Higher-order least squares: assessing partial goodness of fit of linear regression

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Abstract

We introduce a simple diagnostic test for assessing the overall or partial goodness of fit of linear regression. We propose to evaluate the sensitivity of the regression coefficient with respect to changes of the marginal distribution of covariates by comparing the so-called higher-order least squares with the usual least squares estimates. In spite of its simplicity, this strategy is extremely general and powerful, including high-dimensional settings. Specifically, we show that it allows to distinguish between confounded and unconfounded predictor variables as well as determining ancestor variables in linear structural equation models assuming some non-Gaussianity. Thus, we provide a test for partial goodness of fit.

Keywords: causal effects, confounding, model misspecification, nodewise regression, structural equation models

1 Introduction

Linear regression is one of the most commonly used statistical tools to model the relationship between a response and a set of covariates. The regression coefficient corresponding to a particular covariate is usually interpreted as its net effect on the response variable when all else is held fixed. Such an interpretation is essential in many applications and yet could be rather misleading when the linear model assumptions are in question, in particular, when there are hidden confounders.

In this work, we develop a simple but powerful approach to goodness of fit tests for potentially high-dimensional linear models, including also tests for partial goodness of fit of single predictor variables. While hidden confounding is the primary alternative in mind, different deviations from the linear model assumption are in scope as well. The concept of goodness of fit tests is very popular in econometrics where it is referred to as specification tests. For a overview, of such methods see, e.g., Godfrey (1991). Amongst the most famous of these is the testing framework introduced in Hausman (1978) which relies on knowing an estimator that is consistent even under the alternative hypothesis. Another set of related works is Buja et al. (2019a,b), which elaborately discusses deviations from the (linear) model and how distributional robustness links to correctly specified models. For this, they introduce the definition of “well-specified” statistical functionals.

While, in general, it is not possible to resolve the issue of hidden confounding, a number of useful approaches have been developed in recent years to do so by exploiting additional information or assumptions. A very popular approach to leverage the effect of potential confounders is to include
so-called “instrumental variables” into the regression. This is discussed in various places in the literature, see, e.g., the book by Bowden and Turkington (1990). The concept of instrumental variables has been further evolved in Rothenhäusler et al. (2021) leading to anchor regression, which provides predictive guarantees even in situations where the instrumental variables assumptions are not fulfilled. Another line of works that is presented in Gagnon-Bartsch and Speed (2012), Gagnon-Bartsch et al. (2013) or Gerard and Stephens (2017) goes towards using “negative controls”, i.e., variables that are known to be unassociated with the response to remove unwanted variation. Without such negative controls, one can aim to estimate latent factors and adjust for them, see, e.g., Leek and Storey (2007). The approach presented more recently by Wang and Blei (2019) also belongs to this category. A key assumption is that no confounder can influence only a single predictor variable but must have an effect on at least two predictors. For deconfounding in high-dimensional setups, rigorous guarantees are given in Çevid et al. (2020) and Guo et al. (2020) in the regime of dense confounding where the confounder influences many predictors simultaneously. All these techniques, explicitly or implicitly relying on some additional assumptions, are designed to entirely deconfound the problem. In contrast, we develop here an approach which, e.g., does not require dense confounding or valid instrumental variables, yet it still allows to infer some of the predictor variables which have a linear unconfounded effect on the response (see also the next subsection).

1.1 Our contribution

We propose a novel method or methodology, called higher-order least squares (HOLS). It bases its test statistic on the residuals that either come from a least squares or Lasso fit. In that regard, it is related to Shah and Bühlmann (2018) who use “residual prediction” to test for deviation from the linear model. However, our approach does neither assume Gaussian errors nor does it rely on sample splitting, and our novel test statistic has a $\sqrt{n}$ convergence rate (with $n$ denoting the sample size).

Besides that HOLS is leading to a “global” goodness of fit test for the entire model, we also develop a local interpretation that allows detecting which among the $p$ covariates are giving evidence for hidden confounding or non-linear relations. Thus, we strongly increase the amount of extracted information compared to a global goodness of fit test. Especially, even in the case of localised confounding, where various deconfounding techniques fail, we are able to recover the unconfounded regression parameter for a subset of predictors. We present several examples where such a partial goodness of fit test is most applicable.

The work by Buja et al. (2019a,b), especially the second paper, shows how to detect deviations in a linear model using reweighting of the data. Our HOLS technique can be seen as a special way of reweighting, providing also a simple test statistic that tests for well-specification. Distributional robustness, implied by well-specification, is also related to the causal interpretation of a linear model as discussed in Peters et al. (2016). Thus, our HOLS procedure can also be used as a method to infer causal mechanisms. We achieve this with observational data only, i.e., without the need of several, possibly interventional environments. A similar test statistic as in our HOLS procedure is used in Wang and Drton (2020) to construct the causal graph from observational data arising from a non-Gaussian linear structural equation model.

Finally and related to the previous points, our partial goodness of fit test can also be exploited to determine which covariates are ancestors of a response $Y$ in a linear structural equation or causal model. Such information is highly desirable in certain applications from, e.g., biology where
a major task is to find “up-” and “down-stream” variables of a response \( Y \).

## 1.2 Notation

We introduce some notation that we will use throughout this work. Vectors and matrices are written in boldface, while scalars have the usual lettering. This holds for both random and fixed quantities. We use upper case letters to denote a random variable, e.g., \( X \) or \( Y \). We use lower case letters to denote i.i.d. copies of a random variable, e.g., \( x \). If \( X \in \mathbb{R}^p \), then \( x \in \mathbb{R}^{n \times p} \). With a slight abuse of notation, \( x \) can either denote the copies or realisations thereof. We write \( x_j \) to denote the \( j \)-th column of matrix \( x \) and \( x_{-j} \) to denote all but the \( j \)-th column. We write \( H_0 \) to state that equality holds under \( H_0 \). With \( \leftarrow \), we emphasize that an equality between random variables is induced by a causal mechanism. We use \( \odot \) to denote elementwise multiplication of two vectors, e.g., \( x \odot y \). Similarly, potencies of vectors are also to be understood in an elementwise fashion, e.g., \( x^2 = x \odot x \). \( I_n \) is the \( n \)-dimensional identity matrix. \( P_{-j} \) denotes the orthogonal projection onto \( x_{-j} \) and \( P_{-j}^\perp = I_n - P_{-j} \) denotes the orthogonal projection onto its complement. For some random vector \( X \) we have the moment matrix \( \Sigma_X := \mathbb{E}[XX^\top] \). Note that this equals the covariance matrix for centered \( X \). We denote statistical independence by \( \perp \). We write \( e \) to denote a vector for which every entry is 1 and \( e_j \) to denote the unit vector in the direction of the \( j \)-th coordinate axis.

## 2 Low-dimensional higher-order least squares (HOLS)

We develop here the main idea of higher-order least squares (HOLS) estimation.

### 2.1 Univariate regression

It is instructive to begin with the case of simple linear regression where we have a pair of random variables \( X \) and \( Y \). We consider a linear model

\[
Y \leftarrow X \beta + \mathcal{E}, \quad \text{where} \quad X \perp \mathcal{E}, \quad \mathbb{E}[\mathcal{E}] = 0 \quad \text{and} \quad \mathbb{E}[\mathcal{E}^2] = \sigma^2. \tag{1}
\]

We formulate a null hypothesis that the model in (1) is correct and we denote such a hypothesis by \( H_0 \). Estimation of the regression parameter is typically done by the least squares principle

\[
\beta^{\text{OLS}} := \arg\min_{b \in \mathbb{R}} \mathbb{E}[(Y - Xb)^2] = \frac{\mathbb{E}[XY]}{\mathbb{E}[X^2]} H_0 = \beta,
\]

where we use the superscript OLS to denote ordinary least squares. Alternatively, we can premultiply the linear model (1) with \( f(X) \): the parameter minimizing the expected squared error loss is then

\[
\beta^{\text{TFLS}} := \arg\min_{b \in \mathbb{R}} \mathbb{E}[(f(X)Y - f(X)Xb)^2] = \frac{\mathbb{E}[f(X)^2XY]}{\mathbb{E}[f(X)^2X^2]} H_0 \frac{\mathbb{E}[f(X)^2X^2\beta]}{\mathbb{E}[f(X)^2X^2]} = \beta.
\]

