold: First, \( A = (\alpha_{ij}) \) is a matrix with \( \alpha_{ij} = 0 \) for all \( i, j \) where \( V_j \to V_i \notin E \). Second, \( \epsilon = (\epsilon_{e_1}, \ldots, \epsilon_{e_n}) \) is a random vector of errors such that \( E(\epsilon) = 0 \) and \( \text{cov}(\epsilon) = \Omega = (\omega_{ij}) \) is a matrix with \( \omega_{ij} = \omega_{ji} = 0 \) for all \( i, j \) where \( V_i \leftrightarrow V_j \notin E \). Third, for any two disjoint sets \( V', V'' \subseteq V \) such that for all \( V'_i \in V' \) and all \( V''_j \in V'' \), \( V'_i \leftrightarrow V''_j \notin E \), the random vector \( (\epsilon_{e_i})_{V'_i \in V'} \) is independent of \( (\epsilon_{e_j})_{V''_j \in V''} \).

We use the symbol \( \leftarrow \) in equation (1) to emphasise that it describes a generating mechanism rather than just an equality. As a result we can use it to identify the effect of an outside intervention that sets a treatment \( V_i \) to a value \( v_i \) uniformly for the entire population. Such interventions are typically called do-interventions and denoted \( \text{do}(V_i = v_i) \) (Pearl 1995). The edge coefficient \( \alpha_{ij} \) is also called the direct effect of \( V_i \) on \( V_j \) with respect to \( V \). The non-zero error covariances \( \omega_{ij} \) can be interpreted as the effect of latent variables.

**Causal paths and forbidden nodes:** (cf. Perković et al. 2018) A path from \( X \) to \( Y \) in \( G \) is called a causal path from \( X \) to \( Y \) if all edges on \( p \) are directed and point towards \( Y \). We define the descendants
of $X$ in $\mathcal{G}$ as all the nodes $D$, such that there exists a causal path from $X$ to $D$ in $\mathcal{G}$ and denote them $\text{do}(X, \mathcal{G})$. We use the convention that $X \in \text{do}(X, \mathcal{G})$ and for a set $W = \{W_1, \ldots, W_k\}$ that $\text{do}(W, \mathcal{G}) = \bigcup_{i=1}^k \text{do}(W_i, \mathcal{G})$. We define the causal nodes with respect to $(X, Y)$ in $\mathcal{G}$, as all nodes on causal paths from $X$ to $Y$ excluding $X$ and denote them $\text{cn}(X, Y, \mathcal{G})$. We define the forbidden nodes relative to $(X, Y)$ in $\mathcal{G}$ as the descendants of the causal nodes as well as $X$ and denote them $\text{forb}(X, Y, \mathcal{G})$.

**Total effects:** We define the total effect of $X$ on $Y$ as

$$\tau_{yx}(x) = \frac{\partial}{\partial x} E[Y \mid \text{do}(X = x)].$$

In a linear structural equation model the function $\tau_{yx}(x)$ is constant, which is why we simply write $\tau_{yx}$. The path tracing rules by [Wright 1934] allow for the following alternative definition. Consider two nodes $X$ and $Y$ in an acyclic directed mixed graph $\mathcal{G} = (V, E)$ and suppose that $V$ is generated from a linear structural equation model compatible with $\mathcal{G}$. Then $\tau_{yx}$ is the sum over all causal paths from $X$ to $Y$ of the product of the edge coefficients along each such path.

**Two stage least squares estimator:** [Basmann 1957] Consider two random variables $X$ and $Y$, and two random vectors $Z$ and $W$. Let $S_n, T_n$ and $Y_n$ be the random matrices corresponding to taking $n$ i.i.d. observations from the random vectors $S = (X, W), T = (Z, W)$ and $Y$, respectively. Then the two stage least squares estimator $\hat{\tau}_{yx}^{st.w}$ is defined as the first entry of the larger estimator

$$\hat{\tau}_{yx}^{st.w} = Y_n^\top T_n (T_n^\top T_n)^{-1} T_n^\top S_n \{S_n^\top T_n (T_n^\top T_n)^{-1} T_n^\top S_n\}^{-1},$$

where we repress the dependence on the sample size $n$ for simplicity. We refer to the tuple $\{Z, W\}$ as the conditional instrumental set, to $Z$ as the instrumental set and to $W$ as the conditioning set.

**m-separation and latent projection:** [Koster 1999] [Richardson 2003] Consider an acyclic directed mixed graph $\mathcal{G} = (V, E)$, with $V$ generated from a linear structural equation model compatible with $\mathcal{G}$. We can read off conditional independence relationships between the variables in $V$ directly from the acyclic directed mixed graph with a graphical criterion known as $m$-separation. A formal definition is given in the Supplement. We use the notation $S \perp \perp_T T \mid W$ to denote that $S$ is $m$-separated from $T$ given $W$ in $\mathcal{G}$. We also use the convention that $\emptyset \perp \perp_T T \mid W$ always holds.

Consider a subset of nodes $L \subseteq V$. We can use a tool called the latent projection [Richardson 2003] to remove the nodes in $L$ from $\mathcal{G}$ while preserving all $m$-separation statements between subsets of $V \setminus L$. We use the notation $\mathcal{G}^L$ to denote the acyclic directed mixed graph with node set $V \setminus L$ that is the latent projection of $\mathcal{G}$ over $L$. A formal definition of the latent projection is given in the Supplement.

**Covariance matrices and regression coefficients:** Consider random vectors $S = (S_1, \ldots, S_k), T = (T_1, \ldots, T_k)$ and $W$. We denote the covariance matrix of $S$ by $\Sigma_{ss} \in \mathbb{R}^{k_s \times k_s}$ and the covariance matrix between $S$ and $T$ by $\Sigma_{st} \in \mathbb{R}^{k_s \times k_t}$, where its $(i,j)$-th element equals $\text{cov}(S_i, T_j)$. We further define $\Sigma_{st.w} = \Sigma_{st} - \Sigma_{sw}^{-1}\Sigma_{st.w}\Sigma_{w.s}$. If $k_s = k_t = 1$, we write $\sigma_{st.w}$ instead of $\Sigma_{st.w}$. The value $\sigma_{ss.w}$ can be interpreted as the residual variance of the ordinary least squares regression of $S$ on $W$. We also refer to $\sigma_{ss.w}$ as the conditional variance of $S$ given $W$. Let $\beta_{st.w} \in \mathbb{R}^{k_t \times k_t}$ represent the population level least squares coefficient matrix whose $(i,j)$-th element is the regression coefficient of $T_j$ in the regression of $S_i$ on $T$ and $W$. We denote the corresponding estimator as $\hat{\beta}_{st.w}$. Finally, for random vectors $W_1, \ldots, W_m$ with $W = (W_1, \ldots, W_m)$ we use the notation that $\beta_{st.w_1 \cdots w_m} = \beta_{st.w}$ and $\Sigma_{st.w_1 \cdots w_m} = \Sigma_{st.w}$.

**Adjustment sets:** [Shpitser et al. 2010] [Perkovic et al. 2018] We refer to a node set $W$ as a valid adjustment set relative to $(X, Y)$ in $\mathcal{G}$, if $\beta_{yx.w} = \tau_{yx}$ for all linear structural equation models compatible with $\mathcal{G}$. There exists a necessary and sufficient graphical criterion for a set $W$ to be a valid adjustment set, which we give in the Supplement.

## 3 Valid conditional instrumental sets

We now graphically characterise the class of conditional instrumental sets $\{Z, W\}$, such that the two-stage least squares estimator $\hat{\tau}_{yx}^{st.w}$ is consistent for the total effect $\tau_{yx}$.
Definition 3.1. Consider disjoint nodes $X$ and $Y$, and node sets $Z$ and $W$ in an acyclic directed mixed graph $\mathcal{G}$. We refer to $\{Z, W\}$ as a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}$ if the following hold: i) $Z \perp_X W | (X,Y)$ and ii) for all linear structural equation models compatible with $\mathcal{G}$ such that $\Sigma_{XZ, W} \neq 0$, the two-stage least squares estimator $\tau_{yx}$ converges in probability to $\tau_{yx}$.

Condition i) of Definition 3.1 ensures that there exists a linear structural equation model compatible with $\mathcal{G}$ such that $\Sigma_{XZ, W} \neq 0$ and therefore that Condition ii) is never true by default. Condition ii) then ensures that if $\Sigma_{XZ, W} = 0$, which can be checked with observational data, the two-stage least squares estimator $\tau_{yx}^{Z,W}$ is consistent for the total effect $\tau_{yx}$. If $\Sigma_{XZ, W} = 0$, the estimator $\tau_{yx}^{Z,W}$ is generally inconsistent and has non-standard asymptotic theory [Staiger and Stock (1997)], which is why we do not consider this case.

We now provide a full graphical characterization for the class of valid conditional instrumental sets.

Theorem 3.2. Consider disjoint nodes $X$ and $Y$, and node sets $Z$ and $W$ in an acyclic directed mixed graph $\mathcal{G} = (V, E)$. Then $\{Z, W\}$ is a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}$ if and only if (i) $\{Z \cup W\} \cap \text{forb}(X, Y, \mathcal{G}) = \emptyset$, (ii) $Z \perp_X X | (X, Y)$ and (iii) $Z \perp_Y Y | (X, Y)$, where the graph $\tilde{\mathcal{G}}$ is $\mathcal{G}$ with all edges out of $X$ on causal paths from $X$ to $Y$ removed.

The graphical criterion in Theorem 3.2 is similar to the well-known graphical criterion from Pearl (2009) (see also Brito and Pearl (2002a,b)). In fact the two are equivalent for any triple $(X, Y, \tilde{\mathcal{G}})$ such that there is no causal path from $X$ to $Y$ in $\tilde{\mathcal{G}}$ except for the edge $X \rightarrow Y$. The main contribution of Theorem 3.2 is that it gives a necessary and sufficient criterion.

Due to Condition (i) of Theorem 3.2 no valid conditional instrumental set $(Z, W)$ may contain nodes in $\text{forb}(X, Y, \tilde{\mathcal{G}})$. We now show that we can therefore use the latent projection and remove the nodes in $F = \text{forb}(X, Y, \tilde{\mathcal{G}}) \setminus \{X, Y\}$ from our graph $\tilde{\mathcal{G}}$ to obtain the smaller graph $\tilde{\mathcal{G}}^F$, without loosing any relevant information. This is an example of the forbidden projection originally proposed by Write et al. (2020) but in the context of adjustment sets. We formalise this result in the following proposition.

Proposition 3.3. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $\mathcal{G}$. Further let $F = \text{forb}(X, Y, \tilde{\mathcal{G}}) \setminus \{X, Y\}$. Then $\{Z, W\}$ is a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}$ if and only if it is a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}^F$.

We now provide an additional minor proposition regarding the remaining descendants of $X$.

Proposition 3.4. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $\mathcal{G}$ and let $\{Z, W\}$ be a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}$. If $(Z \cup W) \cap \text{de}(X, \tilde{\mathcal{G}}) \neq \emptyset$, then $W$ is a valid adjustment set relative to $(X, Y)$ in $\mathcal{G}$.

By Proposition 3.4 we may only use descendants of $X$ in cases where we can also estimate $\tau_{yx}$ via adjustment. As adjustment is known to be more accurate (e.g. Chapter 5.2.3 of Wooldridge (2010)), we disregard such cases and apply the latent projection to marginalise out any remaining variable in $\text{de}(X, \tilde{\mathcal{G}}) \setminus \{X, Y\}$. Finally, we also assume that $Y \in \text{de}(X, \tilde{\mathcal{G}})$ for simplicity.

Remark 3.5. For the remainder of this paper we consider graphs $\mathcal{G}$ such that $\text{de}(X, \tilde{\mathcal{G}}) = \{X, Y\}$. We use $\tilde{\mathcal{G}}$ to denote the graph $\mathcal{G}$ with the edge $X \rightarrow Y$ removed.
Further, (3) is replaced with the conditional variance \( \sigma \).

Theorem 4.1. Consider nodes \( \{X, W, Z\} \) relative to \( (X, Y) \) in \( G \). By Condition (i) and the fact that \( \text{forb}(X, Y, G) = \{X, Y, E\} \) we only need to consider sets \( Z \) and \( W \) that are disjoint subsets of \( \{A, B, C, D\} \). We first consider potential instrumental sets \( Z \). Since \( C \not\perp Y \mid W \) for all \( W \subseteq \{A, B, C\} \), no \( Z \) may contain \( C \) or we have a violation of Condition (iii).

Further, \( A \perp X \) but \( B \not\perp X \) and \( D \not\perp X \mid W \) for all \( W \subseteq \{A, B, C\} \) and \( W' \subseteq \{A, B, C\} \), respectively. Therefore, any non-empty \( Z \subseteq \{A, B, D\} \) except for \( Z = A \) fulfills Condition (ii), irrespective of \( W \). This means we have six candidates for \( Z : B, D, \{A, B\}, \{A, D\}, \{B, D\} \) and \( \{A, B, D\} \). We now consider the possible conditioning sets \( W \) for each of these six candidates. If \( B \in Z, Z \not\perp Y \mid W \) with \( W \subseteq \{A, C, D\} \) if and only if \( C \notin W \). If \( B \notin Z \) then \( D \in Z \) and \( D \not\perp Y \mid W \subseteq \{A, B, C\} \) if and only if \( B \in W \) or \( C \in W \). Therefore, for the four candidates with \( B \in Z, \{Z, W\} \) is a valid conditional instrumental set if and only if \( W \subseteq \{A, C, D\} \) and \( C \in W \). For example, if \( Z = B \) the possible \( W \) are \( \{C\}, \{A, C\}, \{C, D\} \) and \( \{A, D\} \). For the two candidates with \( B \notin Z, \{Z, W\} \) is a valid conditional instrumental set if and only if \( W \subseteq \{A, B, C\} \) and \( C \notin W \). Therefore, there are \( 4 + 6 + 3 + 2 + 2 + 1 = 18 \) valid conditional instrumental sets relative to \( (X, Y) \) in \( G \).

Finally, consider the graph \( \text{in} \) from Figure \[a\]. It is the forbidden projection graph \( \text{in} \) with \( F = E \) of \( \text{in} \). It is easy to verify that the arguments we gave for \( \text{in} \) also apply to \( \text{in} \) and therefore every valid conditional instrumental set relative to \( (X, Y) \) in \( \text{in} \) is also a valid conditional instrumental set in \( \text{in} \).

4 Accurate and valid conditional instrumental sets

4.1 Asymptotic variance formula for valid conditional instrumental sets

We first present a new formula for the asymptotic variance of the two-stage least squares estimator, which has a simpler dependence on the tuple \( \{Z, W\} \) than the traditional formula. It only holds, however, if the tuple \( \{Z, W\} \) is a valid conditional instrumental set.

Theorem 4.1. Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( G \) such that \( \text{do}(X, G) = \{X, Y\} \). Let \( \{Z, W\} \) be a valid conditional instrumental set relative to \( (X, Y) \) in \( G \) and \( \hat{Y} = Y - \tau_{yx} X \). Then for all linear structural equation models compatible with \( G \) such that \( \Sigma_{xz.w} \neq 0 \), \( \tau_{yzw} \) is an asymptotically normal estimator of \( \tau_{yz} \) with asymptotic variance

\[
a.\text{var}(\hat{\tau}_{yz.w}) = \frac{\sigma_{\hat{y}.w}}{\sigma_{x.z.w} - \sigma_{x.z.w}}.
\]

The new formula in Equation (2) differs in two ways from the traditional asymptotic variance formula which is

\[
a.\text{var}(\tau_{yz.w}) = \left( \eta_{ys.t} (\Sigma_{stst}^{-1} \Sigma_{st}) \right)^{-1},
\]

where \( S = (X, W), T = (Z, W) \) and \( \eta_{ys.t} = \text{var}(Y - \gamma_{ys.t} S) \) is the population level residual variance of the estimator \( \gamma_{ys.t} \). The first change is that in Equation (2), the residual variance \( \eta_{ys.t} \) from Equation (3) is replaced with the conditional variance \( \sigma_{\hat{y}.w} \) of the oracle random variable \( \hat{Y} = Y - \tau_{yx} X \). This is possible because under the assumption that \( \{Z, W\} \) is a valid conditional instrumental set \( \eta_{ys.t} = \sigma_{\hat{y}.w} \). The advantage of this change is that it is easier to describe how the term \( \sigma_{\hat{y}.w} \) behaves as a function of the tuple \( \{Z, W\} \) than \( \eta_{ys.t} \). For example, it is immediately clear that \( \sigma_{\hat{y}.w} \) depends on \( \{Z, W\} \) only via \( W \). We refer to the numerator of Equation (2), \( \sigma_{\hat{y}.w} \) as the residual variance of the estimator \( \tau_{yz} \) or, when \( (X, Y) \) is clear, of the tuple \( \{Z, W\} \). The second change is that in Equation (2), the denominator from Equation (3) is replaced with the difference \( \sigma_{x.z.w} - \sigma_{x.z.w} \). The difference \( \sigma_{x.z.w} - \sigma_{x.z.w} \) measures how much the residual variance of \( X \) on \( W \) decreases if we also add \( Z \) to the conditioning set. Intuitively, this is the information on \( X \) that \( Z \) contains and which was not already contained in \( W \). Based on this intuition, we refer to the denominator of Equation (2), \( \sigma_{x.z.w} - \sigma_{x.z.w} \) as the conditional instrumental strength of the estimator \( \tau_{yz} \) or, when \( (X, Y) \) is clear, of \( \{Z, W\} \).

Another important contribution of Theorem 4.1 is that it also holds for linear structural equation models with non-Gaussian errors. This is a non-trivial result, because Equation (3) is usually derived
under a homoscedasticity assumption on the residuals $Y - \gamma y \perp \Sigma$, which generally does not hold if the errors are non-Gaussian. However, in our proof we show that if $\{Z, W\}$ is a valid conditional instrumental set both Equation (2) and Equation (3) hold, even if the residuals are heteroskedastic.

4.2 Pairwise valid conditional instrumental set comparison

In this section we derive a graphical criterion that for certain pairs of valid conditional instrumental sets, identifies which of the two corresponding two-stage least squares estimators has the smaller asymptotic variance.

**Theorem 4.2.** Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G$ such that $de(X, G) = \{X, Y\}$. Let $\{Z_1, W_1\}$ and $\{Z_2, W_2\}$ be valid conditional instrumental sets relative to $(X, Y)$ in $G$. Let $W_{1\setminus 2} = W_1 \setminus W_2$ and $W_{2\setminus 1} = W_2 \setminus W_1$. If the following four conditions hold

(a) $W_{1\setminus 2} \perp_G Y \mid W_2$,
(b) $W_{1\setminus 2} \perp_G Z_2 \mid W_2$ or $W_{1\setminus 2} \setminus Z_2 \perp_G X \mid Z_2 \cup W_2$,
(c) either i) $W_{2\setminus 1} \setminus Z_1 \perp_G Z_1 \mid W_1$ and $W_{2\setminus 1} \cap Z_1 \perp_G X \mid W_1 \cup (W_{2\setminus 1} \setminus Z_1)$ or
   ii) $W_{2\setminus 1} \perp_G X \mid W_1$,
(d) $Z_1 \setminus (Z_2 \cup W_{2\setminus 1}) \perp_G X \mid Z_2 \cup W_1 \cup W_{2\setminus 1},$

then for all linear structural equation models compatible with $G$ such that $\Sigma_{x,z_1,w_1} \neq 0$ it holds that $a.\var(\hat{\tau}_{y|x|w_2}) \leq a.\var(\hat{\tau}_{y|x|w_1})$.

**Theorem 4.2** is more general in terms of the valid conditional instrumental sets it can compare, than the results from [Kuroki and Cai (2004)] or the result by [vansteelandt and Didelez (2018)]. In particular, it can compare two tuples $\{Z_1, W_1\}$ and $\{Z_2, W_2\}$ with $Z_1 \neq Z_2$ and $W_1 \neq W_2$. As a result the graphical condition of Theorem 4.2 is, however, rather complex. For easier intuition, we can think of it as consisting of two separate parts. Condition (a) verifies that $\{Z_1, W_1\}$ may not provide a smaller residual variance than $\{Z_2, W_2\}$, that is, $\sigma_{\tilde{y}\tilde{w}} \geq \sigma_{\tilde{y}\tilde{w}_2}$. It does so by checking that the covariates in $W_{1\setminus 2}$ are not beneficial in term of reducing the residual variance. Conditions (b) jointly verify that $\{Z_1, W_1\}$ may not provide a larger conditional instrumental strength than $\{Z_2, W_2\}$, that is, $\sigma_{x,z_1,w_1} \leq \sigma_{x,z_2,w_2}$. This requires three conditions because we need to verify in turn that i) the covariates in $W_{1\setminus 2}$ are not beneficial, ii) the nodes in $W_{2\setminus 1}$ are not harmful and iii) the nodes in $Z_1 \setminus (Z_2 \cup W_{2\setminus 1})$ are not beneficial in terms of how they affect the conditional instrumental strength.