More generally, \( \beta^{\text{TFLS}} = \beta^{\text{OLS}} = \beta \) for all \( f(\cdot) \) (for which the moments exist), if \( \mathbb{E}[Y|X] = X \beta \). Using the definition from \[\text{Buja et al. (2019b)}\], this means that the OLS parameter is well-specified. Instead of a generic \( f(\cdot) \), we focus on using the simple function \( f(X) = X \). The estimation principle
is called higher-order least squares, or HOLS for short, as it involves higher-order moments of $X$. This yields
\[
\beta^{HOLS} = \frac{\mathbb{E}[X^3Y]}{\mathbb{E}[X^4]} = \beta.
\]
The motivation to look at HOLS is when $H_0$ is violated, in terms of a hidden confounding variable: Let $H$ be a hidden confounder leading to a model
\[X \leftarrow \mathcal{E}_X + H \rho, \quad Y \leftarrow X \beta + H \alpha + \mathcal{E},\]
where $\mathcal{E}_X$, $H$, and $\mathcal{E}$ are all independent and $\alpha$ and $\rho$ define additional model parameters. In particular, we can compute under such a confounding model that
\[
\beta^{HOLS} - \beta^{OLS} = \rho \alpha \left( \frac{3\mathbb{E}[\mathcal{E}_X^2] \mathbb{E}[H^2] + \rho^2 \mathbb{E}[H^4]}{\mathbb{E}[\mathcal{E}_X^4] + 6 \rho^2 \mathbb{E}[\mathcal{E}_X^2] \mathbb{E}[H^2] + \rho^4 \mathbb{E}[H^4]} - \frac{\mathbb{E}[H^2]}{\mathbb{E}[\mathcal{E}_X^2] + \rho^2 \mathbb{E}[H^2]} \right). \tag{2}
\]
For simplicity, we assumed here $\mathbb{E}[\mathcal{E}_X] = \mathbb{E}[H] = \mathbb{E}[\mathcal{E}] = 0$. In practice, one can get rid of this assumption by including an intercept in the model. If either $\alpha$ or $\rho$ equals to 0, we see that the difference in (2) is 0. This is not surprising as there is no confounding effect when either $X$ or $Y$ is unaffected. However, this is not the only possibility how the difference can be 0. Namely,
\[
\mathbb{E}[H^2] \left( \mathbb{E}[\mathcal{E}_X^4] - 3 \mathbb{E}[\mathcal{E}_X^2]^2 \right) = \rho^2 \mathbb{E}[\mathcal{E}_X^2] \left( \mathbb{E}[H^4] - 3 \mathbb{E}[H^2]^2 \right) \Rightarrow \beta^{HOLS} - \beta^{OLS} = 0.
\]
Especially, if neither $\mathcal{E}_X$ nor $H$ have excess kurtosis, the difference is 0 for any $\rho$. This can be intuitively explained as it corresponds to Gaussian data (up to the moments we consider). For Gaussian $\mathcal{E}_X$ and $H$, one can always write
\[Y = X \beta^{OLS} + \tilde{\epsilon} \quad \text{where} \quad X \perp \tilde{\epsilon},\]
which cannot be distinguished from the null model [1]. Or in other words $\mathbb{E}[Y|X] = X \beta^{OLS}$, i.e., the OLS parameter is well-specified although it is not the parameter $\beta$ that we would like to recover. We discuss this further in Section [3.2]. For other data, one should be able to distinguish $H_0$ from certain deviations when hidden confounding is present. Similar behaviour occurs for a violation of $H_0$ in terms of a non-linear model $Y = f(X, \epsilon)$ which then (typically) leads to $\beta^{HOLS} - \beta^{OLS} \neq 0$.

Formally, one can construct a test based on the sample estimates of $\beta^{HOLS}$ and $\beta^{OLS}$. We consider the centered data
\[\tilde{x} = x - \bar{x} e \quad \text{and} \quad \tilde{y} = y - \bar{y} e \quad \text{and} \quad \tilde{\epsilon} = \epsilon - \bar{\epsilon} e = \left( I_n - \frac{1}{n} ee^\top \right) \epsilon,\]
where we use the upper bar to denote sample means. We can derive
\[\tilde{y} = y - \bar{y} e = x \beta - \bar{x} e \beta + \epsilon - \bar{\epsilon} e = \tilde{x} \beta + \tilde{\epsilon}.
\]
We now obtain $\beta^{OLS}$ from regression through the origin of $\tilde{y}$ versus $\tilde{x}$ with an error term of $\tilde{\epsilon}$ and $\beta^{HOLS}$ from regression through the origin of $\tilde{x} \odot \tilde{y}$ versus $\tilde{x}^2$ with an error term of $\tilde{x} \odot \tilde{\epsilon}$. More precisely, we define
\[\beta^{OLS} := \frac{\tilde{x}^\top \tilde{y}}{\tilde{x}^\top \tilde{x}} \quad \text{and} \quad \beta^{HOLS} := \frac{(\tilde{x}^2)^\top (\tilde{x} \odot \tilde{y})}{(\tilde{x}^2)^\top (\tilde{x}^2)} = \frac{(\tilde{x}^3)^\top (\tilde{y})}{(\tilde{x}^2)^\top (\tilde{x}^2)}.\]
Under $H_0$, one can see that $(\hat{\beta}_{HOLS} - \hat{\beta}_{OLS})$ given $x$ is some known linear combination of $\epsilon$. Assuming further Gaussianity of $\epsilon$, it is conditionally Gaussian. We find

$$
\left(\hat{\beta}_{HOLS} - \hat{\beta}_{OLS}\right) \mid x \sim \mathcal{N}\left(0, \sigma^2 \left(\frac{1}{n} \left(\sum_{i=1}^{n} \tilde{x}_i^3\right)^2 - \frac{1}{n} \left(\tilde{x}^2\right)^2 \left(\tilde{x}_1^2\right)^2 \right)^{-1}\right).
$$

We can calculate this variance except for $\sigma^2$. Further, we can consistently estimate $\sigma^2$, for example, with the standard formula

$$
\hat{\sigma}^2 = \frac{\|\tilde{y} - \tilde{x}_j^{OLS}\|^2}{n-1}.
$$

Thus, we receive asymptotically valid z-tests for the null-hypothesis $H_0$ that the model (1) holds. We treat the extension to non-Gaussian $\epsilon$ in Section 2.2.1 (for the multivariate case directly). As discussed above, in the presence of confounding, we can have that $\beta_{HOLS} \neq \beta_{OLS}$. In such situations, a test assuming (3) will have asymptotic power equal to 1 for correctly rejecting $H_0$ under some conditions. These asymptotic results are discussed in Section 3.1 and Section 3.2.1.

2.2 Multivariate regression

For real data analysis, we typically want to examine the goodness of fit of a linear model with $p > 1$ covariates. We consider the model

$$
Y \leftarrow X^\top \beta + \epsilon, \text{ where } X \perp \epsilon, \quad \mathbb{E}[^\epsilon] = 0 \text{ and } \mathbb{E}[\epsilon^2] = \sigma^2
$$

(4)

with $X \in \mathbb{R}^p$ and $\beta \in \mathbb{R}^p$. Note that $\mathbb{E}[\epsilon] = 0$ can always be enforced by including an intercept in the set of predictors. We formulate a global null hypothesis that the model in (4) is correct and we denote it by $H_0$. The idea is to consider every component $j \in \{1, \ldots, p\}$ separately and work with partial regression. For the population version, we define

$$
\begin{align*}
Z_j &:= X_j - X_{-j}^\top \gamma_j, \quad \text{where } \gamma_j := \arg\min_{\beta \in \mathbb{R}^{p-1}} \left(\text{E}[^{X_j - X_{-j}^\top \beta}]^2 \right) = (\Sigma_{x_{-j}, -j})^{-1} \text{E}[^{X_{-j} X_j}] \\
W_j &:= Y - X_{-j}^\top \zeta_j, \quad \text{where } \zeta_j := \arg\min_{\beta \in \mathbb{R}^{p-1}} \left(\text{E}[^{Y - X_{-j}^\top \beta}]^2 \right) = (\Sigma_{x_{-j}, -j})^{-1} \text{E}[^{X_{-j} Y}].
\end{align*}
$$

(5)

Under $H_0$, it holds that $W_j = Z_j \beta_j + \epsilon$. For $\beta_{OLS} := (\Sigma X)^{-1} \text{E}[^{XY}]$, we find

$$
\beta_{OLS} = \frac{\text{E}[Z_j W_j]}{\text{E}[Z_j^2]} \overset{H_0}{\Rightarrow} \beta_j.
$$

We define the according HOLS parameter by partial regression for every component $j$ separately, namely

$$
\beta_{HOLS}^j := \frac{\text{E}[Z_j^2 W_j]}{\text{E}[Z_j^4]} \overset{H_0}{\Rightarrow} \beta_j.
$$

5
Essentially, $\hat{\beta}^{\text{OLS}}_j \neq \hat{\beta}^{\text{HOLS}}_j$ is a test for $\mathbb{E}[W_j | Z_j] \neq Z_j \beta^{\text{OLS}}_j$. The difference $\hat{\beta}^{\text{OLS}}_j - \hat{\beta}^{\text{HOLS}}_j$ can detect certain local alternatives from the null hypothesis $H_0$. Here, local refers to the covariate $X_j$ whose effect on $Y$ is potentially confounded or involves a non-linearity. The details and some more concrete examples are discussed in Sections 3 and 4.

We turn to sample estimates of these parameters. The residuals are estimated by

$$
\hat{z}_j = x_j - P_{-j}x_j = P_{-j}^\perp x_j \quad \text{and} \\
\hat{w}_j = y - P_{-j}y = P_{-j}^\perp y \overset{H_0}{=} P_{-j}^\perp (x\beta + \epsilon) = \hat{z}_j \beta_j + P_{-j}^\perp \epsilon.
$$

With ordinary least squares, we receive $\hat{\beta}^{\text{OLS}}_j$ from regression of $\hat{w}_j$ versus $\hat{z}_j$, where the error term is $P_{-j}^\perp \epsilon$. Accordingly, we calculate $\hat{\beta}^{\text{HOLS}}_j$ from regression of $\hat{z}_j \odot \hat{w}_j$ versus $\hat{z}_j^2$ with an error term $\hat{z}_j \odot P_{-j}^\perp \epsilon$. Thus, we define

$$
\hat{\beta}^{\text{OLS}} := \frac{\hat{z}_j^\top \hat{w}_j}{\hat{z}_j^\top \hat{z}_j} \quad \text{and} \quad \hat{\beta}^{\text{HOLS}} := \frac{\left(\hat{z}_j^2 \odot \hat{z}_j \odot \hat{w}_j\right)^\top}{\left(\hat{z}_j^2 \odot \hat{z}_j \odot \hat{z}_j\right)} = \frac{\left(\hat{z}_j^3\right)^\top}{\left(\hat{z}_j^2 \odot \hat{z}_j \odot \hat{z}_j\right)} \hat{w}_j.
$$

(6)

This is analogous to the univariate case, where we have $\bar{y}$ instead of $\hat{w}_j$, $\bar{x}$ instead of $\hat{z}_j$ and $(I_n - \frac{1}{n}ee^\top)$ instead of $P_{-j}^\perp$. $(I_n - \frac{1}{n}ee^\top)$ can be thought of as orthogonal projection onto e's complement, which completes the analogy. Again, we see that $(\hat{\beta}^{\text{HOLS}}_j - \hat{\beta}^{\text{OLS}}_j)$ given $x$ is some known linear combination of $\epsilon$, thus, it is conditionally Gaussian for Gaussian $\epsilon$. The same naturally holds for $(\hat{\beta}^{\text{HOLS}}_j - \hat{\beta}^{\text{OLS}}_j)$.

**Theorem 1.** Assume the null hypothesis 4 with Gaussian $\mathcal{E}$. Then

$$
(\hat{\beta}^{\text{HOLS}}_j - \hat{\beta}^{\text{OLS}}_j) \mid x \sim \mathcal{N}\left(0, \sigma^2 \frac{1}{n^2} v^\top v\right), \quad \text{with} \quad v_j = \frac{P_{-j}^\perp (\hat{z}_j^3)}{\frac{1}{n} \left(\hat{z}_j^2 \odot \hat{z}_j \odot \hat{z}_j\right)} - \frac{\hat{z}_j}{\frac{1}{n} \hat{z}_j^\top \hat{z}_j}.
$$

With a consistent estimate of $\sigma^2$, we can thus test the null hypothesis $H_0$. Such a consistent estimate can be obtained, e.g., using the standard formula

$$
\hat{\sigma}^2 = \frac{\|y - x\hat{\beta}^{\text{OLS}}\|^2}{n - p}.
$$

We define for latter reference

$$
\hat{\text{Var}}(\hat{\beta}^{\text{HOLS}}_j - \hat{\beta}^{\text{OLS}}_j) := \hat{\sigma}^2 \frac{1}{n^2} \hat{v}^\top \hat{v}.
$$

(7)

To test for a single variable, we can compare $(\hat{\beta}^{\text{HOLS}}_j - \hat{\beta}^{\text{OLS}}_j)$ to the quantiles of the univariate normal distribution with the according variance. The joint distribution leads to a global test that controls the family-wise error rate (FWER) if $H_0$ is true. Namely, one can look at the maximum test statistic $T = \max_k \left|\hat{\beta}^{\text{HOLS}}_k - \hat{\beta}^{\text{OLS}}_k\right| \sim \max_k |S_k|$, where $S \sim \mathcal{N}(0, \hat{\sigma}^2 \frac{\hat{v}^\top \hat{v}}{n^2})$ can be easily simulated.
Further, one receives multiplicity corrected individual p-values by comparing each \( \tilde{\beta}_j^{HOLS} - \beta_j^{OLS} \) to the distribution of \( \max|S_k| \). This is in analogy to the multiplicity correction suggested by [Bühlmann (2013)](#Buehmann2013). Naturally, other multiplicity correction techniques such as Bonferroni correction are valid as well. Again, all the tests are only asymptotically valid due to the estimation of \( \sigma^2 \).

Algorithm 1 summarizes how to find both raw p-values as well as multiplicity corrected p-values for each variable, \( p_j \) and \( P_j \) respectively, using the correction technique described above. Then, one would reject the global null hypothesis given by model (4) if \( \min_{j} P_j \leq \alpha \), and such a decision procedure provides strong control of the familywise error rate at level \( \alpha \). We will discuss later in the sequel how to use the adjusted p-values \( P_j \) for other purposes than testing the global null-hypothesis \( H_0 \).

**Algorithm 1 HOLS check**

1. for \( j = 1 \) to \( p \) do
2. \( P_{-j} = I_n - x_{-j}(x_{-j}^\top x_{-j})x_{-j}^\top \)
3. Regress \( x_j \) versus \( x_{-j} \) via least squares, denote the residual by \( \tilde{x}_j = P_{-j}x_j \)
4. Regress \( y \) versus \( x_{-j} \) via least squares, denote the residual by \( \tilde{w}_j = P_{-j}y \)
5. \[ \hat{\beta}_j^{OLS} = \tilde{z}_j^\top \tilde{w}_j, \hat{\beta}_j^{HOLS} = \frac{\tilde{z}_j^3}{\tilde{z}_j} \left( \tilde{w}_j \right) \] and \( \hat{v}_j = \frac{P_{-j}(\tilde{z}_j^3)}{n} \left( \frac{1}{\tilde{z}_j^3} - \frac{1}{\tilde{z}_j^2} \right) - \frac{\tilde{z}_j}{n} \tilde{y}_j \)
6. \[ \hat{\sigma}^2 = \frac{\|y - x_\beta^{OLS}\|^2_2}{n - p} \]
7. Create \( n_{\text{sim}} \) i.i.d copies of \( S \sim N(0, \hat{\sigma}^2 \hat{v}^\top \hat{v}/n^2) \), say, \( s^1 \) to \( s^{n_{\text{sim}}} \)
8. for \( j = 1 \) to \( p \) do
9. \( p_j = 2 * \left( 1 - \Phi^{-1} \left( \frac{\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}}{\hat{\sigma}\|\hat{v}_j\|_2} \right) \right) \)
10. \( P_j = \frac{1}{n_{\text{sim}}} \sum_{i=1}^{n_{\text{sim}}} 1\left( \left| \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right| > \|s^i\|_\infty \right) \)

### 2.2.1 Non-Gaussian errors

Naturally, Gaussianity, which is invoked for Theorem 1 is a strong assumption, and we would consider the interpretation of model (4) to be equivalent without requiring Gaussian \( E \). For other distributions, we can invoke the central limit theorem. We make the following extra assumptions:

(A1) The moment matrix \( \Sigma^X \) has positive smallest eigenvalue, i.e., it is invertible and its inverse has bounded eigenvalues.

(A2) \( \mathbb{E}[X_j^6] < \infty \) and \( \mathbb{E}[Z_j^6] < \infty \) \( \forall j \).

Further, let
\[
\tilde{Z}_j^3 := Z_j^3 - X_{-j}^\top \tilde{\gamma}_j, \quad \text{where} \quad \tilde{\gamma}_j := \arg\min_{b \in \mathbb{R}^{p-1}} \mathbb{E}
\left[
(Z_j^3 - X_{-j}^\top b)^2
\right]
= (\Sigma_{-j,-j})^{-1} \mathbb{E}[X_{-j}Z_j^3].
\] (8)
Note that \( \mathbb{E} \left[ \left( \hat{Z}_j^3 \right)^2 \right] \leq \mathbb{E} \left[ Z_j^6 \right] < \infty \).

**Theorem 2.** Assume that the data follows the model (4) and that (A1) - (A2) hold. Let \( p \) be fixed and \( n \to \infty \). Then,

\[
\sqrt{n} \left( \beta^{\text{HOLS}} - \beta^{\text{OLS}} \right) \overset{\mathbb{D}}{\to} \mathcal{N} \left( 0, \sigma^2 \mathbb{E} \left[ VV^\top \right] \right) \\
\frac{1}{n} \hat{\psi}^\top \hat{\psi} \overset{\mathbb{P}}{\to} \mathbb{E} \left[ VV^\top \right],
\]

where \( V_j = \frac{\hat{Z}_j^3}{\mathbb{E} \left[ Z_j^3 \right]} - \frac{Z_j}{\mathbb{E} \left[ Z_j^2 \right]} \).

**Corollary 1.** Assume the conditions of Theorem 2. Consider the decision rule to reject \( H_0 \) iff \( \min_j P_j \leq \alpha \), where \( P_j \) as in Step 10 of Algorithm 1. Then, the familywise error rate is asymptotically controlled at \( \alpha \).

**Simulation example** We create data that follows the model (4). We chose the sample size and dimensionality to be \( n = 100 \) and \( p = 30 \) and sample \( X \) as follows. Let \( \Psi_1, \ldots, \Psi_p \) be i.i.d. random variables. Each of these follows a mixture distribution such that every copy comes from a \( \mathcal{N}(0, 0.5) \) distribution with probability \( \frac{2}{3} \) or from a \( \mathcal{N}(0, 2) \) distribution with probability \( \frac{1}{3} \). Thus, they are 0 mean and unit variance random variables. Then, set \( X_1 = \Psi_1 \) and

\[
X_j = r X_{j-1} + \sqrt{1 - r^2} \Psi_j \quad (\forall j > 1)
\]

This leads to a Toeplitz covariance structure \( \Sigma_X \) with \( \Sigma_X^{ij} = r^{|i-j|} \), where we set \( r = 0.6 \). The coefficient vector \( \beta \) is 5-sparse, and the active predictors are \( \{1, 5, 10, 15, 20\} \), each of which having a coefficient equal to 1. The random error \( \xi \) follows the same non-Gaussian distribution as the \( \Psi_j \).

We run 200 simulations of this setup. For every simulation run, we calculate the p-value per predictor (without multiplicity adjustment). Asymptotically, these p-values would be uniformly distributed as the model assumptions hold true. In Figure 1 we analyse these p-values by looking at their histogram and the empirical cumulative density function (ECDF). The plots are combined over all the \( p = 30 \) covariates. Thus, they are based on 6000 p-values.

We see that even though the error does not have a Gaussian distribution, the p-values still are very close to being uniformly distributed.

### 3 The confounded case and local null hypotheses

In this section and the following, we mainly exploit confounding in linear models as alternative hypothesis since these are the models where our local interpretation is most informative. For a discussion of which interpretations might carry over to more general data structures, we refer to Section 7.1.