The graphical condition also simplifies whenever $W_1 \subseteq W_2$, $W_2 \subseteq W_1$ or $Z_1 \subseteq Z_1$. In the first case, $W_{1\setminus 2} = \emptyset$ and therefore Conditions (a) and (b) are trivially true. In the second, $W_{2\setminus 1} = \emptyset$ and therefore Condition (c) is trivially true. In the third, $Z_1 \setminus Z_2 = \emptyset$ and therefore Condition (d) is trivially true. If $W_1 = W_2$ and $Z_1 \subseteq Z_2$ all four conditions are trivially true. Therefore, the well-known result that adding covariates to the instrumental set is beneficial for the asymptotic variance (e.g. Chapter 12.17 of [Hansen 2019]) is also a corollary of Theorem 4.2.

**Corollary 4.3.** Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G$ such that $de(X, G) = \{X, Y\}$. Let $\{Z_1, W_1\}$ and $\{Z_2, W_2\}$ be valid conditional instrumental sets relative to $(X, Y)$ in $G$.  

![](figure2.png)
If $Z_1 \subseteq Z_2$, then for all linear structural equation models compatible with $\mathcal{G}$ such that $\Sigma_{x,z_1,w} \neq 0$, $a.\var(\hat{\tau}_{yz}] \geq a.\var(\hat{\tau}_{yz})$.

Theorem 4.2 also gives interesting new insights. We first discuss the special case with $Z$ fixed and only $W$ varying. Here, the most important insight is that there exists a class of covariates that practitioners should avoid adding to $W$ because they increase the asymptotic variance. We now illustrate this class along with some other interesting classes of covariates in a series of examples.

**Example 4.4 (Harmful conditioning).** Consider $\mathcal{G}$ from Fig. 2a. We are interested in estimating $\tau_{yx}$ with conditional instrumental sets of the form $\{D,W\}$, where $W \subseteq \{A,B,C\}$. As it holds that forb$(X,Y,\mathcal{G}) = \{X,Y\}$, $D \not\perp_{\mathcal{G}} X$ $| W$ and $D \perp_{\mathcal{G}} Y$ $| W$ for all $W \subseteq \{A,B,C\}$, all tuples of this form are valid conditional instrumental sets relative to $(X,Y)$ in $\mathcal{G}$.

Let $W \subseteq \{B,C\}$ and $W' = W \cup A$. As $A \not\perp_{\mathcal{G}} Y$ $| W$, $A \not\perp_{\mathcal{G}} X$ $| W \cup D$ and $W \not\perp_{\mathcal{G}} W'$ we can apply Theorem 2 with $W_1 = W'$, $W_2 = W$ and $Z_1 = Z_2 = D$. We can therefore conclude that adding $A$ to any $W \subseteq \{B,C\}$ can only harm the asymptotic variance. The reason conditioning on $A$ is harmful, is that $A \perp_{\mathcal{G}} Y$ $| W$ and $A \perp_{\mathcal{G}} X$ $| W \cup B$ but $A \perp_{\mathcal{G}} X$ $| W$. Therefore, $\sigma_{\hat{g}_y,w} = \sigma_{\hat{g}_y,w}$ and $\sigma_{x,w} = \sigma_{x,w}$ but $\sigma_{x,w} \leq \sigma_{x,w}$. The node $A$ is representative of a larger class of covariates that we should avoid conditioning on because they do not affect the residual variance but may reduce the conditional instrumental strength.

**Example 4.5 (Neutral conditioning).** Consider $\mathcal{G}$ from Fig. 2a. We are interested in tuples of the form $\{D,W\}$ and $\{D,W'\}$, with $W \subseteq \{A,C\}$ and $W' = W \cup B$. By Example 4.4, any such tuple is a valid conditional instrumental set relative to $(X,Y)$ in $\mathcal{G}$. Further, as $W \not\perp_{\mathcal{G}} W'$ we can apply Theorem 2 with $W_1 = W'$, $W_2 = W$ and $Z_1 = Z_2 = D$. As $B \not\perp_{\mathcal{G}} Y$ $| W$, $B \perp_{\mathcal{G}} D$ $| W$ and $W \not\perp_{\mathcal{G}} W'$ we can therefore apply Theorem 2 with $W_1 = W'$, $W_2 = W$ and $Z_1 = Z_2 = D$. We can therefore conclude that adding $B$ to any $W \subseteq \{A,C\}$ has no effect on the asymptotic variance. This is due to the fact that $B \perp_{\mathcal{G}} Y$ $| W$ and $B \perp_{\mathcal{G}} D$ $| W$. Therefore, $\sigma_{\hat{g}_y,w} = \sigma_{\hat{g}_y,w}$ and $\sigma_{x,w} = \sigma_{x,w}$ $\sigma_{x,w} - \sigma_{x,w} = \sigma_{x,w} - \sigma_{x,w}$ (see Lemma 4.7 in the Appendix). Conditioning on $B$ has no effect on either the residual variance or the conditional instrumental strength.

**Example 4.6 (Beneficial conditioning).** Consider $\mathcal{G}$ from Fig. 2a and any two tuples of the form $\{D,W\}$ and $\{D,W'\}$, where $W \subseteq \{A,B\}$ and $W' = W \cup C$. As established in Example 4.4, any such tuple is a valid conditional instrumental set relative to $(X,Y)$ in $\mathcal{G}$. Further, $W \not\perp_{\mathcal{G}} W'$ and $C \perp_{\mathcal{G}} D$ $| W$. We can therefore apply Theorem 2 with $W_1 = W$, $W_2 = W'$ and $Z_1 = Z_2 = D$ to conclude that adding $C$ to any $W \subseteq \{A,B\}$ can only improve the asymptotic variance of the estimator. The reason conditioning on $C$ is beneficial, is that $C \perp_{\mathcal{G}} Y$ $| W$ and $C \perp_{\mathcal{G}} D$ $| W$. Therefore, $\sigma_{\hat{g}_y,w} \leq \sigma_{\hat{g}_y,w}$ but $\sigma_{x,w} = \sigma_{x,w} - \sigma_{x,w} - \sigma_{x,w}$. Interestingly, this is still true if we add the edge $C \rightarrow X$ to $\mathcal{G}$, i.e., if $C$ were a confounder. The covariate $C$ is representative of a larger class of covariates that we should aim to condition on because they may reduce the residual variance and do not affect the conditional instrumental strength.

Consider now the graph $\mathcal{G}$ from Fig. 2a and the two tuples $\{\{B,D\}, C\}$ and $\{\{B,D\}, \{A,C\}\}$. By our discussion in Example 4.6, both tuples are valid conditional instrumental sets relative to $(X,Y)$ in $\mathcal{G}$. Further, $A \perp_{\mathcal{G}} X$ $| C$. We can therefore apply Theorem 2 with $W_1 = C$, $W_2 = \{A,C\}$ and $Z_1 = Z_2 = \{B,D\}$ to conclude that conditioning on $A$ can only improve the asymptotic variance of the estimator. The reason conditioning on $A$ is beneficial, is that $A \perp_{\mathcal{G}} Y$ $| C$ and $A \perp_{\mathcal{G}} X$ $| C$ but $A \perp_{\mathcal{G}} X$ $| \{B,C,D\}$. Therefore, $\sigma_{\hat{g}_y,c} = \sigma_{\hat{g}_y,c} \sigma_{x,c} = \sigma_{x,c}$ but $\sigma_{x,c} \leq \sigma_{x,c}$. Interestingly, the valid conditional instrumental set $\{\{A,B,D\}, C\}$ has the exact same residual variance and conditional instrumental strength. Conditioning on the covariate $A$ is therefore beneficial because it acts as a pseudo-instrument.

**Example 4.7 (Ambiguous conditioning).** Consider $\mathcal{G}$ from Fig. 1b. Consider the two tuples $\{D,C\}$ and $\{D,\{B,C\}\}$. By Example 3.6, both tuples are valid conditional instrumental sets relative to $(X,Y)$ in $\mathcal{G}$. Further, as $B \not\perp_{\mathcal{G}} D$ and $D \not\perp_{\mathcal{G}} X$ $| \{C,D\}$ we cannot apply Theorem 2 with either $W_1 = C$ and $W_2 = \{B,C\}$ or vice versa. We can therefore not use Theorem 4.2 to decide what effect adding $B$ to to the conditioning set has on the asymptotic variance. In fact this depends on the underlying linear structural equation model. For verification we consider six linear structural equation models compatible with $\mathcal{G}$ and compute the asymptotic variances of our two candidate tuples in each case.
Table 1: Asymptotic variances for valid conditional instrumental sets in six linear structural equation models compatible with the graph $G_{10}$ from Fig. 1a.

| $Z$ | $W$ | Model 1 | Model 2 | Model 3 | Model 4 | Model 5 | Model 6 |
|-----|-----|---------|---------|---------|---------|---------|---------|
| {D} | C   | 3.13    | 2.70    | 17.52   | 1.30    | 106.73  | 17.55   |
| {D} | {A, C} | 2.16    | 2.46    | 10.81   | 1.20    | 37.65   | 15.50   |
| {D} | {B, C} | 7.00    | 8.83    | 103.73  | 2.02    | 387.41  | 5.45    |
| {D} | {A, B, C} | 4.60    | 7.51    | 36.03   | 1.83    | 65.59   | 4.52    |
| {A, B, D} | C | 1.55    | 2.28    | 3.75    | 1.16    | 9.42    | 3.78    |

of these six models. We summarise the results in Table 4.4 and refer to Section 2 of the Appendix for details. This is an example where a graphical criterion cannot be used to decide which of two valid conditional instrumental sets provides the smaller asymptotic variance.

Since Theorem 4.3 can compare tuples $\{Z_1, W_1\}$ and $\{Z_2, W_2\}$ with $Z_1 \neq Z_2$ and $W_1 \neq W_2$, it also gives interesting new insights regarding covariates that we may add both to $Z$ and $W$ in the form of the following corollary.

**Corollary 4.8.** Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G$ such that $\dependent(X, G) = \{X, Y\}$. Let $\{Z, W \cup S\}$ be a valid conditional instrumental set relative to $(X, Y)$ in $G$. If $\{Z \cup S, W\}$ is a valid conditional instrumental set relative to $(X, Y)$ in $G$, then for all linear structural equation model compatible with $G$ such that $\Sigma_{xz.ws} \neq 0$, it holds that $a.var(\hat{\tau}_{yz.x}) \leq a.var(\hat{\tau}_{yz.x})$.

Intuitively, Corollary 4.8 states that covariates that may be added to both $Z$ and $W$ should be added to $Z$. It can be thought of as a generalization of Corollary 4.3. If we restrict ourselves to the special case that $W'$ is a single node we can also show the following complementary result.

**Proposition 4.9.** Consider nodes $X, Y$ and $N$ in an acyclic directed mixed graph $G$ such that $\dependent(X, G) = \{X, Y\}$. Let $\{Z, W\}$ and $\{Z, W \cup N\}$ be distinct valid conditional instrumental sets relative to $(X, Y)$ in $G$. If $\{Z \cup N, W\}$ is not a valid conditional instrumental set relative to $(X, Y)$ in $G$, then for all linear structural equation models compatible with $G$ such that $\Sigma_{xz.ws} \neq 0$, $a.var(\hat{\tau}_{yz.x}) \leq a.var(\hat{\tau}_{yz.x})$.

Corollaries 4.3 and 4.8 along with Proposition 4.9 are very useful to identify accurate tuples $\{Z, W\}$. We now illustrate this by revisiting first $G_{10}$ and then $G_{20}$.

**Example 4.10.** Consider the acyclic directed mixed graph $G_{10}$ in Fig. 1b. By Example 2.8 there are 18 valid conditional instrumental sets relative to $(X, Y)$ in $G$. Let $\{Z, W\}$ be an arbitrary valid tuple. Suppose that $Z \cup W \neq \{A, B, C, D\}$. If $C \notin W$, then $\{Z, W\}$ is also a valid tuple. We can therefore apply Proposition 4.9 with $A = C$ to conclude that $\{Z, W\}$ is more accurate than $\{Z, W\}$. If any of $A, B$ and $D$ are not in $Z \cup W$ we can add them to $Z$ to obtain a set $Z'$, such that $\{Z', W\}$ is a valid tuple. By Corollary 4.2 this reduces the asymptotic variance. Doing both obtain a more accurate tuple $\{Z', W'\}$, such that $\{Z', W'\}$ is at least as accurate as $\{Z', W'\}$. Since we began from an arbitrary valid tuple, this shows that $\{A, B, D\}$ provides the smallest attainable asymptotic variance among all valid tuples.

**Example 4.11.** Consider the causal acyclic directed mixed graph $G$ in Fig. 2a. We first characterise all valid conditional instrumental sets relative to $(X, Y)$ in $G$. As for $(X, Y)$ in $G_{10}$, we only need to consider disjoint node sets $Z$ and $W$ that are subsets of $\{A, B, C, D\}$. Further, $Z \perp_{G_{10}} Y \mid W$ if and only if $C \notin Z$ and therefore $Z \subseteq \{A, B, D\}$. Finally, $Z \perp_{G_{10}} X \mid W$ if and only if $\{B, D\} \cap Z = 0$ and $D \in W$. Therefore, any valid tuple with respect to $(X, Y)$ in $G$ has to be of the form $\{Z, W\}$, with $Z \subseteq \{A, B, D\}$ non-empty, $W \subseteq \{A, B, C, D\} \setminus Z$ if $Z \neq \{A\}$, and $W \subseteq \{B, C\}$ if $Z = \{A\}$. There are 34 tuples of this form.
Let \( \{ Z, W \} \) be any of these 34 valid tuples. Suppose that \( Z \cup W \neq \{ A, B, C, D \} \). By the same argument as in Example 4.10 we can use Proposition 4.9 and Corollary 4.3 to obtain a more accurate tuple \( \{ Z', W' \} \), such that \( Z \cup W' = \{ A, B, C, D \} \). We can also apply Corollary 4.8 with \( A = \{ A, B, D \} \) and conclude that the valid conditional instrumental set \( \{ A, B, D \} \) is at least as accurate as \( \{ Z', W' \} \). Since we began from an arbitrary valid tuple, this shows that \( \{ \{ A, B, D \}, C \} \) provides the smallest attainable asymptotic variance among all valid tuples. However, as \( A \not\perp_{\overline{G}} X \mid \{ B, C, D \} \) we can apply Theorem 4.2 with \( \{ Z, W \} = \{ \{ A, B, D \} \} \) and therefore Algorithm 1 will output \( \{ \{ B, D \}, C \} \) in this case only \( \{ \{ A, B, D \}, C \} \) provides the smallest attainable asymptotic variance.

### 4.3 Greedy forward procedure

As shown in the previous section the asymptotic variance can behave in complex ways. However, we can in some sense ignore much of this complex behaviour and instead apply the following simple guidelines derived from Corollaries 4.3 and 4.8 along with Proposition 4.9.

**Remark 4.12.** Covariates that can be used as instrumental variables should be used as instrumental variables. Covariates that can only be used as conditioning variables should be used as conditioning variables.

```
input : Acyclic directed mixed graph \( G = (V, E) \) and \( X, Y, Z, W \) such that \( \{ Z, W \} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G \)
output: Valid conditional instrumental set \( \{ Z', W' \} \) relative to \( (X, Y) \) in \( G \) such that
\[
\text{a.var}(\hat{\tau}_{xz}^{z \cdot w}) \leq \text{a.var}(\hat{\tau}_{xz}^{z \cdot w}')
\]
1 begin
2 \( Z' = Z, W' = W, V' = V \setminus \{ \{ X, Y \} \cup Z \cup W \} \)
3 foreach \( N \in V' \) do
4 if \( \{ Z' \cup N, W' \} \) valid and \( N \not\perp_{G} X \mid W \cup Z \) then
5 \( Z' = Z' \cup N \)
6 else if \( \{ Z', W' \cup N \} \) valid and \( N \not\perp_{G} Y \mid W \) then
7 \( W' = W' \cup N \)
8 return \( \{ Z', W' \} \)
```

**Algorithm 1: Greedy forward procedure**

Based on these guidelines we propose the greedy Algorithm 1 that given a valid conditional instrumental set greedily adds covariates to the starting tuple while minimizing the asymptotic variance. We could drop the m-separation checks in Algorithm 1 and it would still greedily minimise the asymptotic variance. We do not consider this variation of Algorithm 1 because it tends to add irrelevant covariates to \( Z \), needlessly growing the output tuple.

**Proposition 4.13.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( G \) such that \( \text{de}(X, G) = \{ X, Y \} \). Let \( \{ Z, W \} \) be a valid conditional instrumental sets relative to \( (X, Y) \) in \( G \). Then applying Algorithm 1 to \( (G, X, Y, Z, W) \) greedily minimises \( \text{a.var}(\hat{\tau}_{xz}^{z \cdot w}') \) at each step.

**Example 4.14.** We now illustrate Algorithm 1 by revisiting \( G_{11} \) and \( G_{12} \). Consider first \( G_{11} \) from Fig. 4.16. Suppose our starting valid conditional instrumental set is \( \{ B, C \} \). Both \( A \) and \( D \) may be added to the instrumental set. However, \( A \not\perp_{\overline{G}} X \mid \{ B, C \} \) and therefore Algorithm 1 will output \( \{ \{ B, D \}, C \} \) if \( A \) is considered before \( D \), and \( \{ \{ A, B, D \}, C \} \) otherwise. Both are better than \( \{ B, C \} \) but in this case only \( \{ \{ A, B, D \}, C \} \) provides the smallest attainable asymptotic variance.

Consider now \( G_{12} \) from Fig. 4.20. Suppose our starting valid conditional instrumental set is \( \{ B, \emptyset \} \). Both \( A \) and \( D \) may be added to the instrumental set. The node \( C \) on the other hand may not be added to the instrumental set but can always be added to the conditioning set. This is true irrespectively of the order in which we consider the three nodes. However, \( A \not\perp_{\overline{G}} X \mid S \), for any \( S \subseteq \{ A, B, C, D \} \) with \( D \in S \). Therefore, Algorithm 1 outputs \( \{ \{ A, B, D \}, C \} \) if the algorithm considers \( A \) before \( D \), and \( \{ \{ B, D \}, C \} \) otherwise. Both are better than \( \{ B, \emptyset \} \) and in this case they even provide the smallest attainable asymptotic variance, as shown in Example 4.17.
4.4 Graphically optimal valid conditional instrumental sets

In Examples 4.11 and 4.10, we identified valid conditional instrumental sets that provide the smallest attainable asymptotic variance among all valid tuples using only the graph. In the closely related literature on accurate valid adjustment sets [Henckel et al. 2022] referred to this property as asymptotic optimality (see also [Kotniszky and Smucler 2020; Witte et al. 2020; Smucler et al. 2022; Runge 2021]). They also proposed a valid adjustment set that for linear structural equation models with independent errors, no asymptotically optimal valid adjustment set may exist. The following example shows that, similarly, an asymptotically optimal valid conditional instrumental set may not exist.

Example 4.15. Consider $G_{2B}$ from Fig. 2b. There are four valid conditional instrumental sets with respect to $(X,Y)$ in $(a)$, $(b)$. Let $A,B,C$ be valid conditional instrumental sets relative to $(X,Y)$ in $G$. We call $A,B,C$ graphically optimal relative to $(X,Y)$ in $G$, if for all valid conditional instrumental sets $Z,W$ relative to $(X,Y)$ in $G$ such that there exists a linear structural equation model $C_1$ compatible with $G$ for which $a.var (\tilde{\sigma}_{x,z|w}^2, C_1) < a.var (\tilde{\sigma}_{y,z|w}^2, C_2)$, there also exists a linear structural equation model $C_2$ compatible with $G$ for which $a.var (\tilde{\sigma}_{x,z|w}^2, C_2) > a.var (\tilde{\sigma}_{y,z|w}^2, C_2)$, where $a.var (\tilde{\sigma}_{x,z|w}^2, C)$ denotes the asymptotic variance of the estimator $\tilde{\sigma}_{x,z|w}^2$ in the linear structural equation model $C$.