We look at the model

\[
X \leftarrow \rho H + \xi_X \\
Y \leftarrow X^\top \beta + H^\top \alpha + \xi,
\]

(9)
where $H \in \mathbb{R}^d$, $E_X \in \mathbb{R}^p$ and $E \in \mathbb{R}$ are independent and centered random variables, and $\alpha \in \mathbb{R}^d$ and $\rho \in \mathbb{R}^{p \times d}$ are fixed model parameters. Thus, there exists some hidden confounder $H$. For the inner product matrices, it holds that

$$
\Sigma_X = \Sigma_{E_X} + \rho \Sigma_H \rho^\top.
$$

Furthermore, we have

$$
\beta^{OLS} = (\Sigma_X)^{-1} \mathbb{E}[XY] = (\Sigma_X)^{-1}(\Sigma_X \beta + \rho \Sigma_H \alpha) = \beta + (\Sigma_X)^{-1} \rho \Sigma_H \alpha.
$$

We will generally refer to $\beta^{OLS}_j \neq \beta_j$, where $\beta_j$ is according to model (9), as confounding bias on $\beta^{OLS}_j$. Further, when writing directly confounded, we mean covariates $j$ for which $X_j \neq E_j$.

Note that we can always reformulate our model both globally and locally as follows

$$
Y = X^\top \beta^{OLS} + \tilde{\epsilon}, \quad \text{with} \quad \mathbb{E}[X \tilde{\epsilon}] = 0, \quad \mathbb{E}[\tilde{\epsilon}] = 0 \quad \text{but (potentially)} \quad X \not\perp \tilde{\epsilon} \quad (10)
$$

$$
W_j = Z_j \beta^{OLS}_j + \tilde{\epsilon}, \quad \text{with} \quad \mathbb{E}[Z_j \tilde{\epsilon}] = 0, \quad \mathbb{E}[\tilde{\epsilon}] = 0 \quad \text{but (potentially)} \quad Z_j \not\perp \tilde{\epsilon} \quad (11)
$$

using the definitions from (5). We now want to see how $\beta^{OLS}$ relates to $\beta$ in certain models. Especially, we are interested in whether there is some potential local interpretation in the sense of distinguishing between “confounded” and “unconfounded” variables. Using the Woodbury matrix identity, we find

$$
\beta^{OLS}_j = \beta_j \quad \text{if} \quad (\Sigma_{E_X})^{-1} \rho = 0 \quad \text{which is implied by}
$$

$$
\left\{ k \in \{1, \ldots, p\} : (\Sigma_{E_X})^{-1}_{jk} \neq 0 \right\} \cap \left\{ l \in \{1, \ldots, p\} : \|e_l^\top \rho\| > 0 \right\} = \emptyset \quad (12)
$$

Figure 1: Results for non-Gaussian design under the global null. On the left: histogram of p-values (unadjusted $p_j$ as in Step 9 of Algorithm 1) over all $p = 30$ predictors. On the right: ECDF of these p-values. The grey dotted line corresponds to the desired uniform distribution.
Thus, if the intersection between covariates that have predictive power for $X_j$ and covariates that are directly confounded is empty, it must hold that $\beta_j^{\text{OLS}} = \beta_j$. Therefore, we can indeed say that for these variables we estimate the true causal effect using ordinary least squares.

To correctly detect these variables, we would like $\beta_j^{\text{HOLS}} = \beta_j^{\text{OLS}} = \beta_j$. As $\beta_j^{\text{HOLS}}$ involves higher-order moments, knowledge of the covariance structure is not sufficient to check this. From (11), we see $\mathbb{E}\left[Z_j^3 \tilde{E}\right] = 0$ is necessary and sufficient to ensure it. Furthermore, having zeroes in the precision matrix is typically related to certain modelling assumptions for which also the higher-order moments are under control. In Section 4, we present such models for which we can characterise a set of variables for which $\beta_j^{\text{HOLS}} = \beta_j^{\text{OLS}} = \beta_j$.

### 3.1 Sample estimates

For a confounded model, the hope is that the global test $\min_j P_j \leq \alpha$, where $P_j$ is the adjusted p-value according to Step 10 in Algorithm 1, leads to a rejection of the modelling assumption (4). Then, one would split the predictors into a set for which we have evidence that $\beta_j^{\text{OLS}} \neq \beta_j$ and a set for which we do not have such evidence based on $P_j$. We consider in the following this local interpretation, showing that we asymptotically control the type-I error and receive power approaching 1. Implicitly, we have to assume that $\beta_j^{\text{HOLS}} - \beta_j^{\text{OLS}} \neq 0$ is a useful proxy for $\beta_j - \beta_j^{\text{OLS}} \neq 0$. In Section 3.2, we discuss cases where this might fail.

Beyond the null model (4), the sample estimates (cf. (6)) are less straightforward to analyse. However, using certain assumptions, one can still assess their asymptotic behaviour for $n \to \infty$. Therefore, we discuss in the following to what limiting quantities the estimates $\hat{\beta}_j^{\text{OLS}} - \hat{\beta}_j^{\text{HOLS}}$ as well as the according variance estimates (cf. (7)) converge to and how fast this convergence is. For all asymptotic results in this section we assume $p$ to be fixed and $n \to \infty$ as in Theorem 2.

**Theorem 3.** Assume that the data follows the model (10) and that (A1)-(A2) hold. Assume further $\sigma^2_{\tilde{E}} = \mathbb{E}\left[\tilde{E}^2\right] < \infty$. Then,

$$
\hat{\beta}_j^{\text{OLS}} = \beta_j^{\text{OLS}} + o_p(1), \quad \hat{\beta}_j^{\text{HOLS}} = \beta_j^{\text{HOLS}} + o_p(1) \quad \text{and} \quad \hat{\text{Var}}\left(\hat{\beta}_j^{\text{HOLS}} - \hat{\beta}_j^{\text{OLS}}\right) = O_p\left(\frac{1}{n}\right),
$$

where $\hat{\text{Var}}\left(\hat{\beta}_j^{\text{HOLS}} - \hat{\beta}_j^{\text{OLS}}\right)$ is according to (7).

Thus, for some fixed alternative $\left|\beta_j^{\text{HOLS}} - \beta_j^{\text{OLS}}\right| > 0$, the absolute z-statistics increases as $\sqrt{n}$.

In order to get some local interpretation, the behaviour for unconfounded variables is of importance. With unconfounded, we mean variables $j$ with $\beta_j^{\text{OLS}} = \beta_j^{\text{HOLS}}$. If $\left|\beta_j^{\text{HOLS}} - \beta_j^{\text{OLS}}\right| = 0$, Theorem 3 is not sufficient to understand the asymptotic behaviour. We refine the results using additional assumptions.

(A3) $\mathbb{E}\left[\left(X_j \tilde{E}\right)^2\right] < \infty \forall j$ \hspace{1cm} (B2) $Z_j \perp \tilde{E}$

(B1) $\mathbb{E}\left[Z_j^2 X_k \tilde{E}\right] = 0 \forall k \neq j$ \hspace{1cm} (B3) $\tilde{Z}_j^3 \perp \tilde{E}$

Note that we use different letters for the assumptions to distinguish between those that are essentially some (mild) moment conditions and those that truly make nodes unconfounded. Obviously, (B2) is not necessary for $\beta_j^{\text{OLS}} = \beta_j^{\text{HOLS}}$, but we will focus on these variables as these are
the ones that are truly unconfounded in the sense that the projected single variable model (11) has an independent error term, while for other variables it can be rather considered an unwanted artefact of our method. Furthermore, the derived asymptotic variance results only apply assuming (B2) and (B3). Assumption (A3) implies a further moment condition. Especially, when considering non-linearities, there exist cases for which (A3) is not implied by (A2). We discuss Assumptions (B1), (B2) and (B3) for certain models in Section 4. Condition (B1) seems to be a bit artificial but is invoked in the proofs. We argue in Section 4 that it is naturally linked to the models in scope.

Theorem 4. Assume that the data follows the model (10) and that (A1) - (A3) hold. Let $j$ be some covariate with $\beta_j^{OLS} = \beta_j^{HOLS}$ for which (B1) - (B3) hold. Then, 

$$\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}) \overset{D}{\rightarrow} N(0, 1).$$

Thus, for these predictors we receive asymptotically valid tests.

Multiplicity correction In order not to falsely reject the local null hypothesis for any covariate with $\beta_j = \beta_j^{OLS} = \beta_j^{HOLS}$ (with probability at least $1 - \alpha$), we need to invoke some multiplicity correction. Analogously to Section 2.2, one can see that $\hat{\beta}^{HOLS} - \hat{\beta}^{OLS} = \hat{v}^\top \hat{e}/n$, which enables the previous multiplicity correction as in Algorithm 1.

Theorem 5. Assume that the data follows the model (10) and that (A1) - (A3) hold. Let $U'$ be the set of variables $j$ for which $\beta_j^{HOLS} = \beta_j^{OLS}$ and (B1) - (B3) hold. Then, 

$$\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}) \overset{D}{\rightarrow} N(0, \sigma^2 \hat{\epsilon}^\top \hat{\epsilon} / n).$$

Corollary 2. Assume the conditions of Theorem 5. Let $H_{0,j} : \beta_j^{OLS} = \beta_j^{HOLS}$. Consider the decision rule to reject $H_{0,j}$ iff $P_j \leq \alpha$, where $P_j$ as in Step 10. of Algorithm 1. Then, the familywise error rate amongst the set $U'$ is asymptotically controlled at $\alpha$.

3.2 What can be detected

Consider the set

$$U = \{j; H_{0,j} \text{ is true}\},$$

where $H_{0,j} : \beta_j^{OLS} = \beta_j^{HOLS}$, (13)

which is the set that we try to infer with our HOLS check. Naturally, one would rather be interested in the set $V = \{j : \beta_j^{OLS} = \beta_j\}$, which consists of the variables for which we can consistently estimate the true causal linear effect according to (9) through linear regression. We use $U$ as proxy for $V$. Therefore, we want to discuss how $U$ relates to $V$ and especially analyse how variables could belong to the difference between the sets. For this, recall our formulation of the model when the global null hypothesis does not hold true in (10) and (11) such that $j \in U$ iff $\mathbb{E}[Z_j^3 \hat{\epsilon}] = 0$.

For any variable $j \in U \setminus V$, certain modelling assumptions, that we discuss in the sequel, cannot be fulfilled as otherwise it would be in $V$ as well. However, these assumptions are not necessary
for $\mathbb{E}[Z_j^2\tilde{E}] = 0$. Especially, the equality always holds if both $\tilde{X}$ and $H$ jointly have Gaussian kurtosis. If they are even jointly Gaussian, then it is clear that $X \perp \tilde{E}$ such that the model \((10)\) has independent Gaussian error. Thus, when using only observational data, it behaves exactly like a model under the global null hypothesis and, naturally, we cannot infer the confounding effect. Apart from Gaussian kurtosis, $j \in U \setminus V$ would be mainly due to spurious cancellation of terms that one does not expect to encounter in arbitrary setups.

For $j \in V \setminus U$, $Z_j$ and $\tilde{E}$ must not be independent. As $Z_j \not\perp \tilde{E}$, the single-covariate model \((11)\) is not a linear model with independent error term. Therefore, one can argue that rejecting the local null hypothesis is the right thing to do in this case. Furthermore, having variables $j \in V$ is usually related to certain model assumptions except for very specific data setups that lead to cancellation of terms. Under these assumptions, $Z_j \perp \tilde{E}$ is then usually implied. An example where $\hat{\beta}_{OLS} = \beta$, but $(potentially)$ $X \not\perp \tilde{E}$ is $\rho \Sigma H \alpha = 0$.

### 3.2.1 Recovery of $U$

Based on our asymptotic results when the global null does not hold true, we would like to construct a method that perfectly detects the unconfounded variables as $n \to \infty$. For this, enhance the definition of $U$ to

\[
\hat{U} = \{j; H_{0,j} \text{ not rejected}\} \text{ and } U = \{j; H_{0,j} \text{ is true}\}, \quad \text{where } H_{0,j} : \hat{\beta}_j^{OLS} = \hat{\beta}_j^{HOLS}. \quad (14)
\]

For some interpretation of $U$, see Section 3.2. The question is how and when can we ensure that

\[
\lim_{n \to \infty} \mathbb{P}[\hat{U} = U] = 1.
\]

This can be split into two problems, namely,

\[
\lim_{n \to \infty} \mathbb{P}[\hat{U} \subseteq U] = 1 \text{ and } \lim_{n \to \infty} \mathbb{P}[\hat{U} \supseteq U] = 1. \quad (15)
\]

The first one corresponds to not wrongly accepting any $H_{0,j}$ and the second one to no wrong rejection. Suppose that we conduct our local $z$-tests at level $\alpha_n$, which varies with the sample size such that $\alpha_n \to 0$ as $n \to \infty$. It will be more convenient to interpret this as a threshold on the (scaled) absolute $z$-statistics, say, $\tau_n$ that grows with $n$, where the $z$-statistics is defined as

\[
s_j = \frac{\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS})}{\sqrt{\text{Var}(\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}))}}.
\]

We refrain from calling it $z_j$ to avoid confusion. We use an additional assumption which is a relaxed version of (B3).

(A4) $\mathbb{E}\left[Z_j^2\tilde{E}\right] < \infty$

**Theorem 6.** Assume that the data follows the model \((10)\) and that (A1) - (A3) hold. Assume that (B1) and (A4) hold $\forall j \in U$. Let $\tau_n$ be the threshold on the absolute $z$-statistics to reject the according null hypothesis with $\tau_n = \sigma(\sqrt{n})$ and $1/\tau_n = \sigma(1)$. Then,

\[
\lim_{n \to \infty} \mathbb{P}[\hat{U} = U] = 1.
\]

In other words, we can choose $\tau_n$ to grow at any rate slower than $\sqrt{n}$.
4 Specific models

In this section, we discuss two types of models where the local interpretation applies. In these settings, there are variables for which $\beta_j = \beta_{j,OLS} = \beta_{j,HOLS}$ and assumptions (B1)-(B3) hold even though the overall data follows the model (9). We note here first that the model of jointly Gaussian $\mathcal{E}_X$, for which the method is suited, is a special case of the model in Section 4.2 below.

4.1 Block independence of $\mathcal{E}_X$

Assume that the errors $\mathcal{E}_X$ can be grouped into two or more independent and disjoint blocks. Denote the block that includes $j$ by $B(j)$. Then, it is clear that $(\Sigma^{\mathcal{E}_X})^{-1} = 0$ if $B(j) \neq B(k)$. If $X_{B(j)} = \mathcal{E}_{B(j)}$, i.e., the confounder has no effect onto $X_{B(j)}$, (12) holds for all covariates in $B(j)$ such that $X_{B(j)}$ is not involved in regressing out the effect of $\mathbf{H}^T \alpha$. Due to the block independence, this yields $X_{B(j)} \perp \tilde{\mathcal{E}}$ and $Z_j \perp \tilde{\mathcal{E}}$, i.e., (B2) is fulfilled. This also ensures $\mathbb{E}[Z_j^3 \tilde{\mathcal{E}}] = 0$. We consider the remaining assumptions: Naturally, the regression $Z_j$ versus $X_{-j}$ only involves $X_{B(j)} \setminus j$ and (B3) holds as well. For (B1), separately consider the case $k \in B(j)$ and $k \notin B(j)$. In the first case, $\mathbb{E}[Z_j^3 X_k \tilde{\mathcal{E}}] = \mathbb{E}[Z_j^3 X_k] \mathbb{E}[\tilde{\mathcal{E}}] = 0$. In the second case, $\mathbb{E}[Z_j^3 X_k \tilde{\mathcal{E}}] = \mathbb{E}[Z_j^3] \mathbb{E}[X_k \tilde{\mathcal{E}}] = 0$.

**Theorem 7.** Assume the data follows the model (9) with errors $\mathcal{E}_X$ that can be grouped into independent blocks. Then, $\beta_{j,HOLS} = \beta_{j,OLS} = \beta_j$ for which $X_{B(j)} = \mathcal{E}_{B(j)}$. Further, (B1)-(B3) hold for which $X_{B(j)} = \mathcal{E}_{B(j)}$.

4.2 Linear structural equation model

From the previous sections, we know that locally unconfounded structures, in the sense that $\beta_j = \beta_{j,OLS}$, are strongly related to zeroes in the precision matrix. Thus, the question arises for what type of models having zeroes in the precision matrix is a usual thing. Besides block independence, which we have discussed in Section 4.1, this will mainly be the case if the data follows a linear structural equation model (SEM). Thus, we will focus on this linear SEM for the interpretation of local, i.e., by parameter, null hypotheses.

To start, assume that there are no hidden variables. So, let $X$ be given by the following linear SEM

$$X_j \leftarrow \Psi_j + \sum_{k \in \text{PA}(j)} \theta_{j,k} X_k \quad j = 1, \ldots, p,$$

where the $\Psi_1, \ldots, \Psi_p$ are independent and centered random variables. We use the notation $\text{PA}(j)$, $\text{CH}(j)$ and $\text{AN}(j)$ for $j$’s parents, children and ancestors. Further, assume that there exists a directed acyclic graph (DAG) representing this structure. For this type of model, we know that a variable’s Markov boundary consists of its parents, its children, and its children’s other parents. For every other variable $k$ outside of $j$’s Markov boundary, we have $(\Sigma^X)^{-1}_{jk} = 0$. Thus, these 0 partial correlations are very usual. In the following, we will analyse how our local tests are especially applicable to this structure.

In the context of linear SEM, hidden linear confounders can be thought of as unmeasured variables. Therefore, we split $X$ which contains all possible predictors into two parts. Let $X_M$ be
the measured variables and $X_N$ the hidden confounder variables. Let $\Psi = (\Psi_1, \ldots, \Psi_p)^\top$ with the according subsets $\Psi_M$ and $\Psi_N$. Then, we can write

$$X = \omega \Psi, \quad X_M = \omega_{M,M} \Psi_M + \omega_{M,N} \Psi_N \quad \text{and} \quad X_N = \omega_{N,M} \Psi_M + \omega_{N,N} \Psi_N$$

for some suitable $\omega \in \mathbb{R}^{p \times p}$, where $\omega_{k,l} = 0$ for $k \neq l$ if $l \not\in \text{AN}(k)$ and $\omega_{k,k} = 1$. Note that $\omega_{M,M}$ is always invertible since it can be written as a triangular matrix with ones on the diagonal if permuted properly. To avoid confusion, we call the parameter if all predictors were observed $\beta^*$. This leads to the definitions

$$\varepsilon_X := \omega_{M,M} \Psi_M, \quad \rho := \omega_{M,N} \quad \text{and} \quad H := \Psi_N$$

such that

$$Y - \varepsilon = X^\top \beta^* = X_M^\top \beta^*_M + X_N^\top \beta^*_N$$

$$= X_M^\top \left( \beta^*_M + \left( \omega_{N,M} \omega_{M,M}^{-1} \right)^\top \beta^*_N \right) + H^\top \left( \omega_{N,N} - \omega_{N,M} \omega_{M,M}^{-1} \omega_{M,N} \right)^\top \beta^*_N := X_M^\top \beta + H^\top \alpha.$$

This is exactly a model as in [1]. When only the given subset is observed we are interested in the parameter $\beta$ as before. We have $\beta_j = \beta_j^*$ iff $(\omega_{N,M} \omega_{M,M}^{-1})^\top \beta_j^* = 0$.

**Theorem 8.** Assume that the data follows the model (16). Let $X_M$ and $X_N$ be the observed and the hidden variables. Denote by $\text{PA}^M(k)$ the closest ancestors of $k$ that are in $M$. Consider some $j \in M$.

If $\not\exists k \in N : (j \in \text{PA}^M(k) \text{ and } \beta_k \neq 0)$, then $\beta_j = \beta_j^*$.