Example 4.15 does not contradict our results from Section 4.3, as these cover the special case of adding a single covariate at a time to a valid tuple. Given that there is generally no asymptotically optimal valid conditional instrumental set we now consider the following property instead.

Definition 4.16. Let $X$ and $Y$ be nodes in an acyclic directed mixed graph $G$ and let $\{Z,W\}$ be a valid conditional instrumental set relative to $(X,Y)$ in $G$. We call $\{Z,W\}$ graphically optimal relative to $(X,Y)$ in $G$, if for all valid conditional instrumental sets $Z',W'$ relative to $(X,Y)$ in $G$ such that there exists a linear structural equation model $C_1$ compatible with $G$ for which $a.var (\tilde{\sigma}_{x,z|w}^2, C_1) < a.var (\tilde{\sigma}_{y,z|w}^2, C_1)$, there also exists a linear structural equation model $C_2$ compatible with $G$ for which $a.var (\tilde{\sigma}_{x,z|w}^2, C_2) > a.var (\tilde{\sigma}_{y,z|w}^2, C_2)$, where $a.var (\tilde{\sigma}_{x,z|w}^2, C)$ denotes the asymptotic variance of the estimator $\tilde{\sigma}_{x,z|w}^2$ in the linear structural equation model $C$.

Graphical optimality is a natural generalization of asymptotic optimality. In particular, if an asymptotically optimal valid conditional instrumental set exists, any graphically optimal valid conditional instrumental set will also be asymptotically optimal. We now give a definition which we will use to construct a conditional instrumental set that is valid and graphically optimal under mild conditions. The definition is a minor generalization of the notion of a Markov blanket in an acyclic directed mixed graph [Richardson 2003].

Definition 4.17. Let $N$ be a node and $W$ a node set in an acyclic directed mixed graph $G$ with node set $V$. Let $dis_W(N,G) = \{A | V_1 \in A \leftrightarrow V_1 \leftrightarrow \cdots \leftrightarrow V_k \leftrightarrow N, V_i \notin W, \ldots, V_k \notin W\}$. Then let $dis_W^+(N,G)$ denote the set $\{dis_W(N,G) \cup \{pa(dis_W(N,G), G)\} \setminus W\}$.

Theorem 4.18. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G$ such that $de(X,G) = \{X,Y\}$. Let $W_o = dis_X^+(Y,G)$ and $Z_o = dis_X^+(X,G) \setminus W_o$. Then the following two statements hold: (i) if $Z_o \neq \emptyset$ then $\{Z_o, W_o\}$ is a valid conditional instrumental set relative to $(X,Y)$ in $G$; (ii) if $Z_o \cap (pa(X,G) \cup \{sib(X,G)\}) \neq \emptyset$ then $\{Z_o, W_o\}$ is also graphically optimal relative to $(X,Y)$ in $G$.
Figure 3: Violin plot of the ratios of the root mean squared error for \( \{ Z^\circ, W^\circ \} \) to the one for the tuple \( \{ Z, W \} \) given on the X-axis. For the labels on the X-axis we use "OLS" to denote the ordinary least squares regression of \( Y \) on \( X \). The black dots mark the geometric mean of the ratios in the respective violin plot.

Our proposed tuple \( \{ Z^\circ, W^\circ \} \) is constructed as follows. We first choose \( W^\circ \) in order to minimise the residual variance of the tuple. With \( W^\circ \) fixed we then in turn choose \( Z^\circ \) from the remaining covariates in order to maximise the conditional instrumental strength. The conditions \( Z^\circ \neq \emptyset \) and \( Z^\circ \cap (\text{pa}(X, G) \cup \text{sib}(X, G)) \neq \emptyset \) ensure that the resulting \( Z^\circ \) is not too small.

We give examples where the two conditions are violated in Section D of the Supplement.

**Example 4.19** (Illustrating Theorem 4.18). We revisit \( G_{1b} \) and \( G_{2a} \) from Figures 1a and 2a, respectively. In \( G_{1b} \) \( Z^\circ = \{ A, B, D \} \) and \( W^\circ = C \). By Example 4.11 \( \{ \{ A, B, D \}, C \} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G_{1b} \) and in fact asymptotically optimal. In \( G_{2b} \) \( Z^\circ = \{ B, D \} \) and \( W^\circ = C \). By Example 4.10 \( \{ \{ B, D \}, C \} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G_{2b} \) and in fact asymptotically optimal. In \( G_{2b} \) \( Z^\circ = \{ A \} \) and \( W^\circ = \{ B, C \} \). By Example 4.15 \( \{ A, \{ B, C \} \} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G_{2b} \). There is no asymptotically optimal valid conditional instrumental set relative to \( (X, Y) \) in \( G_{2b} \). However, \( \{ A, \{ B, C \} \} \) is graphically optimal (see Table 4.4).

5 Simulations

We investigate the finite sample accuracy of \( \{ Z^\circ, W^\circ \} \) and check how it compares to alternative valid conditional instrumental sets. We do so in linear structural equation models compatible with the two graphs \( G_{1b} \) and \( G_{2a} \) from Figures 1a and 2a, respectively.

For each graph, we randomly generate 1000 compatible linear structural equation models as follows. We consider models with either all Gaussian or all uniform errors and uniformly draw the error type. For each node we sample an error variance uniformly on \([0, 1] \) and for each edge an edge coefficient uniformly on \([-2, -0.1] \cup [0.1, 2] \). Any bidirected edge \( V_i \leftrightarrow V_j \) is simply modelled as a
latent variable $V_j \leftarrow L \rightarrow V_j$, with the error variances and edge coefficients generated as for the other nodes and edges. From each linear structural equation model we generate 100 data sets with sample size $n$ and use these to compute the two-stage least squares estimators corresponding to all available valid conditional instrumental sets relative to $(X, Y)$ in our graph. As a non-causal baseline we also compute the ordinary least squares coefficient of $Y$ on $X$. With these 100 estimates per estimator, we compute Monte-Carlo root mean squared errors with respect to the known true total effect $\tau_{yx}$. We do this for the sample sizes $n = 20$ and $n = 500$. To compare the performances, we compute the ratio of the root mean squared error for $\{Z^o, W^o\}$ to the one for each of the alternative estimators. A ratio smaller than 1 indicates that $\{Z^o, W^o\}$ was more accurate than the other estimator, while a ratio larger than 1 indicates the opposite. Fig. 3 shows violin plots of these ratios over the 1000 linear structural equation models. As there are 18 valid conditional instrumental sets relative to $(X, Y)$ in $G_{18}$ we only show the violin plots for a representative subset (see Section E of the Appendix for the remainder).

The violin plots corroborate our results. The optimal tuple $\{Z^o, W^o\}$ outperforms the other tuples, with few of the ratios larger than 1. Interestingly, this is also true for the sample size $n = 20$ even though our results only hold asymptotically. It is not true, however, for the inconsistent ordinary least squares regression, which for $n = 20$ is more accurate than $\{Z^o, W^o\}$ in $G_{18}$ and similarly accurate in $G_{34}$. It is also more accurate than all other valid conditional instrumental sets in both graphs. The fact that this is the case, even though we know the graph, illustrates how important it is to consider statistical accuracy when selecting a conditional instrumental sets. By looking at the relative performance of certain tuples, we can also see that this simulation study corroborates the analyses in the Examples of Section 4.2. For example, in $G_{34}$ the tuple $\{D, \emptyset\}$ performs better than $\{D, A\}$, performs equal to $\{D, B\}$ and performs worse than $\{D, C\}$.

There is another interesting pattern, not directly related to our results. The relative performance of tuples with smaller conditional instrumental strength than $\{Z^o, W^o\}$, improves as the sample size increases from $n = 20$ to $n = 500$. This is for example the case for all tuples with $Z = D$ in $G_{34}$. We believe this is due to the non-standard behaviour of the two-stage least squares estimator in cases with weak conditional instrumental strength, a well-known problem in the literature (Bound et al., 1995; Staiger and Stock, 1997; Stock et al., 2002).

### 6 Illustration

For a simple illustration of our results we consider the analysis of the effect of institutions on economic wealth using settler mortality as an instrument by Acemoglu et al. (2001). In their analysis Acemoglu et al. (2001) consider a variety of different conditioning sets and check that for all of them their estimate of the total effect of institutions on economic growth is positive. They do this as a simple robustness check for their analysis. However, they do not consider how the standard errors differ depending on the choice of conditioning set.

We investigate this for three of the available covariates: latitude, ethnic fragmentation and percentage of population of European ancestry. We summarise the results in Table 6. Latitude and percentage of population with European ancestry are both correlated with settler mortality, as i) tropical diseases were a major cause of settler mortality and ii) low settler mortality lead to a larger settler population. As a result it is unsurprising that adjusting for either leads to larger standard errors. Ethnic fragmentation on the other hand is predictive of economic wealth, as cultural barriers are often also market barriers. As a result it is unsurprising that adjusting for ethnic fragmentation leads to a smaller standard error. Using percentage of population with European ancestry as an additional instrument does lead to a smaller standard error, however. These behaviours are as expected by our theoretical results. The smallest standard error we obtain is less than half the size of the largest, illustrating the potential advantages of applying our results.
| Z                 | W       | estimate | standard error |
|-------------------|---------|----------|----------------|
| settler mort.     | ∅       | 0.94     | 0.16           |
| settler mort.     | latitude| 1.00     | 0.22           |
| settler mort.     | euro. anc. | 0.96    | 0.28           |
| settler mort.     | ethnic frag. | 0.74    | 0.13           |
| {settler mort., euro. anc.} | ∅ | 0.94     | 0.14           |
| {settler mort., euro. anc.} | ethnic frag. | 0.74    | 0.11           |

Table 3: Estimated total effect of institutions on economic wealth and estimated standard errors with varying conditional instrumental sets.

7 Discussion

In this paper we focus on linear structural equation models and the two-stage least squares estimator for the sake for simplicity. However, there are many popular alternative instrumental variable estimators, such as the LIML and the JIVE estimator (Anderson et al. [1949], Phillips and Hale [1977], Angrist et al. [1999]) among many others (Okui et al. [2012], Vansteelandt and Didelez [2018], Emmenegger and Rüblmann [2021]). It remains an interesting research question to what extent our results generalise to these alternative estimators as well as more general settings.

Finally, we would like to point out three other interesting avenues for future research: First, can we graphically characterise when an asymptotically optimal valid conditional instrumental set exists (cf. Runge [2021])? Second, does there exist a valid conditional instrumental set that is graphically optimal and has maximal conditional instrumental strength? Third, can we generalise Theorem 4.2 such that it covers all cases where we can use the graph to decide which of two valid conditional instrumental sets provides the smaller asymptotic variance?

References

Acemoglu, D., Johnson, S., and Robinson, J. A. (2001). The colonial origins of comparative development: An empirical investigation. *American economic review*, 91(5):1369–1401.

Anderson, T. W., Rubin, H., et al. (1949). Estimation of the parameters of a single equation in a complete system of stochastic equations. *The Annals of Mathematical Statistics*, 20(1):46–63.

Angrist, J. D., Imbens, G. W., and Krueger, A. B. (1999). Jackknife instrumental variables estimation. *Journal of Applied Econometrics*, 14(1):57–67.

Angrist, J. D., Imbens, G. W., and Rubin, D. B. (1996). Identification of causal effects using instrumental variables. *Journal of the American statistical Association*, 91(434):444–455.

Basmann, R. L. (1957). A generalized classical method of linear estimation of coefficients in a structural equation. *Econometrica: Journal of the Econometric Society*, pages 77–83.

Bekker, P. A. (1994). Alternative approximations to the distributions of instrumental variable estimators. *Econometrica: Journal of the Econometric Society*, pages 657–681.

Bound, J., Jaeger, D. A., and Baker, R. M. (1995). Problems with instrumental variables estimation when the correlation between the instruments and the endogenous explanatory variable is weak. *Journal of the American statistical association*, 90(430):443–450.

Bowden, R. J. and Turkington, D. A. (1990). *Instrumental variables*. Number 8. Cambridge university press.

Brito, C. and Pearl, J. (2002a). Generalized instrumental variables. In *Proceedings of the Eighteenth Annual Conference on Uncertainty in Artificial Intelligence (UAI-02)*, pages 85–93.
Brito, C. and Pearl, J. (2002b). A new identification condition for recursive models with correlated errors. Structural Equation Modeling, 9(4):459–474.

Buja, A., Berk, R., Brown, L., George, E., Pitkin, E., Traskin, M., Zhan, K., and Zhao, L. (2014). Models as approximations, part I: A conspiracy of nonlinearity and random regressors in linear regression. arXiv:1404.1578.

Emmenegger, C. and Bühlmann, P. (2021). Regularizing double machine learning in partially linear endogenous models. Electronic Journal of Statistics, 15(2):6461–6543.

Hansen, B. E. (2019). Multivariate Analysis (Probability and Mathematical Statistics).

Henckel, L., Perković, E., and Maathuis, M. H. (2022). Graphical criteria for efficient total effect estimation via adjustment in causal linear models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 84(2):579–599.

Hernán, M. A. and Robins, J. M. (2006). Instruments for causal inference: an epidemiologist’s dream? Epidemiology, pages 360–372.

Kinal, T. W. (1980). The existence of moments of k-class estimators. Econometrica: Journal of the Econometric Society, pages 241–249.

Koster, J. T. (1999). On the validity of the markov interpretation of path diagrams of gaussian structural equations systems with correlated errors. Scandinavian Journal of Statistics, 26(3):413–431.

Kuroki, M. and Cai, Z. (2004). Selection of identifiability criteria for total effects by using path diagrams. In Proceedings of the Twentieth Annual Conference on Uncertainty in Artificial Intelligence (UAI-04), pages 333–340, Arlington, Virginia. AUAI Press.

Okui, R., Small, D. S., Tan, Z., and Robins, J. M. (2012). Doubly robust instrumental variable regression. Statistica Sinica, pages 173–205.

Pearl, J. (1995). Causal diagrams for empirical research. Biometrika, 82(4):669–688.

Pearl, J. (2009). Causality. Cambridge University Press, second edition.

Perković, E., Textor, J., Kalisch, M., and Maathuis, M. H. (2018). Complete graphical characterization and construction of adjustment sets in Markov equivalence classes of ancestral graphs. Journal of Machine Learning Research, 18(220):1–62.

Phillips, G. D. A. and Hale, C. (1977). The bias of instrumental variable estimators of simultaneous equation systems. International Economic Review, pages 219–228.

Richardson, T. (2003). Markov properties for acyclic directed mixed graphs. Scandinavian Journal of Statistics, 30(1):145–157.

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

Rotnitzky, A. and Smeucler, E. (2020). Efficient adjustment sets for population average causal treatment effect estimation in graphical models. Journal of Machine Learning Research, 21(188):1–86.

Runge, J. (2021). Necessary and sufficient graphical conditions for optimal adjustment sets in causal graphical models with hidden variables. Advances in Neural Information Processing Systems, 34:15762–15773.

Shpitser, I., VanderWeele, T., and Robins, J. (2010). On the validity of covariate adjustment for estimating causal effects. In Proceedings of the Twenty-Sixth Annual Conference on Uncertainty in Artificial Intelligence (UAI-10), pages 527–536, Corvallis, Oregon. AUAI Press.

Smeucler, E., Sapienza, F., and Rotnitzky, A. (2022). Efficient adjustment sets in causal graphical models with hidden variables. Biometrika, 109(1):49–65.

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Staiger, D. and Stock, J. H. (1997). Instrumental variables regression with weak instruments. *Econometrica: journal of the Econometric Society*, pages 557–586.

Stock, J. H., Wright, J. H., and Yogo, M. (2002). A survey of weak instruments and weak identification in generalized method of moments. *Journal of Business & Economic Statistics*, 20(4):518–529.

Vansteelandt, S. and Didelez, V. (2018). Improving the robustness and efficiency of covariate-adjusted linear instrumental variable estimators. *Scandinavian Journal of Statistics*, 45(4):941–961.

Wermuth, N. (1989). Moderating effects in multivariate normal distributions. *Methodika*, 3:74–93.

Witte, J., Henckel, L., Maathuis, M. H., and Didelez, V. (2020). On efficient adjustment in causal graphs. *Journal of Machine Learning Research*, 21(246):1–45.

Wooldridge, J. M. (2010). *Econometric analysis of cross section and panel data*. MIT press.

Wright, S. (1934). The method of path coefficients. *The Annals of Mathematical Statistics*, 5(3):161–215.

A Preliminaries and known results

A.1 General preliminaries

Covariance matrices and regression coefficients: Consider random vectors \( S = (S_1, \ldots, S_k) \), \( T = (T_1, \ldots, T_k) \) and \( W \). We denote the covariance matrix of \( S \) by \( \Sigma_{ss} \in \mathbb{R}^{k_x \times k_x} \) and the covariance matrix between \( S \) and \( T \) by \( \Sigma_{st} \in \mathbb{R}^{k_x \times k_t} \), where its \((i, j)\)-th element equals \( \text{cov}(S_i, T_j) \). We further define \( \Sigma_{st, w} = \Sigma_{st} - \Sigma_{sw} \Sigma_{ww}^{-1} \Sigma_{st} \). If \( k_x = k_t = 1 \), we write \( \sigma_{st,w} \) instead of \( \Sigma_{st, w} \). The value \( \sigma_{s,w} \) can be interpreted as the residual variance of the ordinary least squares regression of \( S \) on \( W \).

We also refer to \( \sigma_{s,s,w} \) as the conditional variance of \( S \) given \( W \). Let \( \beta_{st,w} \in \mathbb{R}^{k_x \times k_t} \) represent the population level least squares regression coefficient matrix whose \((i,j)\)-th element is the regression coefficient of \( T_j \) in the regression of \( S_i \) on \( T \) and \( W \). We denote the corresponding estimator as \( \hat{\beta}_{st,w} \). Finally, for random vectors \( W_1, \ldots, W_m \) with \( W = (W_1, \ldots, W_m) \) we use the notation that \( \beta_{st,w_1,\ldots,w_m} = \beta_{st,w} \) and \( \Sigma_{st,w_1,\ldots,w_m} = \Sigma_{st,w} \).

Two stage least squares estimator: Consider two random variables \( X \) and \( Y \), and two random vectors \( Z \) and \( W \). Let \( S_n, T_n \) and \( Y_n \) be the random matrices corresponding to taking \( n \) i.i.d. observations from the random vectors \( S = (X, W), T = (Z, W) \) and \( Y \), respectively. Then the two stage least squares estimator \( \hat{\beta}_{y|x,w} \) is defined as the first entry of the larger estimator

\[
\hat{\gamma}_{y|x,t} = Y_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n (S_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n)^{-1},
\]

where we repress the dependence on the sample size \( n \) for simplicity. We refer to the tuple \( \{Z, W\} \) as the conditional instrumental set, to \( Z \) as the instrumental set and to \( W \) as the conditioning set. We also let \( \gamma_{y|x,t} = \Sigma_{yt} \Sigma_{tt}^{-1} \Sigma_{yt} \Sigma_{yt}^{-1} \Sigma_{yt} \) denote the population level two-stage least squares estimator of \( Y \) on \( S \) with instrumental set \( T \), which exists whenever \( \Sigma_{yt} \Sigma_{tt}^{-1} \Sigma_{yt} \) is invertible.

A.2 Graphical and causal preliminaries

Graphs: We consider graphs \( G = (V, E) \) with node set \( V \) and edge set \( E \), where edges can be either directed (\( \rightarrow \)) or bidirected (\( \leftrightarrow \)). If all edges in \( E \) are directed, then \( G \) is a directed graph. If all edges in \( E \) are directed or bidirected, then \( G \) is a directed mixed graph.

Paths: Two edges are adjacent if they have a common node. A walk is a sequence of adjacent edges. A path \( p \) is a sequence of adjacent edges without repetition of a node and may consist of just a single node. The first node \( X \) and the last node \( Y \) on a path \( p \) are called endpoints of \( p \) and we say that \( p \) is a path from \( X \) to \( Y \). Given two nodes \( Z \) and \( W \) on a path \( p \), we use \( p(Z, W) \) to denote the subpath of \( p \)
from $Z$ to $W$. A path from a set of nodes $S$ to a set of nodes $T$ is a path from a node $X \in S$ to some node $Y \in T$. A path from a set $S$ to a set $T$ is proper if only the first node is in $S$ (cf. [Shpitser et al. 2010]). A path $p$ is called directed from $X$ to $Y$ if all edges on $p$ are directed and point towards $Y$. We use $\oplus$ to denote the concatenation of paths. For example, for any path $p$ from $X$ to $Y$ with intermediary node $Z$, $p = p(X,Z) \oplus p(Z,Y)$.