In other words, the causal parameter can only change for variables that have at least one direct descendant in the hidden set which is a parent of $Y$ itself. By direct descendant, we mean that there is a path from $j$ to $k$ that does not pass any other observed variable. We analyse for which variables we can reconstruct this causal parameter using ordinary least squares regression.

**Theorem 9.** Assume that the data follows the model (16). Let $X_M$ and $X_N$ be the observed and the hidden variables. Then,

$$\beta_j^{\text{HOLS}} = \beta_j^{\text{OLS}} = \beta_j \forall j \in M \quad \text{that are not in the Markov boundary of any hidden variable. Further,}$$

$$[\text{B1}]-[\text{B3}] \quad \text{hold } \forall j \in M \quad \text{that are not in the Markov boundary of any hidden variable.}$$

Thus, for those variables, we can a) correctly retrieve the causal parameter using ordinary least squares regression and b) detect that this is the true parameter by comparing it to $\beta_j^{\text{HOLS}}$.

**Simulation example** We assess the performance of our HOLS method in a linear SEM using a simple example. In Figure 2, we show the DAG that represents the setup. For simplicity, the parameters are set such that $X_1$ to $X_7$ all have unit variance. $X_3$ is the only parent of $Y$ and we apply the HOLS method using all but $X_3$ as predictors, i.e., $X_3$ is treated as hidden variable. Following Theorem 9 we know that for variables $X_1$ and $X_5$ to $X_7$ the causal effect on $Y$ is consistently estimated with OLS, while we chose the detailed setup such that there is a detectable confounding bias on $\beta_2^{\text{OLS}}$ and $\beta_4^{\text{OLS}}$. Thus, ideally, our local tests accept the null hypothesis for all but those two covariates.
Figure 2: DAG of the linear SEM. $X_3$ is assumed to be hidden which is depicted by the dashed circle.

For numerical results, we let the sample size grow from $10^2$ to $10^6$. For each sample size, we do 200 simulation runs. On the left-hand side of Figure 3 we show the average absolute $z$-statistics per predictor for the different sample sizes. For $X_2$ and $X_4$ we see the expected $\sqrt{n}$-growth. For the other variables, the empirical averages are close to the theoretical mean, which equals $\sqrt{2/\pi} \approx 0.8$, with a minimum of 0.70 and a maximum of 0.88. Further, we see that the confounding bias on the OLS parameter for $X_4$, which is a child of the hidden variable, is easier to detect than the bias onto the parameter for $X_2$, which is a child’s other parent. The multiplicity corrected p-value for $X_4$ is rejected at level $\alpha = 0.05$ in 91.5% of the cases for $n = 10^3$, while as the null hypothesis for $X_2$ is only rejected with an empirical probability of 3%. For $X_2$, it takes $n = 10^5$ samples to reject the local null hypothesis in 89% of the simulation runs.

Following Section 3.2.1 we should be able to perfectly recover the set $U$ (cf. (13)) as $n \rightarrow \infty$ if we let the threshold on the absolute $z$-statistics grow at the right rate. Therefore, we plot on

Figure 3: Simulation in a linear SEM corresponding to Figure 2. On the left: Average absolute $z$-statistics per covariate for different sample sizes. The dotted lines grow as $\sqrt{n}$ and are fit to match perfectly at $n = 10^5$. On the right: Empirical probability (over 200 simulation runs) of perfectly recovering $U$ (cf. (13)) for different sample sizes.
the right-hand side of Figure 3 the empirical probability of perfectly recovering $U$ over a range of possible thresholds for the different sample sizes. For $n = 10^6$, we could achieve an empirical probability of 1. For $n = 10^5$ the optimum probability is 87%, while as for $n = 10^4$ it is only 19%.

Naturally, perfectly recovering $U$ is a very ambitious goal for smaller sample sizes, and one might want to consider different objectives. In Figure 4, we plot two different performance metrics. On the left-hand side, we plot the empirical probability of not falsely including any variable in $\hat{U}$ against the average intersection size $|\hat{U} \cap U|$. The curve is parametrised implicitly by the threshold on the absolute $z$-statistics in order to reject the local null hypothesis for some variable. Thus, the graphic considers the question of how many variables in $U$ can be recovered while keeping the probability of not falsely including any low. For a sample size of $10^5$, we have an average intersection size of 3.97 allowing for a 10% probability of false inclusions. For $10^4$, it is still 0.995. Thus, we can find (almost) one of the 4 variables in $U$ on average. As we see in Figure 3, the bias on $\beta_{OLS}^4$ is much easier to detect than the bias on $\beta_{OLS}^2$. Thus, keeping the probability of including $X_2$ in $\hat{U}$ low is still an ambitious task. Therefore, we analyse on the right-hand side of Figure 4 how many variables in $U$ we can find while removing a certain amount of confounding signal. We define the remaining fraction as

$$\frac{\|\beta_{OLS}^U - \beta_U\|_1}{\|\beta_{OLS} - \beta\|_1},$$

i.e., how much of the difference $\beta_{OLS} - \beta$ persists in terms of $\ell_1$ norm.

**Figure 4:** Simulation in a linear SEM corresponding to Figure 2. On the left: Probability of not falsely including a variable in $\hat{U}$ versus average intersection size $|\hat{U} \cap U|$ (cf. [14]). On the right: average remaining fraction of confounding signal versus average intersection size $|\hat{U} \cap U|$. It holds that $|U| = 4$. Both curves use the threshold on the absolute $z$-statistics as implicit curve parameter. Note that the legend applies to either plot.
In this SEM, $\beta_{4}^{OLS}$ carries $2/3$ of the confounding signal, $\beta_{2}^{OLS}$ only $1/3$. Accepting $1/3$ of remaining confounding signal, we receive an average intersection size of $3.885$ for a sample size of $10^{3}$. For $10^{4}$, the average is $4$. Thus, if we allow for false inclusion of $X_2$ we can almost perfectly retrieve all of $U$ for sample size $10^{3}$ already.

### 4.2.1 What if X includes descendants of Y?

So far, we have only considered the case where $X$ causally affects $Y$, but potentially, some of $Y$’s parents are missing leading to a potential confounding effect. However, another possibility for $\beta^{OLS}$ to not denote a causal effect is that there are descendants of $Y$ amongst the predictors. This case actually fits our theory from before if interpreted properly. If the model (4) for $Y$ holds true using only the parents as predictors, $Y$ can be naturally included in the assumed linear SEM for $X$ in (16). Then, one can also think of $Y$ as a further predictor variable, which is unobserved. Following (17), $E$ is the confounder. Of course, it holds $\beta^M = \beta$, i.e., $\beta^M_j = 0 \forall j \notin PA(Y)$. Using Theorem 9, we find $\beta^{HOLS}_j = \beta^{OLS}_j = \beta^M_j = 0 \forall j \in M$ that are not in the Markov boundary of $Y$.

Thus, for all variables outside $Y$’s Markov boundary, one can correctly detect that they have no causal effect onto $Y$ ceteris paribus. The variables in the blanket, which includes all the parents, are up to term cancellations all confounded. This can be detected under some conditions, as discussed in Section 3.2.

Naturally, the two cases, not having measured a parental variable or including descendants in the set of predictors, are different in terms of interpretation. For unmeasured variables, our local tests are of more importance since one can detect a set of predictors for which we correctly understand the linear causal effect. For descendants in the predictor set, one could retrieve the true causal model if the separation into ancestors and descendants was known.

Therefore, we suggest a simple diagnostics tool that can potentially detect the ancestors of $Y$ if there are no confounders. Namely, let $f$ be some non-linear function and $X^Y = (Y \ X)^\top$ such that the set of predictors includes $Y$ as well. Denote the index corresponding to $Y$ by 0.

**Theorem 10.** Assume that the data $X^Y$ follows the model (16). Consider the regression $f(Y)$ versus $X^Y$ and denote the according OLS parameter by $\beta^{f,OLS}$. Then,

$$\beta^{f,OLS}_j = 0 \forall j \not\in (\text{AN}(0) \cup 0).$$

Typically, $\beta^{f,OLS}_j \neq 0$ for ancestors as a non-linear function of that ancestor cannot be completely regressed out by the other regressors using only linear terms. For ancestors that are much further upstream, this effect might become vanishingly small. However, this is not such an issue since excluding an ancestor that is not a parent does not change the linear regression parameter if all parents are included. Thus, we suggest testing for $\beta^{f,OLS}_0 = 0$ in order to detect some or even all ancestors of $Y$. In our simulations as well as the real data analysis, we use $f(Y) = Y^3$ as our non-linear function. Note that Theorem 10 also holds for a linear function as then only $\beta^{f,OLS}_0$ is non-zero. In a second step, one can then check with our HOLS procedure whether the estimated set of ancestors is unconfounded. We make things more explicit. Let

$$H^f_{0,j} : \quad \beta^{f,OLS}_j = 0, \quad \text{AN}^*(0) = \left\{ \begin{array}{l} j \neq 0; H^f_{0,j} \text{ is not true} \end{array} \right\} \quad \text{and} \quad \overline{\text{AN}}(0) = \left\{ \begin{array}{l} j \neq 0; H^f_{0,j} \text{ is rejected} \end{array} \right\}.$$

Following Theorem 10, we have $\text{AN}^*(0) \subseteq \text{AN}(0)$.
Theorem 11. Assume that the data $X^{Y}$ follows the model (16), (A1) holds and $E[(X_jf(Y))^2] < \infty \forall j$. Then, we can find a decreasing sequence of significance level $\alpha_n$ to test $H_{0,j}^f$ such that

$$\lim_{n \to \infty} P[\widehat{AN}(0) = AN^*(0)] = 1.$$ 

Thus, we propose to first detect a suggested ancestor set $\widehat{AN}(0)$ and second check whether this might be a linearly unconfounded ancestor set using our HOLS check described in Algorithm 1. If (4) holds true using $X_{\widehat{AN}(0)}$ as predictors, we know from Theorem 2 that this leads to asymptotically valid tests. Note that we ignore the distributional shift implied by this pre-screening step since the detected set approaches a fixed quantity.

In the case where $H_0$ is not true for $X_{AN^*(0)}$, it depends on the difference between $\beta_{OLS}$ and $\beta_{HOLS}$ for this set of predictors whether we can detect this. Usually, this difference is non-zero for some predictors. However, this is not always the case, as discussed in Section 3.2.

We conclude with some remarks. First, for fully Gaussian data, we have $\beta_{j,OLS}^f = 0 \forall j \neq 0$ such that nothing can be detected. Second, there can be cases where $AN^*(0)$ or $\widehat{AN}(0)$ does not include all parents of $Y$ but $H_0$ still holds true for that set, e.g., two independent parents where one is not detected as such. Last, in a mixture of the two issues, missing variables and descendants, the method might fail. Namely, if some descendant is confounded with $Y$ it might be part of $AN^*(0)$.

Thus, the pre-separation is not useful and one would not get local interpretation on the second level test.

Simulation example. We analyse the behaviour of our method detecting ancestors. For this, we reuse the linear SEM given by the DAG in Figure 2, but we try to assess the ancestors of $X_4$ ($X_3$ is not assumed to be hidden anymore). We do a simple linear regression of $f(X_4) = X_3^4$ versus $X_1 \cdots X_7$. From Theorem 10, we know that $\beta_{j,OLS}^f = 0$ for $j \in \{5, 6, 7\}$, while as the setup is such that $\beta_{j,OLS}^f \neq 0$ for $j \in \{1, 2, 3, 4\}$. Thus, all ancestors are detectable.

Again, we vary the sample size from $n = 10^2$ to $n = 10^6$ and do 200 simulation runs for each. In Figure 5, we plot the empirical probability of selecting a proper set of ancestors for different thresholds on the absolute z-statistics. On the left-hand side, we consider selecting all ancestors, i.e., $X_1$, $X_2$, and $X_3$. On the right-hand side, any model that fulfils (4) is accepted, i.e., any combination out of $X_1$, $X_2$, and $X_3$ is ok. Naturally, the first task is much harder to achieve, which can also be seen from the plots. Especially, selecting $X_1$, which is an ancestor but not a parent of $X_4$, is less probable. We see that selecting the full set of ancestors needs a sample size of about $n = 10^5$ to work reliably, while as for $n = 10^2$ we can select a well-specified model with high probability. (For the optimal threshold, the empirical probability is 98.5%.) Naturally, including $X_1$ is of less importance since its causal effect onto $X_4$ is 0 when fixing $X_2$ and $X_3$. Thus, recovering the full set of ancestors is not necessary in practice even though we can guarantee it for large enough sample sizes.

5 Real data example

We analyse the flow cytometry dataset presented by Sachs et al. (2005). It contains cytometry measurements of 11 phosphorylated proteins and phospholipids. There is a “ground truth” on how
Figure 5: Detection of the ancestors of variable $X_4$ in the linear SEM corresponding to Figure 2 with no hidden variables. On the left: Empirical probability of selecting the full true model ($X_1$, $X_2$, and $X_3$ but none of $X_5$, $X_6$, and $X_7$). On the right: Empirical probability of selecting a true model according to (4) (any out of $X_1$, $X_2$, and $X_3$ but none of $X_5$, $X_6$, and $X_7$). Note that the legend is split over both plots.

these quantities affect each other, the so-called consensus network (Sachs et al., 2005). Data is available from various experimental conditions, some of which being interventional environments. The dataset has been further analysed in various projects, see, e.g., Mooij and Heskes (2013), Meinshausen et al. (2016) and Taeb and Bühlmann (2021). Following these works, we consider the data from 8 different environments, 7 of which being interventional.

In a first analysis, we trust the consensus network from Sachs et al. (2005). For each node, we go through all environments, fit a linear model using all its claimed parents as predictors, and assess the goodness of fit of the model using our HOLS check. In the consensus network, there is one bidirected edge between the variables PIP2 and PIP3. We include it as a parent for either direction. For each suggested edge, we collect the p-values from the linear model fit in all environments keeping only those where the edge passes the subsequent local HOLS check at level $\alpha = 5\%$ without multiplicity correction. In Table 1a we report the minimum p-value per edge sorted by increasing p-value. Additionally, we show the number of environments in which the check is passed. Note that there is one p-value of 0 reported corresponding to a t-value of 174, which exceeds the precision that can be obtained with the standard R-function `lm`.

In a second analysis, we deviate from the consensus network and estimate the ancestor set using our technique described in Section 4.2.1. Thus, the model that is fit for each node varies now over the different environments. We use $f(Y) = Y^3$ as the non-linear function and include predictors that lead to a (Bonferroni corrected) p-value of less than 5%. Then, we fit a linear model using the estimated set of predictors and calculate a combined p-value which is the maximum of the (uncorrected) p-values obtained from the ancestor detection step and the linear model fit. We
do this for each environment keeping only those p-values, where the edge passes the subsequent HOLS check at level $\alpha = 5\%$. In Table 1b we report the minimum p-value per edge sorted by increasing p-value. Additionally, we show in how many environments the edge was suggested as ancestor relationship and in how many of these it passed the subsequent HOLS check. Trusting the consensus network, we see that the edge RAF $\rightarrow$ MEK is the most significant. However, using ancestor detection, the opposite direction is suggested more often and leads to even more significant results. This is in accordance with the direction of this edge being disputed in the literature, e.g., the aforementioned projects all report the direction MEK $\rightarrow$ RAF. Further, every edge of the consensus network passes the HOLS check in at least one environment. Some pass it even in all environments. Though, those connections do not appear to be very significant based on the linear model fits. This is in agreement with [Taeb and Bühlmann (2021)], where none of these is reported.

Using our ancestor detection, the top edge is the one that is bidirected in the consensus network, while the second-ranked edge is part of the consensus network. Further, we see some edges that appear either in the consensus or in some of the cited work or both, but also some that have not been reported there. The third-ranked edge, p38 $\rightarrow$ PKC, is such an example. All the cited projects

| Edge          | Passing | p-value |
|---------------|---------|---------|
| RAF $\rightarrow$ MEK | 3       | 0       |
| PKA $\rightarrow$ Akt   | 3       | 1.5e-120|
| PKA $\rightarrow$ Erk    | 5       | 3.8e-69 |
| PKC $\rightarrow$ JNK     | 3       | 5.9e-55 |
| PIP2 $\rightarrow$ PIP3   | 1       | 6.5e-40 |
| PIP3 $\rightarrow$ PLCg   | 5       | 1.4e-36 |
| PKC $\rightarrow$ p38     | 1       | 7.1e-34 |
| PIP3 $\rightarrow$ PIP2   | 1       | 9.6e-08 |
| PLCg $\rightarrow$ PKC    | 6       | 0.016   |
| PLCg $\rightarrow$ PIP2   | 1       | 0.027   |
| PKC $\rightarrow$ RAF     | 8       | 0.046   |
| PKC $\rightarrow$ PIP2     | 8       | 0.057   |
| PKA $\rightarrow$ RAF     | 8       | 0.086   |
| PKA $\rightarrow$ p38      | 8       | 0.12    |
| PIP3 $\rightarrow$ Akt    | 8       | 0.2     |
| PKA $\rightarrow$ JNK      | 8       | 0.21    |
| MEK $\rightarrow$ Erk      | 8       | 0.42    |

Table 1: (a) the model is taken from the consensus network. The second column reports the number of environments in which the edge passes the HOLS check. The p-value is the minimum of the p-values from linear regression in environments, where the edge passes the HOLS check. (b) the model is estimated using our ancestor detection technique (cf. 4.2.1). The second column reports the number of environments in which the edge is suggested by our technique and the third column reports in how many of these the edge passes the HOLS check. The p-value per environment is the maximum of the p-values from ancestor detection and the subsequent linear model fit. We report the minimum p-value over environments in which the edge passes the HOLS check.
claim the opposite direction for this edge. For this, two things shall be noted. First, our ancestor detection technique assumes the data to follow a linear SEM. This is of course questionable in nature and if it fails to hold true, there is also no guarantee that the number of suggested non-ancestors is controlled. Second, although global linearity can not be guaranteed, the fact that we still find a decent number of suggested edges that pass the HOLS check, at least in some environments, leads to the impression that the assumption of some local unconfounded linear structures is not unrealistic, see also the discussion in Section 7.1.

Lastly, we want to mention that our ancestor detection technique was able to make edges pass the HOLS check that did not pass in the consensus model. For example, in one environment, the edge PIP3 → PIP2 is rejected to be linearly unconfounded in the consensus model

\[
\text{PIP2} \leftarrow \text{PIP3} + \text{PLCg}
\]

but accepted in the model

\[
\text{PIP2} \leftarrow \text{PIP3},
\]

which our method suggested. In light of our analysis of linear SEMs, this could be induced, e.g., by the following structures

\[
\begin{array}{c}
\text{PIP3} \\
\rightarrow \\
\text{PIP2} \\
\rightarrow \\
\text{PLCg}
\end{array}
\quad
\begin{array}{c}
\text{PIP3} \\
\rightarrow \\
\text{H} \\
\rightarrow \\
\text{PIP2} \\
\rightarrow \\
\text{PLCg}
\end{array}
\]

where \( H \) is a hidden variable.

We can also analyse our results in the light of invariant causal prediction, see, e.g., Peters et al. (2016), where one typically assumes that interventions do not change the underlying graph except for edges that point towards the node that is intervened on. This assumption is highly questionable in practice, and our findings, which vary a lot over different environments, indicate that the assumption is likely not fulfilled in the given setup.