Ancestry: If $X \rightarrow Y$, then $X$ is a parent of $Y$ and $Y$ is a child of $X$. If there is a directed path from $X$ to $Y$, then $X$ is an ancestor of $Y$ and $Y$ a descendant of $X$. If $X \leftrightarrow Y$, then $X$ and $Y$ are siblings. We use the convention that every node is an ancestor, descendant and sibling of itself. The sets of parents, ancestors, descendants and siblings of $X$ in $G$ are denoted by $pa(X,G)$, $an(X,G)$, $de(X,G)$ and $sib(X,G)$, respectively. For sets $S$, let $pa(S,G) = \bigcup_{X \in S} pa(X,G)$, with analogous definitions for $an(S,G)$, $de(S,G)$ and $sib(S,G)$.

Colliders: A node $V_j$ is a collider on a path $V_1 \cdots V_j \cdots V_m$ if $p$ contains a subpath of the form $V_{j-1} \rightarrow V_j \leftarrow V_{j+1}, V_{j-1} \leftrightarrow V_j$ or $V_{j-1} \leftrightarrow V_j \rightarrow V_{j+1}$. A node $V$ on a path $p$ is called a non-collider on $p$ if it is neither a collider on $p$ nor an endpoint node of $p$.

Directed cycles, directed acyclic graphs and acyclic directed mixed graphs: A directed path from a node $X$ to a node $Y$, together with the edge $Y \rightarrow X$ forms a directed cycle. A directed graph without directed cycles is called a directed acyclic graph and a directed mixed graph without directed cycles is called an acyclic directed mixed graph.

Blocking, d-separation and m-separation: (Cf. Definition 1.2.3 in Pearl 2009 and Section 2.1 in Richardson 2003) Consider an acyclic directed mixed graph $G = (V,E)$, with $V$ generated from a linear structural equation model compatible with $G$. We can read off conditional independence relationships between the variables in $V$ directly from the acyclic directed mixed graph with the following graphical criterion. Let $S$ be a set of nodes in an acyclic directed mixed graph. A path $p$ is blocked by $S$ if (i) $p$ contains a non-collider that is in $S$, or (ii) $p$ contains a collider $C$ such that no descendant of $C$ is in $S$. A path that is not blocked by a set $S$ is open given $S$. If $S,T$ and $W$ are three pairwise disjoint sets of nodes in an acyclic directed mixed graph $G$, then $W$ m-separates $S$ from $T$ in $G$ if $W$ blocks every path between $S$ and $T$ in $G$. We then write $S \perp_{G} T \mid W$. Otherwise, we write $S \not\perp_{G} T \mid W$. We use the convention that for any two disjoint node sets $S$ and $T$ it holds that $\emptyset \perp_{G} S \mid T$.

Markov property and faithfulness: (Cf. Definition 1.2.2 2009) Let $S$, $T$ and $W$ be disjoint sets of random variables. We use the notation $S \perp T \mid W$ to denote that $S$ is conditionally independent of $T$ given $W$. A density $f$ is called Markov with respect to an acyclic directed mixed graph $G$ if $S \perp_{G} T \mid W$ implies $S \perp T \mid W$ in $f$. If this implication holds in the other direction, then $f$ is faithful with respect to $G$.

Causal paths and forbidden nodes: (cf. Perković et al. 2018) Let $X$ and $Y$ be nodes in an acyclic directed mixed graph $G$. A path from $X$ to $Y$ in $G$ is called a causal path from $X$ to $Y$ if all edges on $p$ are directed and point towards $Y$. We define the causal nodes with respect to $(X,Y)$ in $G$, as all nodes on causal paths from $X$ to $Y$ excluding $X$ and denote them $cn(X,Y,G)$. We define the forbidden nodes relative to $(X,Y)$ in $G$ as the descendants of the causal nodes as well as $X$ and denote them forb$(X,Y,G)$.

Total effects: We define the total effect of $X$ on $Y$ as

$$\tau_{yx}(x) = \frac{\partial}{\partial x} \mathbb{E}[y \mid do(x=x)].$$

In a linear structural equation model the function $\tau_{yx}(x)$ is constant, which is why we simply write $\tau_{yx}$. The path tracing rules by [Wright, 1934] allow for the following alternative definition. Consider two nodes $X$ and $Y$ in an acyclic directed mixed graph $G = (V,E)$ and suppose that $V$ is generated from a linear structural equation model compatible with $G$. Then $\tau_{yx}$ is the sum over all causal paths from $X$ to $Y$ of the product of the edge coefficients along each such path. Given a set of random variables $W = \{W_1, \ldots, W_k\}$ we also define $\tau_{wx}$ to be the stacked column vector with $i$th entry $\tau_{wix}$. Finally, let $\tau_{wx;w_1 \ldots w_{n-1}}$ be the sum over all causal paths from $X$ to $W_i$ that does not contain nodes in $W_{i+1}$ of the product of the edge coefficients along each such path.
Linear structural equation model: Consider an acyclic directed mixed graph $G = (V, E)$, with nodes $V = (V_1, \ldots, V_p)$ and edges $E$, where the nodes represent random variables. The random vector $V$ is generated from a linear structural equation model compatible with $G$ if

$$V \leftarrow AV + \epsilon,$$

such that the following three properties hold: First, $A = (\alpha_{ij})$ is a matrix with $\alpha_{ij} = 0$ for all $i, j$ where $V_j \rightarrow V_i \notin E$. Second, $\epsilon = (\epsilon_{v_1}, \ldots, \epsilon_{v_p})$ is a random vector of errors such that $E(\epsilon) = 0$ and $\text{cov}(\epsilon) = \Omega = (\omega_{ji})$ is a matrix with $\omega_{ji} = \omega_{ij} = 0$ for all $i, j$ where $V_i \leftrightarrow V_j \notin E$. Third, for any two disjoint sets $V', V'' \subseteq V$ such that for all $V_i \in V'$ and all $V_j \in V''$, $V_i \leftrightarrow V_j \notin E$, the random vector $(\epsilon_{v_i})_{v_i \in V'}$ is independent of $(\epsilon_{v_j})_{v_j \in V''}$.

Given the matrices $A$ and $\Omega$ it holds that

$$\Sigma_{vv} = (\text{Id} - A)^{-T} \Omega (\text{Id} - A)^{-1},$$

that is, the covariance matrix of a linear causal model is completely determined by the tuple of matrices $(A, \Omega)$.

Gaussian linear structural equation model: If the errors in a linear structural equation model are jointly normal we refer to the linear structural equation model as a Gaussian linear structural equation model. Such a model is completely determined by the tuple of matrices $(A, \Omega)$ which is why we will use $(A, \Omega)$ to denote the corresponding Gaussian linear structural equation model.

Latent projections and causal acyclic directed mixed graphs. (Richardson et al. 2017) Let $G$ be an acyclic directed mixed graph with node set $V$ and let $L \subset V$. We can use a tool called the latent projection (Richardson 2003) to remove the nodes in $L$ from $G$ while preserving all m-separation statements between subsets of $V \setminus L$. We use the notation $G^L$ to denote the acyclic directed mixed graph with node set $V \setminus L$ that is the latent projection of $G$ over $L$. The latent projection $G^L$ of $G$ over $L$ is an acyclic directed mixed graph with node set $V \setminus L$ and edges in accordance with the following rules: First, $G^L$ contains a directed edge $W_i \rightarrow W_j$ if and only if there exists a causal path $W_i \rightarrow \cdots \rightarrow W_j$ in $G$ with all non-endpoint nodes in $L$. Second, $G^L$ contains a bi-directed edge $W_i \leftrightarrow W_j$ if and only if there exists a path between $W_i$ and $W_j$, such that all non-endpoints are non-colliders in $L$ and the edges adjacent to $W_i$ and $W_j$ have arrowheads pointing towards $W_i$ and $W_j$, respectively.

The following is an important property of the latent projection for acyclic directed mixed graphs: if $V$ is generated from a linear structural equation model compatible with the acyclic directed mixed graph $G$ then $V \setminus L$ is generated from a linear structural equation model compatible with $G^L$.

Valid adjustment sets: (Shpitser et al. 2010; Perković et al. 2018) We refer to a node set $W$ as a valid adjustment set relative to $(X, Y)$ in $G$, if $X, Y \not\in W$ for all linear structural equation models compatible with $G$. Consider node sets $X, Y$ and $W$ in an acyclic directed mixed graph $G$. Then $W$ is a valid adjustment set relative to $(X, Y)$ in $G$ if i) $W \cap \text{forb}(X, Y, G) = \emptyset$ and ii) $W$ blocks all non-causal paths from $X$ to $Y$.

Example A.1 (Linear structural equation model, causal nodes and forbidden nodes). Consider the graph $G_1$ from Fig. 4a. Then the following generating mechanism is an example of a linear structural
A continuous function in $\Sigma$ by continuity. Finally, $(\text{Id}_\Sigma G)$ is invertible as a strictly diagonally dominant matrix. Let $A, B, C \in \mathbb{R}$ be mean random vectors with finite variance, with $C$ possibly of length zero. Then

$$\Sigma_{aa, bc} = \Sigma_{aa, b} - \beta_{ac, b} \Sigma_{cc, b} \beta_{ac, b}^T.$$\n
Lemma A.3. (e.g. [Henckel et al., 2022]) Let $A, B, C$ and $D$ be mean $0$ random vectors with finite variance, with $C$ possibly of length zero. Then

$$\beta_{ab, c} = \beta_{ab, cd} + \beta_{ad, bc} \beta_{bc, d}.$$\n
Lemma A.4. (Wermuth [1989]) Let $A, B, C$ and $D$ be mean $0$ random vectors with finite variance, with $C$ possibly of length zero. If $B \not\perp D \mid C$ or $A \not\perp D \mid B, C$, then $\beta_{ab, c} = \beta_{ab, cd}$. Furthermore, if $A \not\perp D \mid B, C$, then $\Sigma_{aa, bc} = \Sigma_{aa, bc}$.\n
Lemma A.5. Consider an acyclic directed mixed graph $G = (V, E)$ and let $(A, \Omega)$ be a Gaussian linear structural equation model compatible with $G$ with $\Omega$ a strictly diagonally dominant matrix. Let $F \subseteq E$ and let $(A_F(e), \Omega_F(e))$ denote the Gaussian linear structural equation model $(A, \Omega)$ where the edge coefficients and error covariances corresponding to the edges in $F$ replaced with some value $\epsilon > 0$. Then

$$\lim_{\epsilon \to 0} \Sigma_{ab, c}(A_F(e), \Omega_F(e)) = \Sigma_{ab, c}(A_F(0), \Omega_F(0))$$

for any $A, B, C \subseteq V$.\n
Proof. The proof is based on the fact that as continuous functions in $\epsilon$, $\lim_{\epsilon \to 0} A_F(e) = A_F(0)$ and $\lim_{\epsilon \to 0} \Omega_F(e) = \Omega_F(0)$, and as we will show, $\Sigma_{ab, c}(\Omega_F(e), A_F(e))$ is a continuous function at $(A_F(0), \Omega_F(0))$. We show this in two steps by first showing that $\Sigma_{uv}(\Omega_F(e), A_F(e))$ is a continuous function at $(A_F(0), \Omega_F(0))$ and second showing that $\Sigma_{ab, c}(\Sigma_{uv})$ is a continuous function at $(A_F(0), \Omega_F(0))$.

Regarding the first step,

$$\Sigma_{uv}(A, \Omega) = (\text{Id} - A)^{-T} \Omega (\text{Id} - A)^{-1}$$

is a continuous function in $\Omega$ and $(\text{Id} - A)^{-1}$. It therefore remains to check that $(\text{Id} - A_F(0))$ is invertible to show it is continuous at $(A_F(0), \Omega_F(0))$. To see this note that $(A_F(0), \Omega_F(0))$ is compatible with the graph $G'$, which is the graph $G$ with the edges in $F$ removed. As $G$ is acyclic, so is $G'$ and as a result $(\text{Id} - A_F(0))$ is invertible. Therefore,

$$\lim_{\epsilon \to 0} \Sigma_{uv}(\Omega_F(e), A_F(e)) = \lim_{\epsilon \to 0} (\text{Id} - A_F(e))^{-T} \Omega_F(e)(\text{Id} - A_F(e))^{-1}$$

$$= \lim_{\epsilon \to 0} (\text{Id} - A_F(e))^{-T} \Omega_F(e) \lim_{\epsilon \to 0}(\text{Id} - A_F(e))^{-1}$$

$$= (\text{Id} - A_F(0))^{-T} \Omega_F(0)(\text{Id} - A_F(0))^{-1}$$

by continuity. Finally,

$$\Sigma_{ab, c}(\Sigma_{uv}) = \Sigma_{ab} - \Sigma_{ac} \Sigma_{bc}^{-1} \Sigma_{cb}$$

is a continuous function at $\Sigma_{uv}(A_F(0), \Omega_F(0))$ by the fact that since $\Omega_F(0)$ is invertible as a strictly diagonally dominant matrix by the Levy-Desplques theorem, so is $\Sigma_{uv}(A_F(0), \Omega_F(0))$.
\textbf{B Proofs for Section 3}

\textbf{Theorem B.1.} Consider disjoint nodes X and Y, and node sets Z and W in an acyclic directed graph \( G = (V, E) \). Then \( \{Z, W\} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G \) if and only if (i) \( Z \cup W \) \( \cap \) \( \text{forb}(X, Y, G) = \emptyset \), (ii) \( Z \not \subseteq X \mid W \) and (iii) \( Z \perp \perp Y \mid W \), where the graph \( \tilde{G} \) is \( G \) with all edges out of X on causal paths from X to Y removed.

\textit{Proof.} \( \implies \) : We first show directly that under the three conditions, \( \hat{\gamma}_{yz, t} \) consistently estimates \( \gamma_{yz} \) for any linear structural equation model compatible with \( G \) such that \( \Sigma_{yz, w} \neq 0 \). By the fact that \( Z \perp \perp X \mid W \) there exist linear structural equation model compatible with \( G \), such that \( \Sigma_{yz, w} \neq 0 \), so consider such a model and let \( S = (X, W) \) and \( T = (Z, W) \). Consider the whole vector valued two-stage least squares estimator \( \hat{\gamma}_{yz, t} \), whose first entry defines our estimator \( \hat{\gamma}_{yz} \). Let \( \gamma = (\gamma_{yz}, \beta_{gw}) \), with \( \bar{Y} = Y - \gamma_{yz}X \) and let \( \epsilon = Y - \gamma S \). Then

\[
\hat{\gamma}_{yz, t} - \gamma = Y_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n \{S_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n \}^{-1} - \gamma = \epsilon_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n \{S_n^T T_n (T_n^T T_n)^{-1} T_n^T S_n \}^{-1} \frac{1}{n} S_n^T T_n (T_n^T T_n)^{-1} \frac{1}{n} T_n^T \epsilon_n,
\]

where \( S_n, T_n \) and \( \epsilon_n \) are the random matrices corresponding to taking \( n \) i.i.d. observations from \( S, T \) and \( \epsilon \), respectively. By assumption \( \Sigma_{yz, w} \neq 0 \) and we can therefore conclude with Lemma B.3 that \( \Sigma_{yt} \Sigma_{tz}^{-1} \Sigma_{zw} \) is invertible. With the continuous mapping theorem it follows that the limit in probability of \( (\hat{\gamma} - \gamma) \) is \( \Sigma_{yt} \Sigma_{tz}^{-1} \Sigma_{zw} \) by Lemma B.5 and it therefore follows that \( \hat{\gamma}_{yz} \) converges in probability to \( \gamma \) which implies that \( \hat{\gamma}_{yz, t} \) converges to \( \gamma_{yz} \).

Consider first \( \Sigma_{ew} \). Clearly, \( \Sigma_{ez} = \text{cov}(Y - \gamma S, Z) = \text{cov}(Y - \gamma S, W, W) = 0 \) by the fact that \( \beta_{gw} = \Sigma_{gw} \Sigma_{zw}^{-1} \). Consider now \( \Sigma_{ez} = \text{cov}(Y - \gamma_{yz}X - \beta_{gw}W, Z) = \sigma_{gz} - \beta_{gw} \sigma_{zw} = \sigma_{gz, w} \). It therefore suffices to show that \( Y \perp \perp Z \mid W \) to conclude that \( \Sigma_{ez} = 0 \). By condition (i), \( (Z \cup W) \cap \text{forb}(X, Y, G) = \emptyset \) and therefore \( Z \) and \( W \) are also nodes in the latent projection graph \( G^F \) over \( F = \text{forb}(X, Y, G) \setminus \{X, Y\} \), so we can without loss of generality consider the smaller linear structural equation model compatible with \( G^F \) instead. We can apply Lemma B.3 to this model where we use that since Condition (iii) holds for \( G \) it also holds for \( G^F \) by Lemma B.5 and it therefore follows that \( Y \perp \perp Z \mid W \).

\( \iff \) : By our definition of a conditional instrumental set, Condition (i) is trivially required and ensures that there exists a linear structural equation model compatible with \( G \) such that \( \Sigma_{xz, w} \neq 0 \). We now show that if either of the other two conditions are violated there exists a linear structural equation model compatible with \( G \) such that \( \Sigma_{xz, w} \neq 0 \) and for which \( \hat{\gamma}_{yz, t} \) does not consistently estimate \( \gamma_{yz} \).

By the same argument as given at the beginning of the proof for the \( \iff \) case, \( \Sigma_{yz, w} \neq 0 \) suffices to conclude that the estimator \( \hat{\gamma}_{yz, t} \) converges to some unique limit \( \gamma \), that is characterized by the fact that \( \Sigma_{zt} = 0 \) with \( \epsilon = Y - \gamma S \). We now show that this limit vector \( \gamma \) cannot have \( \gamma_{yz} \) as the first entry if either Condition (i) or (iii) are violated by contradiction. So assume that the first entry of \( \gamma \) is \( \gamma_{yz} \).

We have shown already that if the first entry of \( \gamma \) is \( \gamma_{yz} \) then the remaining entries have to form the vector \( \beta_{gw} \) as otherwise \( \Sigma_{ew} \neq 0 \). This implies, as shown above, that \( \Sigma_{ew} = 0 \) corresponds to \( \Sigma_{gz, w} = 0 \). It therefore suffices to show that \( Y \perp \perp Z \mid W \) for some Gaussian linear structural equation model compatible with \( \Sigma_{xz, w} = 0 \) to show that \( \Sigma_{ew} \neq 0 \). If Condition (i) is violated such a model exists by Lemma B.5. If Condition (i) is not violated but Condition (ii) holds we can construct again the graph \( G^F \). By Lemma B.3 Condition (ii) being violated for \( G \) implies that \( Y \not \subseteq G^F \) \( Z \mid W \). Therefore, we can invoke Lemma B.4 to conclude that there exists a Gaussian linear structural equation model such that \( \Sigma_{gz, w} \neq 0 \) in this case as well.

\( \square \)

\textbf{Lemma B.2.} Consider two random variables X and Y, and two random vectors Z and W. Let \( S = (X, W) \) and \( T = (Z, W) \). Then \( \Sigma_{st} \Sigma_{tt}^{-1} \Sigma_{sz} \) is invertible if and only if only if \( \Sigma_{sz, w} \neq 0 \).
Proof. Using $\beta_{st} = \Sigma_{st}\Sigma_{tt}^{-1}$ it follows that $\Sigma_{st}\Sigma_{tt}^{-1}\Sigma_{tt} = \beta_{st}\Sigma_{tt}\beta_{tt}^\top$. As $S = (X, W)$ and $T = (Z, W)$ it follows that
\[
\beta_{st} = \begin{bmatrix} \beta_{xz,w} & \beta_{yw,z} \\ 0 & Id \end{bmatrix}.
\]
Here we use that $\beta_{nn,v} = \Sigma_{nn} = 1$ and $\beta_{nw,v} = 0$ for any random variable $N$ and random vector $V$, as $N \perp V | N$ and $\Sigma_{NN}\Sigma_{NN}^{-1} = 1$. As $\beta_{zw} = \Sigma_{xz,w}\Sigma_{zw,w}^{-1}$, it follows that $\beta_{zw}$ is of maximal rank if and only if $\Sigma_{xz,w} \neq 0$. As $\Sigma_{tt}$ is a positive-definite matrix, $\beta_{st}\Sigma_{tt}\beta_{tt}^\top$ is positive definite if and only if $\beta_{st}$ has maximal rank by standard properties of positive definiteness.

\[\boxempty\]

Lemma B.3. Let $X$ and $Y$ be nodes and $Z$ and $W$ node sets in an acyclic directed mixed graph $G$, such that $(Z \cup W) \cap \text{forb}(X, Y, G) \neq \emptyset$ and $X \not\text{ind} Z \mid W$. Then there exists a linear structural equation model compatible with $G$, such that
\[
\tilde{Y} \perp Z \mid W,
\]
where $\tilde{Y} = Y - \tau_{yz} X$.

Proof. As the statement is trivial for $\text{forb}(X, Y, G) = \emptyset$, we can assume that $Y \in \text{do}(X, G)$. We will now construct a Gaussian linear structural equation model in which $\beta_{yz,w} \neq 0$. This suffices to prove our claim since $\beta_{yz,w} \neq 0$ if and only if $\Sigma_{yz,w} \neq 0$ and we consider Gaussian linear structural equation models. To do so we first derive an equation for $\beta_{yz,w}$ that does not depend on $\tilde{Y}$.

Consider a Gaussian linear structural equation model compatible with $G$. We augment $G$ as well as the underlying linear structural equation model by adding $\tilde{Y}$ to $V$ as well as the edges $X \rightarrow \tilde{Y}$ and $Y \rightarrow \tilde{Y}$ with edge coefficients $-\tau_{yz}$ and 1, respectively, to $E$. We denote the augmented graph with $G'$. Clearly the augmented model is still a linear structural equation model. In particular
\[
\begin{align*}
(i) & \quad \beta_{yz,w} = \beta_{yz,xw} + \beta_{yz,zw}\beta_{xz,w}, \\
(ii) & \quad \beta_{yz,xw} = \beta_{yz,xw} + \beta_{yy,zw}\beta_{yz,xw} = \beta_{yz,xw} \quad \text{and} \\
(iii) & \quad \beta_{yz,zw} = \beta_{yz,yzw} + \beta_{yy,zw}\beta_{yz,zw} = -\tau_{yz} + \beta_{yz,zw},
\end{align*}
\]
where we use that $\text{pa}(\tilde{Y}, G') = \{X, Y\}, \text{do}(\tilde{Y}, G') = \{\tilde{Y}\}$ and that as a result $Z \cup W$ is an adjustment set relative to $\{(X, Y), \tilde{Y}\}$ since there are no forbidden nodes and no non-causal paths. We now show that there exists a linear structural equation model compatible with $G'$, such that
\[
\beta_{yz,w} = \beta_{yz,xw} + (\beta_{yx,zw} - \tau_{yz})\beta_{xz,w} \neq 0,
\]
where we consider $G$ again, as our new expression for $\beta_{yz,w}$ does not depend on $\tilde{Y}$ directly. Let $p$ be a proper path from $Z$ to $X$ open given $W$. Such a path exists by assumption. If $p$ contains colliders $C_1, \ldots, C_h$, such that $\text{do}(C, G) \cap W \neq \emptyset$ let $q_1, \ldots, q_k$ be the corresponding causal paths from $C_1, \ldots, C_h$ to $W$, respectively. If any of the $q_i$ paths contain $X$, replace $p$ with $p(Z, C_i) \oplus q_i(C_i, X)$ for the smallest such $i$ and if $p$ and $q_i$ intersect at another node $I$ but $C_i$ replace $p$ with $p(Z, C_i) \oplus q_i(C_i, I) \oplus p(I, X)$, ensuring that $p$ and the $q_i$'s only intersect at the $C_i$'s. Set all edge coefficients and error covariances not corresponding to edges either on $p, q_1, \ldots, q_k$ or on causal paths from $X$ to nodes in $\text{forb}(X, Y, G)$ to 0. Consider the graph $G''$ with the 0 coefficient edges dropped and all other edge coefficients and error covariances set to a positive value to ensure faithfulness. Note that $\text{forb}(X, Y, \text{G''}) = \text{forb}(X, Y, G)$, there exists at most one edge (stemming from $p$) into $X$ in $G''$ and $p$ is also open given $W$ in $G''$.

Suppose there exists a path from $Z$ to $Y$ in $G''$ that is open given $W$ and that does not contain $X$. We will show that there then exists a walk from $Z$ to $Y$ open given $W$ that does not contain $X$. We first show by contraposition that for any collider $C$ on $k$, $X \notin \text{do}(C, G'')$, irrespective of whether $k$ is open or not. So suppose there exists a collider $C$ such that $X \in \text{do}(C, G'')$ and consider the causal path $k'$ from $C$ to $X$. the path $k'$ consists of nodes in $\text{an}(X, G)$ and therefore must consist of edges on $p$ and the $q_i$‘s by construction of $G''$. As it ends with an edge into $X$, the only possible such edge in $G''$ lies specifically on $p$. Further the node adjacent to $X$ may not be a collider on $p$ and hence may not
lie on any of the paths $q_i$. Therefore the next edge on $k'$ is also on $p$. By iterative application we can conclude the same for all other edges on $k'$ and thus $k'$ is a subsegment of $p$. But the same argument holds for the two edges into $C$ on $k$, but as $p$ is a path it cannot contain three edges adjacent to $C$ and we get a contradiction. Therefore we have $X \notin \text{de}(C, \mathcal{G})$ for any collider $C$ on $k$ but as $k$ is open given $W$ we do have $W \cap \text{de}(C, \mathcal{G}'''') \neq \emptyset$ for any collider $C$. Adding the causal paths from any collider $C$ to the node in $W$ and back we obtain a walk in $\mathcal{G}'''$ from $Z$ to $Y$ that is open given $W$ and that does not contain $X$. If a walk from $Z$ to $Y$ that is open given $W$ and that does not contain $X$ exists we are done by the fact that all three terms $\beta_{yz.zw}, \tau_{yx}$ and $\beta_{zx.zw}$ depend only on walks that begin or end in $X$ and our model is faithful to $\mathcal{G}'''$. If for example we set all edge coefficients and error covariances for the edges adjacent to $X$ to some value $\epsilon > 0$ in a Gaussian linear structural equation model $(A, \Omega)$ compatible with $\mathcal{G}'''$ that has a diagonally dominant $\Omega$, then as $\epsilon$ goes to 0 so do $\beta_{yz.zw}$ and $\beta_{zx.zw}$ by Lemma A.5 and $\tau_{yx}$ by Wright’s path tracing rule. This is not the case for $\beta_{yz.zw}$ as by the walk we assume to exist, $Y \notin \mathcal{G}'''$ $Z \mid W$, where $\mathcal{G}'''$ is the graph $\mathcal{G}'''$ with the edges adjacent to $X$ dropped.

Therefore, we can suppose that all paths from $Z$ to $Y$ that are open given $W$ contain $X$. As $X$ must be a non-collider on any such path by nature of $\mathcal{G}'''$ all such paths are therefore blocked given $W$ and $X$. Further, by the fact that $X \notin \text{de}(C, \mathcal{G}'''')$ for all colliders $C$ on any path from $Z$ to $Y$, the addition of $X$ to the conditioning set also does not open any new paths. It thus follows that $Z \perp_{\mathcal{G}''''} Y \mid \{X\} \cup W$ and we can conclude that $\beta_{yz.zw} = 0$. By the assumption that $Y \in \text{de}(X, \mathcal{G}'''')$ as well as the existence of $p$, $\tau_{yx} \neq 0$ and $\beta_{zx.zw} \neq 0$. But $\beta_{yz.zw} = \tau_{yx}$ for all distribution compatible with $\mathcal{G}'''$ if and only if $W \cup Z$ is an adjustment set relative to $(X, Y')$ in $\mathcal{G}'''$ (see Perkovic et al. [2018]). But as $(W \cup Z) \cap \text{forbi}(X, Y, \mathcal{G}'''') \neq \emptyset$ this is not the case and we can conclude that there exists a distribution such that $\beta_{yz.zw} \neq 0$. \hfill $\square$

Lemma B.4. Consider two nodes $X$ and $Y$, and two node sets $Z$ and $W$ in an acyclic directed mixed graph $\mathcal{G} = (V, E)$ such that $\text{de}(X, \mathcal{G}) \subseteq \{X, Y\}$ and $V$ is generated from a linear structural equation model compatible with $\mathcal{G}$. Let $\mathcal{G}' = Y \sim \tau_{yx}.X$. Then $Z \perp_{\mathcal{G}'} Y \mid W$ implies $Z \perp_{\mathcal{G}} Y \mid W$, where $\mathcal{G}$ is the graph $\mathcal{G}$ with the edge $X \rightarrow Y$ removed. Further, if $Z \notin \mathcal{G}' Y \mid W$ there exists a Gaussian linear structural equation model compatible with $\mathcal{G}$ such that $Z \perp_{\mathcal{G}} Y \mid W$.

Proof. Consider first the special case that $Y \notin \text{de}(X, \mathcal{G})$. In this case $\mathcal{G}' = Y$ and $\mathcal{G} = \mathcal{G}$. Therefore the claims follow from the fact that linear structural equation model is compatible to the graph it is generated according to and that linear structural equation models with all positive coefficients are faithful to their graph by Wright’s path tracing rules.

Suppose for the remainder of the proof that $\text{de}(X, \mathcal{G}) = \{X, Y\}$. We first prove that $Z \perp_{\mathcal{G}} Y \mid W$ implies $Z \perp_{\mathcal{G}'} Y \mid W$. By the assumption $\text{de}(X, \mathcal{G}) = \{X, Y\}$,

\[ \mathcal{G}' = \sum_{\forall i \in \text{pa}(Y, \mathcal{G})} \alpha_{yi} V_i + \epsilon_Y - \tau_{yx} X = \sum_{\forall i \in \text{pa}(Y, \mathcal{G})} \alpha_{yi} V_i + \epsilon_Y, \]

as $\tau_{yx} = \alpha_{yx}$ and $\text{pa}(Y, \mathcal{G}) = \{X\} \cup \text{pa}(Y, \mathcal{G})$, where we use that the only causal path between $X$ and $Y$ is the edge $X \rightarrow Y$ and Wright’s path tracing rule. As $\text{de}(Y, \mathcal{G}) = \{Y\}$ this suffices to show that the distribution of $\tau_{yx}$, which is $V$ with $Y$ replaced by $\mathcal{G}'$, is generated according to a linear structural equation model compatible with $\mathcal{G}$. By the fact that linear structural equation models are Markov with respect to the graphs they are generated according to, the claim follows.

Regarding the second claim, consider a Gaussian linear structural equation model with all positive edge coefficients compatible with $\mathcal{G}$. Then the linear structural equation model compatible with $\mathcal{G}$ we construct also has all positive edge coefficients and is therefore faithful to $\mathcal{G}$. Thus, $Z \notin \mathcal{G} Y \mid W$ implies $Z \perp_{\mathcal{G}} Y \mid W$. \hfill $\square$

Lemma B.5. Consider disjoint nodes $X$ and $Y$ in an acyclic directed mixed graph $\mathcal{G}$. Let $F = \text{forbi}(X, Y, \mathcal{G}) \setminus \{X, Y\}$ and let $\mathcal{G}$ denote the graph $\mathcal{G}$ with all edges out of $X$ on causal paths from $X$ to $Y$ removed. Further let $\mathcal{G}' = \mathcal{G} F$ be the graph $\mathcal{G} F$ with the edge $X \rightarrow Y$ removed. Then $\mathcal{G}'$ and $\mathcal{G} F$ are the same graph.

Proof. Clearly, $\mathcal{G}'$ and $\mathcal{G} F$ contain the same nodes. We will now show that $\mathcal{G}'$ and $\mathcal{G} F$ also contain the same edges.
Assume first that \( Y \notin \text{de}(X, G) \). Then \( \text{forb}(X, Y, G) = \emptyset \) and there are also no edges to remove. Therefore, both \( \tilde{G}^F \) and \( G^F \) are equal to \( G \).

Assume now that \( Y \in \text{de}(X, G) \) and consider any edge \( e \) in \( G^F \). If \( e \) is an edge in \( G \), then it has to be an edge between two nodes not in \( F \). As a result it is not removed in the pruning step forming \( \tilde{G} \) unless it is the edge \( X \rightarrow Y \) or in the latent projection step forming \( G^F \) from \( G \). Therefore, \( e \) is also an edge in \( G^F \) unless it is the edge \( X \rightarrow Y \). If \( e \) is not an edge in \( \tilde{G} \) then it has to correspond to a path \( p \) in \( G \) of the form \( V_i \rightarrow \cdots \rightarrow V_j, V_i \leftarrow \cdots \rightarrow V_j \) or \( V_i \leftarrow \cdots \rightarrow V_j \), such that all nodes but \( V_i \) and \( V_j \) are in \( F \). If \( p \) contains none of the edges removed in the construction of \( \tilde{G} \) it will clearly be mapped to the same edge \( e \) in \( G^F \) it corresponds to in \( G^F \). If it does contain such an edge then edge has to be without loss of generality the first edge on \( p \) as \( X \notin F \). Therefore, we can assume that \( V_i = X \) and that the first edge on \( p \) is of the form \( \rightarrow \). As the only node in \( \text{de}(X, G) \) that is not in \( F \) is \( Y \) it follows that \( p \) in fact has to be of the form \( X \rightarrow \cdots \rightarrow Y \). Therefore \( p \) will be mapped to the edge \( X \rightarrow Y \) in \( G^F \), that is \( e \) is the edge \( X \rightarrow Y \). As the edge \( X \rightarrow Y \), if it exists, is itself removed in \( \tilde{G} \) we can therefore conclude that \( G^F \) cannot contain the edge \( X \rightarrow Y \) and that this is the only edge in which it may differ from \( G^F \). We can thus conclude that \( G^F = \tilde{G}^F \).

\( \square \)

B.1 Proof of Proposition 3.3

**Proposition B.6.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( G \) and let \( F = \text{forb}(X, Y, G) \setminus \{X, Y\} \). Then \( \{Z, W\} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( G \) if and only if it is a valid conditional instrumental set relative to \( (X, Y) \) in \( G^F \).

**Proof.** \( \implies \) : Suppose that \( \{Z, W\} \) is a valid conditional instrument set in \( G \). Then \( \{Z \cup W\} \cap \text{forb}(X, Y, G) = \emptyset \) and therefore both \( Z \) and \( W \) are also node sets in \( G^F \). As \( \text{forb}(X, Y, G^F) = \{X, Y\} \) it also follows that \( \{Z \cup W\} \cap \text{forb}(X, Y, G^F) = \emptyset \). Further, \( Z \not\perp_{G^F} X \mid W \) implies that \( Z \not\perp_{G^F} X \mid W \) by the fact that the latent projection preserves all m-separation statements among node sets disjoint with \( F \). Finally, by Lemma B.5, \( G^F \) is a latent projection graph of the graph \( G \) from Theorem 3.2. Therefore, \( Z \perp_{\tilde{G}} Y \mid W \) by the same m-separation argument.

\( \iff \) : Suppose that \( \{Z, W\} \) is a valid conditional instrument set in \( G^F \). As \( Z \) and \( W \) are node sets in \( G^F \) which do not contain \( X \) or \( Y \), it follows that \( \{Z \cup W\} \cap \text{forb}(X, Y, G) = \emptyset \). The other two properties follow again by the fact that the latent projection preserves m-separation statements.

\( \square \)

B.2 Proof of Proposition 3.4

**Proposition B.7.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( G \) and let \( \{Z, W\} \) be a valid conditional instrumental set relative to \( (X, Y) \) in \( G \). If \( \{Z \cup W\} \cap \text{de}(X, G) = \emptyset \), then \( W \) is a valid adjustment set relative to \( (X, Y) \) in \( G \).

**Proof.** We will prove our claim by contradiction. So consider a valid tuple \( \{Z, W\} \) such that \( \{Z \cup W\} \cap \text{de}(X, G) = \emptyset \) and suppose that there exists a non-causal path \( p \) from \( X \) to \( Y \) that is open given \( W \). We will now construct a path \( q \) from \( Z \) to \( Y \) that is open given \( W \) in \( \tilde{G} \), where \( G \) is the graph obtained by deleting all the first edges out of \( X \) on causal paths from \( X \) to \( Y \) in \( G \).

We first note that as a non-causal path from \( X \) to \( Y \), \( p \) is also a path in \( \tilde{G} \). Further, consider any node \( N \) in \( G \) and any node \( M \) in the set \( \text{de}(N, G) \setminus \text{de}(N, \tilde{G}) \). By assumption there exists a causal path from \( N \) to \( M \) in \( G \) but not in \( \tilde{G} \). Therefore, any such causal path needs to contain an edge of the form \( X \rightarrow C \) with \( C \in \text{cn}(X, Y, G) \). Therefore, \( M \in \text{forb}(X, Y, G) \). It follows that for any node \( N \) that if \( W \cap \text{de}(N, G) = \emptyset \) it also holds that \( W \cap \text{de}(N, \tilde{G}) = \emptyset \). We can therefore conclude that \( p \) is also open given \( W \) in \( \tilde{G} \).

Suppose now that \( Z \cap \text{de}(X, G) \neq \emptyset \) and let \( A \in Z \cap \text{de}(X, G) \). By the assumption that \( A \in \text{de}(X, G) \) there exists a directed path \( p' \) from \( X \) to \( A \). As \( \{Z, W\} \) is a valid tuple, \( \{Z \cup W\} \cap \text{forb}(X, Y, G) = \emptyset \) and therefore \( p' \) is not a subpath of a causal path from \( X \) to \( Y \) in \( G \). Therefore it is also a path in \( \tilde{G} \). We first suppose that \( p' \) is open given \( W \) in \( \tilde{G} \). Let \( I \) be the first node on \( -p' \) that is also on \( p \) and consider \( q = -p'(Z, I) \oplus p(I, Y) \), where \( -p' \) denotes the reversed path \( p \) that goes from \( A \) to \( X \). As \( p' \) is open given \( W \) as well as a directed path, it follows that \( I \notin W \) and \( I \) may not be a
collider on \( q \). Hence, \( q \) is a path from \( A \) to \( Y \) that is open given \( W \) in \( \mathcal{G} \) and thus \( \{ Z, W \} \) is not a valid conditional instrumental set.

Now suppose that \( p' \) is not open given \( W \), i.e. it contains at least one node \( B \), such that \( B \in W \cap \text{de}(X, \mathcal{G}) \). Therefore this case reduces to the case that there exists a node \( B \in W \cap \text{de}(X, \mathcal{G}) \), which we will now consider. By the assumption that \( \{ Z, W \} \) is a valid conditional instrumental set, there exists a path \( p'' \) from some node \( A' \in \mathcal{G} \) to \( X \) open given \( W \). As \( (Z \cup W) \cap \text{forb}(X, Y, \mathcal{G}) = \emptyset \), \( p'' \) must be a path in \( \mathcal{G} \) as it would otherwise contain a collider that is in \( \text{forb}(X, Y, \mathcal{G}) \), contradicting our assumption that it is open given \( W \). Let \( I \) be the node closest to \( A' \) on \( p'' \) that is also on \( p \) and consider \( q = p''(A', I) \oplus p(I, Y) \). If \( I \) is a non-collider on \( q \) and \( I \notin W \) we are done. Suppose that \( I \) is a non-collider on \( q \) and \( I \in W \). But then \( I \) must be a non-collider on \( p \) contradicting our assumptions. Suppose now that \( I \) is a collider on \( q \). As \( p'' \) is open given \( W \) this implies that either \( W \cap \text{de}(I, \mathcal{G}) \neq \emptyset \) or \( p''(I, X) \) is directed towards \( X \), by the fact that there exists a node \( B \in W \cap \text{de}(X, \mathcal{G}) \) in turn implies that \( W \cap \text{de}(I, \mathcal{G}) \neq \emptyset \). Thus, \( q \) is open given \( W \), yielding a contradiction.

In the special cases where \( I = Y \) or \( I = X, q \) is a subpath of \( p'' \), respectively \( p \) and our claim trivially follows. Finally, in the special case that \( I \in Z \), \( p(I, Y) \) is an open path between \( Z \) and \( Y \) given \( W \) in \( \mathcal{G} \).

\[ \square \]

C Proofs for Section 4

C.1 Proof of Theorem 4.1

**Theorem C.1.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( \mathcal{G} \) such that \( \text{de}(X, \mathcal{G}) = \{X, Y\} \). Let \( \{Z, W\} \) be a valid conditional instrumental set relative to \( (X, Y) \) in \( \mathcal{G} \) and \( Y = Y - \gamma_{yx} X \). Then for all linear structural equation models compatible with \( \mathcal{G} \) such that \( \Sigma_{x.z} \neq 0 \), \( \widehat{\tau}_{yx} \) is an asymptotically normal estimator of \( \tau_{yx} \) with asymptotic variance

\[
\text{a.var}(\widehat{\tau}_{yx}) = \frac{\sigma_{\gamma y.w}}{\sigma_{x.z} - \sigma_{x.z.w}}.
\]  

(5)

**Proof.** By Theorem 3.2 \( \widehat{\tau}_{yx} \) is a consistent estimator of the total effect \( \tau_{yx} \). By Lemma C.2 it is an asymptotically normal estimator with asymptotic variance

\[
E[(\delta_{x,w} - \delta_{x,z.w})^2 \kappa_{y,t}^2] = \frac{E[(\delta_{x,w} - \delta_{x,z.w})^2 \kappa_{y,t}^2]}{E[(\delta_{x,w} - \delta_{x,z.w})^2]^2},
\]

with \( \delta_{x,w} = X - \beta z \), \( \delta_{x,z.w} = X - \beta z W - \beta z Z \) and \( \kappa_{y,t} = Y - \gamma_{y,t} S \), where \( S = (X, W) \) and \( T = (Z, W) \). Here, \( \gamma_{y,t} \) denotes the vector of regression coefficients for the two-stage least square regression of which \( \gamma_{y,t} \) is the entry corresponding to \( X \). By Lemma C.3 \( \kappa_{y,t} = (\delta_{x,w} - \delta_{x,z.w}) \perp \kappa_{y,t} \) and as a result the asymptotic variance simplifies to

\[
E[\kappa_{y,t}^2] = \frac{E[(\delta_{x,w} - \delta_{x,z.w})^2]}{E[(\delta_{x,w} - \delta_{x,z.w})^2]^2}.
\]

By Lemma C.6 \( E[(\delta_{x,w} - \delta_{x,z.w})^2] = \sigma_{x,z.w} - \sigma_{x,z.w} \). Lastly, we have shown in the proof of Theorem 3.2 that \( \gamma_{y,t} = (\gamma_{yx}, \beta y.w) \), where \( \gamma_{yx} \). Therefore, \( E[\kappa_{y,t}^2] = E[\delta_{y.w}^2] = \sigma_{\gamma y.w} \), where \( \delta_{y.w} = Y - \beta y.w \).

\[ \square \]

**Lemma C.2.** Consider two random variables \( X \) and \( Y \), and two random vectors \( Z \) and \( W \). Suppose that \( (X, Y, Z, W) \) has mean 0 and finite variance, and that \( \Sigma_{x.z} \neq 0 \). Let \( S = (X, W) \) and \( T = (Z, W) \) and consider the two-stage least squares estimator of \( Y \) on \( X \) using the tuple \( \{Z, W\} \), denoted \( \gamma_{yx} \). Then \( \gamma_{yx} \) converges in probability to some limit \( \gamma_{yx} \) and \( n^{1/2}(\gamma_{yx} - \gamma_{yx} \) converges in distribution to a normally distributed random variable with mean 0 and variance

\[
E[(\delta_{x,w} - \delta_{x,z.w})^2 \kappa_{y,t}^2] = \frac{E[(\delta_{x,w} - \delta_{x,z.w})^2 \kappa_{y,t}^2]}{E[(\delta_{x,w} - \delta_{x,z.w})^2]^2},
\]

with \( \delta_{x,w} = X - \beta z \), \( \delta_{x,z.w} = X - \beta z W - \beta z Z \) and \( \kappa_{y,t} = Y - \gamma_{y,t} S \). Here, \( \gamma_{y,t} \) denotes the vector of regression coefficients for the two-stage least square regression.
Lemma C.3. Consider nodes $X$ and $W$, with $Y = \beta_{xt}T$ the fitted value from the first stage regression of $X$ on $T$. We can apply Corollary 11.1 from Buja et al. (2014) to this regression and obtain that $n^{1/2}(\hat{\gamma}_{px} - \gamma_{px})$ converges in distribution to a normally distributed random variable with variance 

$$E[\delta_{x,w}^2] \quad E[\hat{\delta}_{x,w}^2]^2,$$

where $\delta_{x,w} = X - \beta_{xw}W$. Further, as $X = X - (X - \beta_{xt}T) = X - \delta_{x,zw}$ it follows that

$$\delta_{x,w} = \hat{X} - \beta_{xw}W = X - \beta_{xw}W - \delta_{x,zw} = \delta_{x,w} - \delta_{x,zw},$$

concluding our proof.

The following two lemmas, which are adaptations of Lemma B.3 and B.4 of Henckel et al. (2022), respectively, rely on the insight that we can rewrite any population level residual in a linear structural equation model as a linear function in the errors $\epsilon$ of the underlying model. For example, given node sets $A$ and $B$ in an acyclic directed mixed graph $G = (V, E)$, such that $V$ is generated from a linear structural equation model,

$$A = \beta_{ab}B = \sum_{W \in V} \tau_{aw} \epsilon_w = \sum_{Z \in B} \left( \beta_{az.b} \sum_{W \in V} \tau_{zw} \epsilon_w \right),$$

where $B = B \setminus \{Z\}$.

Lemma C.3. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G = (V, E)$, such that $V$ is generated from a linear structural equation model compatible with $G$ and $\text{cl}(X, G) = \{X, Y\}$. Let $\{Z, W\}$ be a valid conditional instrumental set relative to $(X, Y)$ in $G$. Then the random variables $\delta_{x,w} - \delta_{x,zw}$ and $\delta_{y,w}$ are independent.

Proof. Our proof relies extensively on Lemma C.4 and is closely related to the proof of Lemma B.3 in Henckel et al. (2022). For every node $A \in V$ in a linear structural equation model $V$ it holds that

$$A = \sum_{b \in V} \tau_{ab} \epsilon_b.$$
By Lemma C.4 it follows that there exists a path $p_1$ from some node $A \in Z$ to $M$ in $\mathcal{G}$ that is open given $W$ and whose last edge points into $M$. In addition, there also exists a path $p_2$ from $M$ to $Y$ in $\mathcal{G}$ that is open given $W$ and whose first edge points into $M$. Let $I$ be the first node on $p_1$ that also lies on $p_2$ and consider the path $q = p_1(I, A) \cup p_2(I, Y)$. We will now show that $q$ is open given $W$. If $I = A$ or $I = Y$, $q$ is a subpath of either $p_1$ or $p_2$ and therefore open given $W$. If $I = M$, $q$ is open as $M \in W$ is a collider on $q$. Suppose now that $I \notin \{A, Y, M\}$ is a non-collider on $q$. Then $I$ may not be a collider on both $p_1$ and $p_2$. Since both $p_1$ and $p_2$ are open given $W$ it therefore follows that $I \notin W$ and therefore $q$ is open given $W$. Suppose now that $I \notin \{A, Y, M\}$ is a collider on $q$. If $I$ is also a collider on either $p_1$ or $p_2$ it follows that $I \in W$ and we are done. If $I$ is not a collider on either $p_1$ or $p_2$, then $p_1$ either of the form $A \cdots \rightarrow I \rightarrow \cdots M$ or $A \cdots \leftrightarrow I \rightarrow \cdots M$. As $p_1(I, M)$ is open given $W$ and $M \in W$ it follows that $\text{de}(I, \tilde{G}) \cap W \neq \emptyset$ and therefore $q$ is open given $W$.

Suppose now that $M \notin W$. Consider first the case $M = Y$. As $Y \notin W$ and $\text{de}(Y, \mathcal{G}) = \{Y\}$ it follows that the coefficient corresponding to $\epsilon_0$ in the equation for $\delta_{z.w} - \delta_{x.zw}$ is always 0. We can therefore disregard this case. Consider now the case that $M \in Z$. There then exists a path $p$ from $M \in Z$ to $Y$ in $\mathcal{G}$ that is open given $W$ and we are done. Finally, suppose $M \notin Z \cup W \cup \{Y\}$. It then follows that there exists a path $p_1$ from some node $A \in Z$ to $M$ in $\mathcal{G}$ that is open given $W$. In addition, there also exists a path $p_2$ from $M$ to $Y$ in $\mathcal{G}$ that is open given $W$ and $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$. Let $I$ be the first node on $p_1$ that also on $p_2$ and consider $q = p_1(A, I) \cup p_2(I, Y)$. If $I = A$ or $I = Y$, $q$ is a subpath of either $p_1$ or $p_2$ and therefore open given $W$. If $I = M$, $q$ is open by the fact that $M \notin W$ and $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$, irrespectively of whether it is a collider or a non-collider on $q$. Suppose now that $I \notin \{A, Y, M\}$ is a non-collider on $q$. Then $I$ may not be a collider on both $p_1$ and $p_2$. Since both $p_1$ and $p_2$ are open given $W$ it therefore follows that $I \notin W$ and therefore $q$ is open given $W$. Suppose now that $I \notin \{A, Y, M\}$ is a collider on $q$. If $I$ is also a collider on either $p_1$ or $p_2$ it follows that $I \in W$ and we are done. If $I$ is not a collider on either $p_1$ or $p_2$, then $p_1$ either of the form $A \cdots \rightarrow I \rightarrow \cdots M$ or $A \cdots \leftrightarrow I \rightarrow \cdots M$. As $p_1(I, M)$ is open given $W$ and $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$ it follows that $\text{de}(I, \tilde{G}) \cap W \neq \emptyset$ and therefore $q$ is open given $W$.

Consider now Case ii): $\text{sib}(S, \tilde{G}) \cap S' \neq \emptyset$. This implies that their exists a pair of nodes $M$ and $M'$, such that $M \in \text{sib}(M', \tilde{G})$, the coefficient for $\epsilon_m$ in the equation for $\delta_{x.w} - \delta_{x.zw}$ is non-zero and the coefficient for $\epsilon_m'$ in the equation for $\delta_{z.w}$ is non-zero. Suppose first that $M \in W$. In this case there exists a path $p$ from some node $A \in Z$ to $M$ that ends with an edge into $M$ and is open given $W$. Suppose also that $M' \in W$. If $M'$ lies on $p$ than it must be a collider on $p$ and therefore $p(A, M')$ is a path from $Z$ to $M'$ that is open given $W$ and whose last edge points into $M'$. If $M'$ does not lie on $p$ we can simply add the edge $M \leftrightarrow M'$ to $p$ to also obtain such a path. If $M' \notin W$ we have therefore reduced this case to the corresponding case in Case i). If $M' \notin W$, then we know that there either exists a causal path from $M'$ to $Y$ that is open given $W$ or $\text{de}(M', \tilde{G}) \cap W \neq \emptyset$ and there must exist a path from $M'$ to $Y$ that is open given $W$. In both cases we can use the edge $M' \leftrightarrow M'$ to construct a path from $Y$ to $M'$ that is open given $W$ and whose last edge is into $M$. Again we have reduced the problem to the corresponding case in Case i).

Suppose now that $M \notin W$. If $M' \notin W$ we can argue as for the case $M \in W$ and $M' \notin W$. Lastly, suppose that both $M$ and $M'$ are not in $W$. Again we have four cases to consider: a) $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$ and $\text{de}(M', \tilde{G}) \cap W \neq \emptyset$, b) $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$ and $\text{de}(M', \tilde{G}) \cap W = \emptyset$, c) $\text{de}(M, \tilde{G}) \cap W = \emptyset$ and $\text{de}(M', \tilde{G}) \cap W \neq \emptyset$, and d) $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$ and $\text{de}(M', \tilde{G}) \cap W = \emptyset$. In Case a), there exists a path $p_1$ from $Z$ to $M$ that is open given $W$ as well as a path $p_2$ from $M$ to $Y$ that is open given $W$. As $\text{de}(M, \tilde{G}) \cap W \neq \emptyset$ we can use the edge $M' \leftrightarrow M'$ to either extend $p_2$ to a path from $M' \rightarrow Y$ that is open given $W$ or $M'$ lies on $p_2$ and $p_2(M, Y)$ is such a path. In either case we have reduced this to the corresponding setting in Case i). In Case a), there exists a path $p_1$ from $Z$ to $M$ that is open given $W$ as well as a causal path $p_2$ from $M'$ to $Y$ that is open given $W$. As $p_2$ is causal path, $M'$ may not be a collider on $p_2$, so we can again either enlarge $p_2$ with the edge $M' \leftrightarrow M'$ or use $p(M, Y)$ instead to reduce this to the corresponding setting in Case i). The same arguments apply to Cases c) and d).

In conclusion, the set nodes whose errors have non-zero coefficients in the equation for $\delta_{z.w}$ and the corresponding set for $\delta_{x.w} - \delta_{x.zw}$ are disjoint. In addition, there also exist no bi-directed edges between any two nodes from the two sets. By our assumption on the independences that hold between the errors in a linear structural equation model, we can therefore conclude that $\delta_{z.w} \perp \delta_{x.w} - \delta_{x.zw}$.

Lemma C.4. Consider nodes $A$ and $M$, and node sets $Z$ and $W = \{W_1, \ldots, W_k\}$ in an ADMG $\mathcal{G} =$
(V, E), such that V = {V1, ..., Vq} is generated from a linear structural equation model compatible with G. Let T = (Z, W) and consider the residual δa.w = A − βaw W. If the coefficient for ϵm in the equation for δa.w is non-zero, then there are two cases: First, if M ∈ W then there exists a path p from A to M that ends with an edge pointing into M and which is open given W. Second, if M ∉ W, then there exists a causal path from M to some node M′ ∈ {A} ∪ W such that the coefficient of ϵm′ is non-zero and there exists a path from A to M that is open given W.

Consider also the difference of residuals δa.w − δa.zw = βaw T − βaw W. If the coefficient for ϵm in the equation for δa.w − δa.zw is non-zero, then there exist two cases: First, if M ∈ W then there exists a path p from Z to M that ends with an edge pointing into M and which is open given W. Second, if M ∉ W, then there exists a causal path from M to some node M′ ∈ (Z ∪ W) such that the coefficient of ϵm′ is non-zero and there exists a path from M to Z that is open given W.

**Proof.** The first statement is a generalization of Lemma B.4 of Henckel et al. (2022), which is for directed acyclic graphs, to acyclic directed mixed graph. Using Lemma C.5, it can be shown with the exact same arguments as in the proof of Lemma B.4 which we now give for completeness.

We first rewrite the random variable δa.w as a linear combination of the errors from the underlying linear structural equation model as follows:

\[ \delta_{a,w} = A - \beta_{aw} W = \sum_{V_j \in V} \tau_{aw,j} \epsilon_j - \sum_{V_j \in V} \beta_{aw} \tau_{wv,j} \epsilon_j = \sum_{V_j \in V} \gamma_j \epsilon_j, \]

with \( \gamma_j = \tau_{aw,j} - \beta_{aw} \tau_{wv,j} \) the coefficient corresponding to \( \epsilon_j \).

We now prove the first half of the first statement of the Lemma by contraposition. So suppose \( M \in W \) and assume that there is no path from A to M that is open given W and end with an edge pointing into M. Under these assumption Lemma C.5 holds and therefore

\[ \gamma_m = \tau_{aw,j} - \beta_{aw} \tau_{wv,j} = 0, \]

where we assume that \( M = W_j \).

We now prove the second half of the first statement of the Lemma. So suppose \( M ∉ W \) and let \( W^\prime = \{W_1, ..., W_k, A\} \). Then

\[ \gamma_m = \tau_{aw} - \beta_{aw} \tau_{wv,j} = \sum_{W_1 \in W^\prime} \tau_{w_1,m,w_1'} (\tau_{aw,j} - \beta_{aw} \tau_{w_1,j}) = \sum_{W_1 \in W^\prime} \tau_{w_1,m,w_1'} \gamma_j, \]

where we use that by Lemma B.7 of Henckel et al. (2022), \( \tau_{w,m} = \sum_{W_1 \in W^\prime} \tau_{w_1,m,w_1'} \tau_{w_1,w_j} \). Lemma B.7, although stated for directed acyclic graphs, also holds for acyclic directed mixed graphs as all of its arguments only depend on the linear structural equation model via the matrix of edge coefficients A. Therefore, \( \gamma_m \) is only non-zero if there exists a \( W_j \in W \) such that \( \tau_{w_1,m,w_1'} \neq 0 \) and \( \gamma_w \neq 0 \), that is, if there exists a causal path p from M to some \( W_j \in W^\prime \) (that does not contain other nodes in \( W^\prime \)) and the coefficient for \( \tau_{w_1,j} \) is non-zero. The latter implies that there exists a path \( p' \) from A to \( W_j \) that is open given W and whose last edge points into \( W_j \) by what we have already shown in this proof.

It remains to show that there exists a path from M to A that is open given W. If \( W_j = A \), p is such a path so assume this is not the case. Consider the first node I on p where p and p′ intersect and let \( q = p(M, I) \oplus p'(I, A) \). If \( I = M \) or \( I = A \), q is a subpath of p′ respectively p and therefore open given W. Suppose first that \( I \in W \). Then as \( I = W_j \) as \( W_j \) is the only node in W on p. But then \( W_j \) is a collider by the fact that the edge on p′ points into \( W_j \) and p is causal. Therefore, q is open given W. If \( I \notin W \) then by the fact that any node on p has \( W_j \) as a descendant by nature of p, \( W_j \in \text{de}(I, G) \) and therefore q is open irrespective of whether I is a collider on q or not.
For the second statement of the lemma we will show that if the coefficient for $M$ in the equation for $\delta_{z,w}$, denoted $\gamma_m'$, is zero, so is the one in the equation for $\delta_{a,w} - \delta_{a,z,w}$, denoted $\gamma_m$. We can write

$$
\gamma_m = \beta_{az,w} \tau_{zw} + \beta_{aw,z} \tau_{wm} - \beta_{aw} \tau_{wm} \\
= \beta_{az,w} \tau_{zw} + \beta_{aw,z} \tau_{wm} - (\beta_{aw,z} + \beta_{az,w} \beta_{zw}) \tau_{wm} \\
= \beta_{az,w} \tau_{zw} - \beta_{az,w} \beta_{zw} \tau_{wm}
$$

where we use Lemma A.3 to plug in $\beta_{aw} = \beta_{aw,z} + \beta_{az,w} \beta_{zw}$. This coefficient is zero whenever

$$
\gamma_m' = \tau_{zw} - \beta_{zw} \tau_{wm} = 0.
$$

But since we can apply the first half of the Lemma to $\gamma_m'$, our statement follows. \[\square\]

**Lemma C.5.** Consider node sets $Z$ and $W = \{W_1, \ldots, W_k\}$ in an acyclic directed mixed graph $G = (V, E)$, such that $V$ is generated from a linear structural equation model compatible with $G$. Let $W_j$ be some node in $W$, such that all paths from $Z$ to $W_j$ that end with an edge of the form $\rightarrow$ or $\leftrightarrow$ are blocked by $W$, then

$$
\tau_{zw_j} = \beta_{zw} \tau_{zw_j}.
$$

**Proof.** We show our claim in two steps. First we construct an enlarged linear structural linear equation model, such that there exists valid adjustment sets with respect to $(W_j, Z)$ and $(W_j, W_{-j})$. We use these to replace the terms $\tau_{zw_j}$ and $\tau_{uw_j}$ in Equation (6) with ordinary least squares coefficients. Second, we apply Lemma A.3 to the ordinary least squares coefficients corresponding to $\tau_{zw_j}$ and then simplify the resulting equation by using Lemma A.4 to arrive at Equation (6).

We first enlarge the underlying linear structural equation model as follows. For every node in $V \in \text{sib}(W_j, G)$ add a node $\epsilon_v$, a directed edge from $\epsilon_v$ to $V$ and a bidirected edge from $\epsilon_v$ to $W_j$. Let $G' = (V', E')$ denote this enlarged model and its causal graph. Consider the set $P' = \text{pa}(W_j, G) \cup \text{sib}(W_j, G')$ and two sets $A \subseteq \text{de}(W_j, G) \setminus \{W_j\}$ and $B \subseteq V \setminus \text{de}(W_j, G)$. By construction the set $P' \cup B$ does not contain any descendants of $W_j$. In addition, any non-causal path from $W_j$ to $B$ that starts with an edge into $W_j$, must contain a node in $P' \cup B$ that is a non-collider. The latter is due to the fact that by the construction of $G'$ no node in $\text{sib}(W_j, G')$ may be a collider on any path. Therefore, $P' \cup B$ is a valid adjustment set with respect to $(W_j, A)$. In particular, $\tau_{zw_j} = \beta_{zw_j, p'}$ and $\tau_{w_{-j}w_j} = \beta_{w_{-j}w_j, p'}$, where $W_{-j} = W \setminus \{W_j\}$. Applying this to equation (6) we obtain

$$
\tau_{zw_j} = \beta_{zw_j, p'} = \beta_{zw_j, w_{-j}p''} + \beta_{zw_j, w_{-j}p''} \beta_{w_{-j}w_j, p'} = \beta_{zw, p'} \tau_{zw_j},
$$

where we use Lemma C.7 in the second step and where $P''$ is some maximal subset of $P'$, such that the covariance matrix of $(\hat{W}, P'')$ has full rank. The covariance matrix $(W_j, P')$ is of full rank by our construction of $G'$. Note that by assumption $P' \perp_{G'} Z | W$, as any path that would contradict this statement could be extended to a path from $Z$ to $W_j$ whose last edge points into $W_j$ and that is open given $W$. As a result $\beta_{zw, p''} = \beta_{zw}$ and our claim follows. \[\square\]

**Lemma C.6.** Consider a random variable $X$, and two random vectors $Z$ and $W$. Then

$$
E[(\delta_{z,w} - \delta_{x,z,w})^2] = \sigma_{x,x,w} - \sigma_{z,x,z,w},
$$

where $\delta_{z,w} = X - \beta_{zw} W$ and $\delta_{x,z,w} = X - \beta_{xw,z} W - \beta_{x,z,w} Z$.

**Proof.**

$$
E[(\delta_{z,w} - \delta_{x,z,w})^2] = E[\delta_{z,w}^2] - 2E[\delta_{z,w} \delta_{x,z,w}] + E[\delta_{x,z,w}^2] \\
= \sigma_{z,w} - 2E[\delta_{x,z,w} \delta_{x,z,w}] + \sigma_{z,w}.
$$
Further,
\[
E[\delta_{x,w}\delta_{z,w}] = E[(X - \beta_{x,w}W)(X - \beta_{x,w}Z)] \\
= \sigma_{xz} - \Sigma_{xwu}\beta_T^{T} \Sigma_{xwu} - \beta_{xwu}\Sigma_{zu} + \beta_{xwu}\Sigma_{zu}\beta_T^{T} + \beta_{xwu}\Sigma_{zu}\beta_T^{T} \\
= (\sigma_{xz} - \beta_{xwu}\Sigma_{zu}) + \beta_{xwu}\Sigma_{zu}\beta_T^{T} + \beta_{xwu}\Sigma_{zu}\beta_T^{T} \\
= 2\beta_{xwu}\Sigma_{zu}\beta_T^{T} \\
= \sigma_{xz} - \beta_{xwu}\Sigma_{zu} \\
= \sigma_{xz}.
\]

As a result,
\[
E[(\delta_{x,w} - \delta_{z,w})^2] = \sigma_{xzw} - \sigma_{xzw}
\]
follows.

**Lemma C.7.** Let \( A, B, C \) and \( D \) be mean 0 random vectors with finite variance, such that \( \Sigma_{e_1e_2} \) with \( E_1 = (B, C, D) \), is not of full rank but \( \Sigma_{e_2e_2} \) and \( \Sigma_{e_3e_3} \), with \( E_2 = (B, C) \) and \( E_3 = (B, D) \), are of full rank. Then
\[
\beta_{ab,c} = \beta_{ab,c'd} + \beta_{ad,be'}\beta_{db,c},
\]
where \( C' \) is any maximally sized subset of \( C \), such that \( \Sigma_{e_4e_4} \) with \( E_4 = (B, C', D) \) is of full rank.

**Proof.** Regressing \( A \) on \( B, C' \) and \( D \), yields the equation
\[
A = \beta_{ab,c'd}B + \beta_{ac',be'}C' + \beta_{ad,be'}D + \epsilon_{a,be'd}.
\]
Regressing \( D \) on \( B, C \), yields the equation
\[
D = \beta_{db,c}B + \beta_{dc,b}C + \epsilon_{d,be'}.
\]
Plugging the latter equation into the former yields
\[
A = (\beta_{ab,c'd} + \beta_{ad,be'}\beta_{db,c})B + \beta_{ac',be'}C' + \beta_{ad,be'}\beta_{dc,b}C + \beta_{ad,be'}\epsilon_{d,be'} + \epsilon_{a,be'd}.
\]
We can rewrite this equation as
\[
A = (\beta_{ab,c'd} + \beta_{ad,be'}\beta_{db,c})B + \beta_{ac',be'}C' + \epsilon',
\]
where \( \beta_{ab,c} \) is some real-valued vector of length \( |C| \) and \( \epsilon' = \beta_{ad,be'}\epsilon_{d,be'} + \epsilon_{a,be'd} \). As \( E[\epsilon_{a,be'd}(B, C', D)] = 0 \) it follows that it also holds that \( E[\epsilon_{a,be'd}(B, C, D)] = 0 \) by our assumptions on \( C \). We can therefore conclude that \( E[\epsilon(B, C)] = 0 \). Our claim then follows by the uniqueness of the ordinary least squares regression coefficient \( (\beta_{ab,c}, \beta_{ac,b}) \).

**C.2 Proof of Theorem 4.2.**

**Theorem C.8.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( G \) such that \( \text{de}(X, G) = \{X, Y\} \). Let \( \{Z_1, W_1\} \) and \( \{Z_2, W_2\} \) be valid conditional instrumental sets relative to \( (X, Y) \) in \( G \). Let \( W_{12} = W_1 \setminus W_2 \) and \( W_{21} = W_2 \setminus W_1 \). If the following four conditions hold
(a) \( W_{12} \perp_{G} Y \mid W_2 \),
(b) \( W_{12} \perp_{G} Z_2 \mid W_2 \text{ or } W_{12} \perp_{G} Z_2 \cup Z_2 \setminus \{Z_2 \cup W_2, \}
(c) \text{ either } i) \ W_{21} \setminus Z_1 \perp_{G} Z_1 \mid W_1 \text{ and } W_{21} \setminus \cup Z_1 \perp_{G} X \mid W_1 \cup (W_{21} \setminus Z_1) \text{ or } \n ii) \ W_{21} \setminus \cup_{G} X \mid W_1,
(d) \ Z_1 \setminus (Z_2 \cup W_{21}) \perp_{G} X \mid Z_2 \cup W_1 \cup W_{21},
\]

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then for all linear structural equation models compatible with $G$ such that $\Sigma_{x,z_1} \neq 0$, $a.\text{var}(\hat{\tau}_{yz}^{2, w_2}) \leq a.\text{var}(\hat{\tau}_{yz}^{2, w_1})$.

Proof. By the m-separation assumptions we can apply both Lemma C.9 and Lemma C.10, which both hold for all linear structural equation models compatible with $G$. Therefore, $\sigma_{\tilde{y}y, w_1} \geq \sigma_{\tilde{y}y, w_2}$ and $\sigma_{x,z_1w_1} \leq \sigma_{x,z_2w_1}$ for all linear structural equation models compatible with $G$.

Given a linear structural equation model such that $\Sigma_{x,z_1} \neq 0$ it also holds that $\sigma_{x,z_1w_1} - \sigma_{x,z_1w_1} = \Sigma_{x,z_1} - \Sigma_{x,z_1w_1} \Sigma_{x,z_1w_1}^{-1} \Sigma_{x,z_1w_1} > 0$. By Lemma C.10 it follows that similarly $\sigma_{x,z_2w_2} - \sigma_{x,z_2w_2} - \sigma_{x,z_1w_1} > 0$. As the claim is for linear structural equation models such that $\Sigma_{x,z_1} \neq 0$, we can therefore apply Theorem 4.1 to both $\{Z_1, W_1\}$ and $\{Z_2, W_2\}$ and conclude that $a.\text{var}(\hat{\tau}_{yz}^{2, w_1}) = \sigma_{\tilde{y}y, w_1}/\sigma_{x,z_1w_1}$ and $a.\text{var}(\hat{\tau}_{yz}^{2, w_2}) = \sigma_{\tilde{y}y, w_2}/\sigma_{x,z_2w_2}$. The claim then follows by the fact that $\sigma_{\tilde{y}y, w_1} \geq \sigma_{\tilde{y}y, w_2}$ and $\sigma_{x,z_1w_1} \leq \sigma_{x,z_2w_2}$ as shown above.

Lemma C.9. Consider disjoint nodes $X$ and $Y$, and node sets $W_1$ and $W_2$ in an acyclic directed mixed graph $G = (V, E)$, such that $V$ is generated from a linear structural equation model compatible with $G$ and $\text{de}(X, G) = \{X, Y\}$. Let $\hat{Y} = Y - \tau_{yz} X$, with $\tau_{yz}$ the total effect of $X$ on $Y$. If $W_1 \setminus W_2 \not\perp \!\!\!\!\perp \hat{Y} \mid W_2$, then $\sigma_{\tilde{y}y, w_1} \leq \sigma_{\tilde{y}y, w_2}$.

Proof. As we assume that $W_{1,2} \not\perp \!\!\!\!\perp \hat{Y} \mid W_2$ it follows that $W_{1,2} \not\perp \!\!\!\!\perp \hat{Y} \mid W_2$ by Lemma B.4. It follows that $\sigma_{\tilde{y}y, w_1} \geq \sigma_{\tilde{y}y, w_1} \mid w_2 = \sigma_{\tilde{y}y, w_2}$ holds.

Lemma C.10. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $G = (V, E)$, such that $V$ is generated from a linear structural equation model compatible with $G$ and $\text{de}(X, G) = \{X, Y\}$. Let $(Z_1, W_1)$ and $(Z_2, W_2)$ be two pairs of disjoint node sets in $G$ and define $W_{1,2} = W_1 \setminus W_2$ as well as $W_{2,1} = W_2 \setminus W_1$. If the following three conditions hold

(a) $W_{1,2} \not\perp \!\!\!\!\perp Z_2 \mid W_1 \setminus W_2$ or $W_{1,2} \not\perp \!\!\!\!\perp Z_2 \mid Z_2 \cup W_2$ and
(b) either i) $W_{2,1} \setminus Z_1 \not\perp \!\!\!\!\perp Z_1 \mid W_1$ and $W_{2,1} \setminus Z_1 \not\perp \!\!\!\!\perp X \mid W_1 \cup (W_{2,1} \setminus Z_1)$ or ii) $W_{2,1} \setminus Z_1 \not\perp \!\!\!\!\perp X \mid W_1$ and
(c) $Z_1 \setminus (Z_2 \cup W_{2,1}) \not\perp \!\!\!\!\perp X \mid Z_2 \cup W_1 \cup W_{2,1}$,

then $\sigma_{x,z_2} - \sigma_{x,z_2w_2} \geq \sigma_{x,z_1} - \sigma_{x,z_1w_1}$.

Proof. Let $A = W_{1,2}$ and $C = W_{2,1}$ to unclutter the notation. By Condition (a) it follows that $\sigma_{x,z_2} - \sigma_{x,z_2w_2} \geq \sigma_{x,z_1} - \sigma_{x,z_1w_1}$ with $C' = C \setminus Z_1$. This follows either by first applying Lemma C.11 with $B = C'$ and then using that if $C \cap Z_1 \not\perp \!\!\!\!\perp X \mid (W_1 \cup C')$, $\sigma_{x,z_2w_2} = \sigma_{x,z_1w_1}$ or by applying the latter argument to all of $C$ using the alternative assumption $C \not\perp \!\!\!\!\perp X \mid W_1$. By Condition (b), it holds that $\sigma_{x,z_1w_1} \geq \sigma_{x,z_1z_2} \geq \sigma_{x,z_1w_1} - \sigma_{x,z_1z_2w_2}$. Hence,

$\sigma_{x,z_2} - \sigma_{x,z_2w_2} \geq \sigma_{x,z_1} - \sigma_{x,z_1w_1}$.

Finally, by Condition (c) it follows that

$\sigma_{x,z_2} - \sigma_{x,z_2w_2} = \sigma_{x,z_2} - \sigma_{x,z_2w_2} \leq \sigma_{x,z_2w_2} - \sigma_{x,z_2w_2} \leq \sigma_{x,z_2w_2} - \sigma_{x,z_2w_2}$,

with $A' = A \setminus Z_2$. This follows either by applying Lemma C.11 with $B = A \setminus Z_2$ or by the fact that if $(A \setminus Z_2) \not\perp \!\!\!\!\perp X \mid Z_2 \cup W_2$, then $\sigma_{x,z_2w_2} = \sigma_{x,z_2w_2}$ holds.
Lemma C.11. Consider a node $X$ and two disjoint node sets $Z$ and $W$ in an acyclic directed mixed graph $\mathcal{G} = (V, E)$ such that the distribution of $V$ is compatible with $\mathcal{G}$. Let $W = A \cup B$ be a partition of $W$, i.e. $A \cap B = \emptyset$, and suppose that $A \perp_{\mathcal{G}} Z \mid B$. Then

$$\sigma_{xx, ab} - \sigma_{xx, zab} = \sigma_{x, b} - \sigma_{xx, zb}.$$ 

Proof. Using Lemma A.4 we can conclude that

$$\sigma_{xx, ab} - \sigma_{xx, zab} = \beta_{xx, ab} \sigma_{zz, ab} \tau_{xx, ab} = \beta_{xx, b} \sigma_{zz, b} \tau_{xx, b} = \sigma_{x, b} - \sigma_{xx, zb}$$

holds.

C.3 Proof of Proposition 4.9

Proposition C.12. Consider nodes $X, Y$ and $N$ in an acyclic directed mixed graph $\mathcal{G}$ such that $\text{de}(X, \mathcal{G}) = \{X, Y\}$. Let $\{Z, W\}$ and $\{Z, W \cup N\}$ be distinct valid conditional instrumental sets relative to $(X, Y)$ in $\mathcal{G}$. If $\{Z \cup N, W\}$ is not a valid conditional instrumental set relative to $(X, Y)$ in $\mathcal{G}$, then for all linear structural equation models compatible with $\mathcal{G}$ such that $\Sigma_{xx, w} \neq 0$, $a.\text{var}(\hat{\tau}_{yw}) \leq a.\text{var}(\tilde{\tau}_{yw})$.

Proof. We will show our claim by showing that $\{Z, W\}$ and $\{Z, W \cup N\}$ being valid conditional instrumental sets while $\{Z \cup N, W\}$ is not, implies that $N \not \perp_{\mathcal{G}} Y \mid W$ and $N \perp_{\mathcal{G}} Z \mid W$. Using this we can apply Theorem 4.2 with $Z_1 = Z_2 = Z, W_1 = W$ and $W_2 = W \cup N$ to conclude the proof.

We first show that $N \not \perp_{\mathcal{G}} Y \mid W$. The fact that $\{Z, W \cup N\}$ is a valid conditional instrumental set implies that $\{Z \cup N, W\}$ fulfills Condition (i) of Theorem 3.2. Similarly, the fact that $\{Z, W\}$ is a valid conditional instrumental set, implies that $\{Z \cup N, W\}$ also fulfills Condition (ii). Therefore $\{Z \cup N, W\}$ not being a valid conditional instrumental set, requires a violation of Condition (iii), i.e., a path $p$ from $N$ to $Y$ in $\mathcal{G}$ that is open given $W$.

We now show that $N \not \perp_{\mathcal{G}} X \mid W$ by contradiction, so suppose that $N \not \perp_{\mathcal{G}} Z \mid W$. We have shown that $N \not \perp_{\mathcal{G}} Y \mid W$. Thus there exists a $p$ from some node $A \in Z \cup N$ open given $W$ as well as a path $p'$ from $N$ to $Y$ open given $W$ that does not contain the edge $X \rightarrow Y$. Note, first that $p$ may also not contain the edge $X \rightarrow Y$, as by the assumption that $\text{de}(Y, \mathcal{G}) = \{Y\}$, the node $Y$ would have to be a collider on $p$ contradicting our assumption that it be open given $W$. Let $I$ be the first node where these paths intersect and consider the concatenated path $q = p(A, I) \oplus p'(I, Y)$. We will now sequentially discuss the possible properties of $I$ and show that in all the possible cases $q$ is either open given $W$ or $W \cup N$.

Suppose first that $I = N$. Then if $N$ is a collider $q$ is open given $W$. If not, $q$ is open given $W \cup N$. Suppose second that $I$ is a non-collider on $q$. Then it also has to be a non-collider on either $p$ or $p'$. Therefore, $I \not \in W$ and $q$ is trivially open given $W$. Suppose third that $I$ is a collider on $q$. Then $q$ is open if $\text{de}(I, \mathcal{G}) \cap W \neq \emptyset$. We can therefore assume that $\text{de}(I, \mathcal{G}) \cap W = \emptyset$. Then $p(I, N)$ must be of the form $I \rightarrow \cdots \rightarrow N$, as otherwise some node in $\text{de}(I, \mathcal{G})$ would have to be a collider on $p(I, N)$, contradicting our assumption that $p$ is open given $W$. Thus, $N \in \text{de}(I, \mathcal{G})$ and $q$ is an open path given $W \cup N$. Lastly, if $I = Y$ then $q = p(A, Y)$ is open given $W$ as a subpath of $p$. The existence of the paths $p$ and $p'$ therefore contradicts our assumption that both $\{Z, W\}$ and $\{Z, W \cup N\}$ are valid conditional instrumental sets.

C.4 Proof of Proposition 4.13

Proposition C.13. Consider nodes $X$ and $Y$ in an acyclic directed mixed graph $\mathcal{G}$ such that $\text{de}(X, \mathcal{G}) = \{X, Y\}$. Let $\{Z, W\}$ be a valid conditional instrumental sets relative to $(X, Y)$ in $\mathcal{G}$. Then applying Algorithm 1 to $(\mathcal{G}, X, Y, Z, W)$ greedily minimises $a.\text{var}(\hat{\tau}_{yw})$ at each step.

Proof. Consider a step of Algorithm 1 given a valid tuple $\{Z', W'\}$ and node $N$. We will now show that in all possible cases Algorithm 1 uses $N$ in a manner that greedily minimises the asymptotic variance.

Suppose first that $\{Z' \cup N, W'\}$ is a valid tuple and $N \not \perp_{\mathcal{G}} X \mid W \cup Z$. Then by Corollary 4.3 $\{Z' \cup N, W'\}$ is more accurate than $\{Z', W'\}$. Further, if $\{Z', W' \cup N\}$ is valid tuple, it is less accurate.
than \( \{Z' \cup N, W'\} \) by Corollary 4.8. Therefore, adding \( N \) to \( Z' \) greedily minimises the two-stage least squares estimator’s asymptotic variance.

Suppose now that \( \{Z' \cup N, W'\} \) is a valid tuple and \( N \perp \!\!\!\perp X \mid W \cup Z \). Then we can apply Theorem 4.2 with \( \{Z_1, W_1\} = \{Z' \cup N, W'\} \) and \( \{Z_2, W_2\} = \{Z', W'\} \) to conclude that \( \{Z', W'\} \) is at least as accurate as \( \{Z' \cup N, W'\} \). Further, as \( \{Z' \cup N, W'\} \) is by assumption a valid tuple it follows that \( Z' \cup N \perp \!\!\!\perp Y \mid W' \). This implies that \( N \perp \!\!\!\perp Y \mid Z' \cup W' \) by the weak union property of m-separation. Therefore, Algorithm 1 discards \( N \), i.e., does not add it to either \( Z' \) or \( W' \) irrespectively of whether \( \{Z', W' \cup N\} \) is valid. We have already shown that this greedily minimizes the asymptotic variance.

Finally, suppose that \( \{Z' \cup N, W'\} \) is not valid but \( \{Z', W' \cup N\} \) is. In this case, \( \{Z', W' \cup N\} \) is more accurate than \( \{Z', W'\} \) by Proposition 4.9. Further, as \( \{Z' \cup N, W'\} \) is not valid while \( \{Z', W'\} \) and \( \{Z', W' \cup N\} \) are it follows that \( Z' \cup N \perp \!\!\!\perp Y \mid W' \) by Theorem 3.2. Combined with \( Z' \perp \!\!\!\perp Y \mid W' \) this implies that \( N \not\perp \!\!\!\perp Y \mid W' \cup Z' \), as otherwise we would have a contradiction to the contraction property of m-separation. Therefore, Algorithm 1 will always add \( N \) to \( W' \) in this case and we have shown that this greedily minimises the asymptotic variance.

\[ \square \]

C.5 Proof of Theorem 4.18

Theorem C.14. Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( \mathcal{G} \) such that \( \text{de}(X, \mathcal{G}) = \{X, Y\} \). Let \( W^0 = \text{dir}_+^0(Y, \mathcal{G}) \) and \( Z^0 = \text{dir}_+^0(X, \mathcal{G}) \cup \overline{W^0} \). Then the following two statements hold:

(i) if \( \overline{Z^0} \neq \emptyset \) then \( \{Z^0, W^0\} \) is a valid conditional instrumental set relative to \( (X, Y) \) in \( \mathcal{G} \); (ii) if \( \overline{Z^0} \cap (\text{pa}(X, \mathcal{G}) \cup \text{si}(X, \mathcal{G})) \neq \emptyset \) then \( \{Z^0, W^0\} \) is also graphically optimal relative to \( (X, Y) \) in \( \mathcal{G} \).

Proof. We first show that if \( \overline{Z^0} \neq \emptyset \) then \( \{Z^0, W^0\} \) is a valid conditional instrumental set. By Lemma C.15 \( Z^0 \perp_{\!\!\!\!\perp} Y \mid W^0 \). Further, by construction of \( Z^0 \) and our assumption that \( Z^0 \neq \emptyset \) there exists a path \( p \) from any node in \( Z^0 \) to \( X \) consisting entirely of colliders in \( Z^0 \cup W^0 \). Hence, \( Z^0 \not\perp \!\!\!\perp X \mid W^0 \).

We now consider the second statement of the theorem. First we will show that for any valid conditional instrumental set \( \{Z, W\} \), such that \( C = W^0 \setminus W \neq \emptyset \), we can use Theorem 4.2 to conclude that

\[ a.\text{var}(\hat{z}_{yx}^o \setminus w) \leq a.\text{var}(\hat{z}_{yx}^o) \cdot \frac{\sigma_{\hat{y}y, w^0}(\sigma_{xx, w^o} - \sigma_{xx, w^o z^o})}{\sigma_{\hat{y}y, w}(\sigma_{xx, w^o} - \sigma_{xx, w^o z^o})} \]

By Lemma C.15 \( W \setminus W^0 \perp_{\!\!\!\!\perp} Y \mid W^0 \) and as a result Condition 4 holds. By Lemma C.16 Conditions 3 and 4 hold. By the assumption that \( C = \emptyset \), Condition 3 trivially holds and our claim follows.

We can therefore suppose that \( C \neq \emptyset \) for the remainder of the proof.

Let \( \{Z, W\} \) be a valid conditional instrumental set in \( \mathcal{G} \), such that \( C = W^0 \setminus W \neq \emptyset \) and consider the ratio of asymptotic variances.

\[ \frac{a.\text{var}(\hat{z}_{yx})}{a.\text{var}(\hat{z}_{yx}^o \setminus w)} = \frac{\sigma_{\hat{y}y, w^0}(\sigma_{xx, w^o} - \sigma_{xx, w^o z^o})}{\sigma_{\hat{y}y, w}(\sigma_{xx, w^o} - \sigma_{xx, w^o z^o})} \]

We will now construct a Gaussian linear structural equation model such that this ratio is smaller than 1. To keep our notation readable we make the dependence of our conditional variances on the underlying Gaussian linear structural equation model explicit only when necessary.

Let \( F' \) be the set of all edges that are the first on any proper path from \( W^0 \) to \( X \) that is open given \( Z^0 \). Similarly, let \( F'' \) be the set of all edges that are first on any proper path from \( W^0 \) to \( X \) that is open given the empty set. We then define the following class of Gaussian linear structural equation models. Let \( (\mathcal{A}, \Omega) \) be a Gaussian linear structural equation model compatible with \( \mathcal{G} \) such that all non-zero entries of \( \mathcal{A} \) and \( \Omega \) are non-zero, and \( \Omega \) is strictly diagonally dominant. Let \( (\mathcal{A}_F(\epsilon), \Omega_F(\epsilon)) \) be the Gaussian linear structural equation model, such that the edge coefficients and error covariances corresponding to edges in \( F = F' \cup F'' \) are replaced with the value \( \epsilon > 0 \). As all edge coefficients and error covariances are positive for any \( \epsilon > 0 \), \( (\mathcal{A}_F, \Omega_F(\epsilon)) \) is faithful to \( \mathcal{G} \). Thus, \( \sigma_{xx, w^o} \neq 0 \) and \( \sigma_{xx, w^o z^o} \neq 0 \) for any \( \epsilon > 0 \).

We first make two observations that hold for any Gaussian linear structural equation model compatible with \( \mathcal{G} \). Let \( A = W \setminus W^0 \) and \( C = W^0 \setminus W \). By Lemma C.15 \( \sigma_{\hat{y}y, w^0} = \sigma_{\hat{y}y, aw^o} = \sigma_{\hat{y}y, wc} \).
Therefore,
\begin{equation}
0 < \frac{\sigma_{\tilde{g}\tilde{y},w^\epsilon}}{\sigma_{\tilde{g}\tilde{y},w}} = \frac{\sigma_{\tilde{g}\tilde{y},w^\epsilon} - \Sigma_{\tilde{g}c, w^\epsilon} \Sigma_{\tilde{g}c, w^\epsilon}^T}{\sigma_{\tilde{g}\tilde{y},w}} = 1 - q, \quad q \geq 0.
\end{equation}

Second,
\begin{equation}
\frac{\sigma_{xx.w^\epsilon} - \sigma_{xx.w^\epsilon}}{\sigma_{xx.w^\epsilon}} \leq \frac{\sigma_{xx.w^\epsilon} - \sigma_{xx.w^\epsilon}}{\sigma_{xx.w^\epsilon}} \leq \frac{\sigma_{xx.w^\epsilon} - \sigma_{xx.w^\epsilon}}{\sigma_{xx.w^\epsilon}}.
\end{equation}

with $W' = W \setminus Z^\circ$ and $Z' = Z \setminus Z^\circ$.

By Lemma \[\text{A.5}\] the limit for any conditional covariance as a function of $\epsilon$, with $\epsilon \to 0$ exists and is the corresponding conditional covariance in the model $(A_F(0), \Omega_F(0))$. Clearly, $(A_F(0), \Omega_F(0))$ is also compatible with the truncated acyclic directed mixed graph $G'$ with the edges in $F$ removed and we can therefore invoke additional m-separation statements as implied by $G'$.

By assumption on $Z^\circ$, there exists a path from some node in $Z^\circ$ to $X$ consisting entirely of colliders in $Z^\circ$. Clearly no edge in this path is adjacent to any node in $W^\circ$ and therefore no edge is in $F$. Thus, $Z^\circ \not\mathcal{L}_{G'} X | W^\circ$. By construction $(A_F(0), \Omega_F(0))$ is faithful to $G'$. Therefore,
\[
\lim_{\epsilon \to 0} (\sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) - \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0))) = \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) - \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) > 0.
\]

This allows us to conclude that
\[
\lim_{\epsilon \to 0} \frac{a.\var{\tilde{g}\tilde{y},w^\epsilon}(A_F(0), \Omega_F(0))}{a.\var{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))} = \frac{\sigma_{\tilde{g}\tilde{y},w^\epsilon}(A_F(0), \Omega_F(0)) - \sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))}{\sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))} = 1 - \frac{\sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))}{\sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))} = 1 - q^0 < 1.
\]

Combined with Equation \[\text{6}\] we have
\[
\lim_{\epsilon \to 0} \frac{a.\var{\tilde{g}\tilde{y},w^\epsilon}(A_F(0), \Omega_F(0))}{a.\var{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))} = (1 - q^0) \frac{\sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0)) - \sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))}{\sigma_{\tilde{g}\tilde{y},w}(A_F(0), \Omega_F(0))} = 1 - q^0 < 1.
\]

By construction of $F$, $W^\circ \perp_{G'} X$ and therefore
\[
\lim_{\epsilon \to 0} \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx}(A_F(0), \Omega_F(0)).
\]

We will now show that, similarly $S \perp_{G'} X | Z^\circ$ for any $S \subseteq V \setminus (Z^\circ \cup \{X, Y\})$. This allows us to conclude that
\[
\lim_{\epsilon \to 0} \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx}(A_F(0), \Omega_F(0))
\]
and
\[
\lim_{\epsilon \to 0} \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx,w^\epsilon}(A_F(0), \Omega_F(0)) = \sigma_{xx}(A_F(0), \Omega_F(0)).
\]

To do so we show that any proper path from some node $A \in S$ to $X$ that is open given $Z^\circ$ contains an edge in $F$. Let $p$ be such a path. Clearly $p$ may not contain $Y$ and be open given $Z^\circ$. Further, any other node adjacent to $X$ is either in $Z^\circ$ or $W^\circ$. If the latter is the case we are done, so suppose
that \( p \) contains a subsegment \( p(Z, X) \) chosen to be of maximal possible length, such that every node in \( p(Z, X) \), except for \( X \) is in \( Z^o \). Let \( N \) be the node before \( Z \) on \( p \) and consider \( p(N, X) \). By assumption \( p(N, X) \) may not contain a non-collider and thus must be of the form

\[
N \rightarrow Z \leftrightarrow \cdots \leftrightarrow X \text{ or } N \leftrightarrow Z \leftrightarrow \cdots \leftrightarrow X.
\]

In either case, to not contradict our assumption that \( p(Z, X) \) is of maximal length, \( N \in W^o \) must hold. Thus the edge \( N \rightarrow Z \), respectively \( N \leftrightarrow Z \), is in \( F^* \) and our claim follows.

Using these limit statements we can conclude

\[
\lim_{\epsilon \to 0} \frac{a.var(\hat{\tau}_{\epsilon, 0}^Z, w_o(A_F(\epsilon), \Omega_F(\epsilon)))}{a.var(\hat{\tau}_{\epsilon, 0}^Z, w_o(A_F(\epsilon), \Omega_F(\epsilon)))} \leq (1 - q^0) < 1.
\]

Therefore, there exists an \( \epsilon > 0 \), such that the Gaussian linear structural equation model \((A_F(\epsilon), \Omega_F(\epsilon))\) is compatible with and faithful to \( \mathcal{G} \) and the asymptotic variance provided by \( \{Z, W^o\} \) is larger than the one provided by \( \{Z^o, W^o\} \).

**Lemma C.15.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( \mathcal{G} \) with node set \( V \) such that \( \text{de}(X, \mathcal{G}) = \{X, Y\} \). Let \( W^0 = \text{dis}^+_X(Y, \mathcal{G}) \), then for any \( S \subseteq V \setminus (W^o \cup \{X, Y\}) \)

\[
S \perp_{\mathcal{G}} Y \mid W^o.
\]

**Proof.** Let \( p \) be a proper path from some node \( A \in S \) to \( Y \) in \( \mathcal{G} \). We will now show that \( p \) is blocked by \( W^o \). Every node adjacent to \( Y \) in \( \mathcal{G} \) is either in \( W^o \) or \( X \). If it is \( X \), then as \( \text{de}(X, \mathcal{G}) = \emptyset \), \( X \) is a collider on \( p \) and \( p \) is closed given \( W \). Therefore suppose that \( p \) contains at least one node \( W \in W^o \), such that \( p(W, Y) \) consists, except for \( Y \), of nodes in \( W^o \). Choose \( W \in W^o \), such that \( p(W, Y) \) consists, except for \( Y \), of nodes in \( W^o \) and is of maximal length. If \( p(W, Y) \) contains a non-collider then we can conclude that \( p(W, Y) \) and therefore \( p \) is blocked by \( W^o \). Suppose that this is not the case. Then \( p(W, Y) \) must be of the forms

\[
W \leftrightarrow W^f \leftrightarrow \cdots \leftrightarrow Y \text{ or } W \rightarrow W^f \leftrightarrow \cdots \leftrightarrow Y,
\]

with possibly \( W = W^f \). In the latter case \( W \neq A \) is a non-collider on \( p \) and we can again conclude that \( p \) is blocked by \( W^o \). Suppose that \( W \) and all other nodes in \( p(W, Y) \), except for \( Y \), are colliders on \( p \). Then \( p \) must be of the form

\[
\cdots \leftrightarrow W \leftrightarrow \cdots \leftrightarrow Y \text{ or } \cdots \rightarrow W \leftrightarrow \cdots \leftrightarrow Y,
\]

either of which contradicts our assumption that \( p(W, Y) \) is of maximal length. Thus, \( p \) is blocked by \( W^o \) and \( Z^o \perp_{\mathcal{G}} Y \mid W^o \) follows.

**Lemma C.16.** Consider nodes \( X \) and \( Y \) in an acyclic directed mixed graph \( \mathcal{G} \) with node set \( V \), such that \( \text{de}(X, \mathcal{G}) = \{X, Y\} \). Let \( W^o = \text{dis}^+_X(Y, \mathcal{G}) \) and \( Z^o = \text{dis}^+_X(X, \mathcal{G}) \setminus W^o \), then for any \( S \subseteq V \setminus (W^o \cup Z^o \cup \{X, Y\}) \)

\[
S \perp_{\mathcal{G}} X \mid W^o \cup Z^o.
\]

**Proof.** Follows by the same arguments as given for Lemma C.15.

## D Additional examples

### D.1 Additional example for Section 3

**Example D.1** (Valid conditional instrumental sets). To illustrate Theorem 3.2 and Lemma 3.3 we consider the graph \( \mathcal{G}_1 \) from Fig. 2. We are interested in classifying all valid conditional instrumental
sets relative to \((V_4, V_6)\) in \(G_1\). By Condition (i) of Theorem 3.2 no valid conditional instrumental set \(\{Z, W\}\) may contain any nodes in \(\text{for}b(V_4, V_6, G) = \{V_4, V_5, V_6, V_7\}\). Therefore, we only need to consider sets \(Z, W \subseteq \{V_1, V_2, V_3\}\). For Condition (ii) to hold, there must exist a path from \(Z\) to \(X\) that is open given \(W\) in \(G_1\). For any \(V_i\) with \(i \in \{1, 2, 3\}\) there exist three paths to \(X\) in \(G_1\): the path ending with the edge \(V_1 \rightarrow V_4\), the one ending with the edge \(V_5 \leftarrow V_4\) and the one ending with the edge \(V_5 \leftrightarrow V_6\). The latter two always include \(V_6\) as a collider and as \(\text{de}(V_6, G) = \{V_6, V_7\}\) this implies that they are both always closed given any \(W \in \{V_1, V_2, V_3\}\). The first path on the other hand does not contain a collider and is therefore only closed if there exists a node \(V_j \in W\) with \(j < i\). Therefore, Condition (ii) holds if and only if there exists an \(i \in \{1, 2, 3\}\), such that \(V_i \in Z\) and for all \(j < i, V_j \notin W\). Finally, for Condition (iii) to hold there must not be a path from \(Z\) to \(Y\) that is open given \(W\) in the graph \(G_1\), which is the graph \(G_1\) but with the edge \(V_1 \rightarrow V_5\) removed. For any \(V_i\) with \(i \in \{1, 2, 3\}\) there exist two paths to \(Y\) in \(G_1\): the path ending with the edge \(V_3 \rightarrow V_6\) and the one ending with the edge \(V_4 \leftrightarrow V_6\). The latter always includes \(V_4\) as a collider and as \(\text{de}(V_4, G_1) = \emptyset\) it is always closed given any \(W \in \{V_1, V_2, V_3\}\). The first path on the other hand does not contain a collider and is therefore only closed if there exists a node \(V_j \in W\) with \(j > i\). Therefore, Condition (iii) holds if and only if for all \(i \in \{1, 2, 3\}\), such that \(V_i \in Z\) there exists a \(j > i\) such that \(V_j \in W\). It follows that there are five possible valid conditional instrumental sets relative to \(V_4, V_6\) in \(G_1\): \(\{V_1, V_2\}, \{V_1, V_3\}, \{V_1, V_4\}, \{V_1, V_2, V_3\}\) and \(\{V_2, V_3\}\).

### D.2 Additional example for Section 4.4

To illustrate the role of the two conditions on \(Z^o\) made in Theorem 4.18 consider the acyclic directed mixed graphs in Fig. 5a and 5b denoted here as \(G_{4a}\) and \(G_{4b}\), respectively. Again, we are interested in estimating \(\gamma_{yx}\). In \(G_{4a}\), \(Z^o = \emptyset\), even though \(\{A, \emptyset\}\) is a valid conditional instrumental set relative to \((X, Y)\) in \(G_{4a}\). It is therefore an example, where \(\{Z^o, W^o\}\) is not a valid conditional instrumental set, even though one exists. In \(G_{4b}\), \(Z^o = A\) and \(W^o = \{B, C\}\), which is a valid conditional instrumental set relative to \((X, Y)\) in \(G_{4b}\). However, \(Z^o \cap (\text{pa}(X, G_{4b}) \cup \text{si}(X, G_{4b})) = \emptyset\). As a result in many Gaussian linear structural equation model compatible with \(G_{4b}\) the instrumental strength of \(\{A, \{B, C\}\}\), \(\sigma_{zx, bc} - \sigma_{zx, abc}\) will be small.

### E Supplementary material for simulations

We now provide some additional information regarding the simulations in our main paper. Reproducible code is made available at https://github.com/henckell/CodeEfficientCIS.

#### E.1 Simulation from Section 4

We first explain how we obtain the 6 models in Table 4.7 and 4.8 respectively. By Theorem 4.1 the asymptotic variances we are interested in only depend on the linear structural equation model via the matrices \(A\) and \(\Omega\). Based, on this we actually pick 6 tuples \((A, \Omega)\) that are compatible with the graph in Figure 1b and 2b respectively, rather than linear structural equation models. We select each tuple \((A, \Omega)\) randomly by drawing the non-zero entries of our two matrices as follows: For each node we sample an error variance uniformly on [0.5, 1] and for each edge an edge coefficient uniformly on
Any bidirected edge \( V_i \leftrightarrow V_j \) is simply modelled as a latent variable \( V_i \leftarrow L \rightarrow V_j \), with the error variances and edge coefficients generated as for the other nodes and edges. This random procedure is similar to the one we used in our simulation study to generate linear structural equation models randomly.

### E.2 Simulation from Section 4

For completeness we also provide violin plots for all alternative valid conditional instrumental sets in our simulation study from Section 4. In addition we also add violin plots for the ratio of the theoretical asymptotic standard deviation of \( \{ Z^o, W^o \} \) to the alternative valid tuple per Theorem 4.1. These plots arguably represent the case for \( n = \infty \), except for the biased ordinary least squares estimator.

The plots for \( G_1 \) are given in Fig. 6. We dropped the alternative valid tuple \( \{ \{ B, D \}, \{ A, C \} \} \) from the figure because it has the exact same asymptotic variance as the optimal tuple \( \{ \{ A, B, D \}, \{ A, C \} \} \) (see Example 4.10). As a result adding it would heavily distort the violin plots. The plots for \( G_2 \) are given in Fig. 7 and 8. We dropped the alternative valid tuple \( \{ \{ A, B, D \}, C \} \) from the figure because it has the exact same asymptotic variance as the optimal tuple \( \{ \{ A, B, D \}, \{ A, C \} \} \) (see Example 4.11). As a result adding it would heavily distort the violin plots.
Figure 6: Violin plot of the ratios of the root mean squared error, respectively the asymptotic standard deviation, for \( \{Z^0, W^0\} \) to the one for the tuple \( \{Z, W\} \) given on the X-axis. For the labels on the X-axis we use "OLS" to denote the ordinary least squares regression of \( Y \) on \( X \). The black dots mark the geometric mean of the ratios in the respective violin plot.
Figure 7: Violin plot of the ratios of the root mean squared error, respectively the asymptotic standard deviation, for \{Z^o, W^o\} to the one for the tuple \{Z, W\} given on the X-axis. For the labels on the X-axis we use "OLS" to denote the ordinary least squares regression of Y on X. The black dots mark the geometric mean of the ratios in the respective violin plot.
Figure 8: Violin plot of the ratios of the root mean squared error, respectively the asymptotic standard deviation, for \( \{Z^o, W^o\} \) to the one for the tuple \( \{Z, W\} \) given on the X-axis. For the labels on the X-axis we use "OLS" to denote the ordinary least squares regression of \( Y \) on \( X \). The black dots mark the geometric mean of the ratios in the respective violin plot.