6 High-dimensional data

We now turn to high-dimensional situations. We assume the global null hypothesis (4) but allow for \( p \) to diverge with and even exceed \( n \). If \( p - 1 \geq n \), \( P_{-j} = I_n \), i.e., the identity matrix. Using least squares regression, the residuals \( \hat{z}_j \) and \( \hat{w}_j \) would both be 0 and the sample estimates we described before are no longer defined. Instead, we apply the debiased Lasso introduced in Zhang and Zhang (2014) and further discussed in van de Geer et al. (2014). To obtain an estimate \( \hat{\beta}_{\text{OLS}} \), we use a standard debiased Lasso, which converges to the true \( \beta \) under certain assumptions discussed in van de Geer et al. (2014).

From the debiased Lasso, we receive \( \hat{z}_j = \mathbf{x}_j - \mathbf{x}_{-j} \hat{\mathbf{\gamma}}_j \), where \( \hat{\mathbf{\gamma}}_j \) is obtained by regressing \( \mathbf{x}_j \) versus \( \mathbf{x}_{-j} \) using the Lasso, and \( \hat{\mathbf{w}}_j = \mathbf{y} - \mathbf{x}_{-j} \hat{\beta}_{-j} \) with \( \hat{\beta} \) coming from the Lasso fit of \( \mathbf{y} \) versus \( \mathbf{x} \).
Since
\[ \hat{\beta}_j^{OLS} = \frac{\hat{z}_j^T \hat{w}_j}{\hat{z}_j^T x_j} \]
it would be intuitive to use \( \hat{\beta}_j^{HOLS} = \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \).

However, this might lead to an uncontrollable approximation error since \( \mathbb{E} \left[ Z_j^3 X_{-j} \right] \neq 0 \). As a remedy, we suggest a second level of orthogonalisation based on \( \hat{Z}_j^3 \) and \( \hat{\gamma}_j \) as defined in (8).

Naturally, we have \( \hat{Z}_j^3 = Z_j^3 \) iff \( \mathbb{E} \left[ Z_j^3 X_{-j} \right] = 0 \) and always \( \mathbb{E} \left[ \hat{Z}_j^3 X_{-j} \right] = 0 \). To approximate \( \hat{Z}_j^3 \) we use the Lasso for the regression \( \hat{z}_j^3 \) versus \( x_{-j} \) leading to \( \hat{z}_j^3 = x_j^3 - x_{-j} \hat{\gamma}_j \). We define \( \hat{\beta}_j^{HOLS} \) as
\[
\hat{\beta}_j^{HOLS} := \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \hat{w}_j = \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \left( y - x_{-j} \hat{\beta}_{-j} \right) = \beta_j + \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) x_{-j} \left( \beta_j - \hat{\beta}_{-j} \right)/n + \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \epsilon.
\]

In the end, we are interested in the difference between \( \hat{\beta}_j^{HOLS} \) and \( \hat{\beta}_j^{OLS} \). We apply Algorithm 2 where we make use of the (asymptotic) normality of the non-vanishing term in this difference. For non-Gaussian \( \mathcal{E} \), a multiplicity correction method that does not rely on exact Gaussianity of this remainder might be preferred since the CLT does not apply for dimensions growing too fast.

**Algorithm 2** HOLS check for \( p > n \)

1. Regress \( y \) versus \( x \) via Lasso with a penalty parameter \( \lambda \), denote the estimated regression coefficients by \( \hat{\beta} \)
2. for \( j = 1 \) to \( p \) do
3. Regress \( x_j \) versus \( x_{-j} \) via Lasso with a penalty parameter \( \lambda_j \), denote the residual by \( \hat{z}_j \)
4. Regress \( \hat{z}_j^3 \) versus \( x_{-j} \) via Lasso with a penalty parameter \( \hat{\lambda}_j \), denote the residual by \( \hat{z}_j^3 \)
5. \( \hat{w}_j = y - x_{-j} \hat{\beta}_{-j} \)
6. \( \hat{\beta}_j^{OLS} = \frac{\hat{z}_j^T \hat{w}_j}{\hat{z}_j^T x_j} \), \( \hat{\beta}_j^{HOLS} = \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \hat{w}_j \) and \( \hat{v}_j = \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) x_j / \left( \frac{\hat{z}_j^3}{\hat{z}_j^3 \times x_j} \right) \hat{z}_j - \hat{z}_j^3 \)
7. \( \hat{\sigma}^2 = \frac{||y - x \hat{\beta}||^2}{n - ||\hat{\beta}||^2_0} \) (or any other reasonable variance estimator)
8. Create \( n_{sim} \) i.i.d copies of \( S \sim \mathcal{N} \left( 0, \hat{\sigma}^2 \frac{1}{n^2} \hat{\nu}^T \hat{\nu} \right) \), say, \( s^1 \) to \( s^{n_{sim}} \)
9. for \( j = 1 \) to \( p \) do
10. \( p_j = 2 \times \left( 1 - \Phi^{-1} \left( \frac{\left| \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right|}{\hat{\sigma} \left( \frac{1}{n} ||\hat{v}_j||_2 \right)} \right) \)
11. \( P_j = \frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} 1 \left( \left| \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right| > \left| s_i \right| \right) \)

We provide here the main result to justify Algorithm 2 invoking additional assumptions on the dimensionality and sparsity of the problem. We use the definitions \( s := ||\beta||_0 \), \( s_j := ||\gamma_j||_0 \) and \( \tilde{s}_j := ||\tilde{\gamma}_j||_0 \) to denote the different levels of sparsity.
Thus, well specification of $\beta$ - (C6) hold ($\forall$).

Assume that the data follows the model (4) with sub-Gaussian

Theorem 12.

We have mainly focused on linear models, i.e., the data is either generated by model (4) or model (9).

To close, we provide a quick outlook and some concluding remarks.

7 Discussion

7.1 Beyond linearity

We have mainly focused on linear models, i.e., the data is either generated by model [1] or model [9]. Naturally, this assumption might be questionable in practice. Therefore, we provide some intuition about how HOLS might be applied in a more general setup. As we only detect misspecification of the OLS coefficient without identifying the type of misspecification, one should not try to over-interpret the effect of the regressors in $\hat{\beta}^{OLS}$ without identifying the type of misspecification, one should not try to over-interpret

variables in $\hat{\beta}^{OLS}$.

More details can be found in the supplemental material.

$$Y = X^{\top} \beta^{OLS} + f_{non-linear}(X) + \epsilon, \text{ where } f_{non-linear}(X) = \mathbb{E}[Y|X] - X^{\top} \beta^{OLS} \text{ and } \mathbb{E}[\epsilon|X] = 0.$$ $W_{j} = Z_{j} \beta^{OLS} + f_{non-linear}(X) + \epsilon.$

Thus, well specification of $\beta^{OLS}$ implies $\mathbb{E}[f_{non-linear}(X)|Z_{j}] = 0$, i.e., after linearly adjusting for $X_{-j}$, $X_{j}$ does not have any predictive power for $f_{non-linear}(X)$. If it does not have any predictive
power after linear adjustment, it would be a natural conclusion that it does not have predictive power after optimally adjusting for $X_j$ implying that $f_{\text{non-linear}}(X)$ can be written as function of $X_{-j}$ only. This would then imply

$$E[Y|X_j = x_j + 1, X_{-j} = x_{-j}] - E[Y|X_j = x_j, X_{-j} = x_{-j}] = \beta_j^{\text{OLS}} \forall x_j, x_{-j}. $$

Except for Gaussian data, such a linear relationship must be either causal or due to very pathological data setups. Excluding such unusual constellations, the conclusion is that for $j \in U$ there must be a true causal linear effect from $X_j$ to $Y$ keeping the other predictors fixed, which can be consistently estimated using OLS. Of course, if there are no locally linear structures it might well be that $U = \emptyset$ such that the local tests are not more informative than the global test. However, there is also nothing to be lost by exploiting this local view.

Note that the asymptotic results presented in Sections 3.1 and 3.2.1 hold for non-linear data as well since they only assume model (10), which is the most general formulation.

7.2 Conclusion

We have introduced the so-called HOLS check to assess the goodness of fit of linear models. It is based on the dependence between residuals and predictors in misspecified models, leading to non-vanishing higher moments. Besides checking whether the overall model might hold true, the method allows to detect a set of variable for which linear regression consistently estimates a true (unconfounded) causal effect for certain model classes.

Of particular interest are linear structural equation models, for which our method allows for very precise characterisations regarding which least squares parameters are causal effects. Furthermore, we suggest a simple related technique with which one can detect the ancestors for any given variable in a linear structural equation model. Both results require non-Gaussianity.

Finally, we show how the HOLS method can be extended to high-dimensional datasets based on the idea of the debiased Lasso (Zhang and Zhang, 2014; van de Geer et al., 2014). This extension comes very naturally as our HOLS check involves nodewise regression just as the debiased Lasso.

We complement our theory with several simulation studies as well as a real data example. The simulations, while generally supporting our asymptotic results, show that sometimes one might require a rather large sample size in order to perfectly distinguish between confounded and unconfounded parameter estimates.

A drawback of our method is that it does not distinguish whether a model is misspecified due to confounding or due to non-linearities in the model. Therefore, an interesting follow-up direction would be to extend our methodology and theory from linear to non-linear SEM using more flexible regression methods. This could allow to detect local causal structures in non-linear settings as well.

Further simulation results as well as proofs and extended theory can be found in the supplemental material. Code scripts to reproduce the results presented in this paper are available here [https://github.com/cschultheiss/HOLS](https://github.com/cschultheiss/HOLS).

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26
A Proofs

A.1 Proof of Theorem 1

Following the definitions of $\hat{\beta}_{OLS}^j$ and $\hat{\beta}_{HOLS}^j$, we have $\hat{\beta}_{HOLS}^j - \hat{\beta}_{OLS}^j = \frac{1}{n} \hat{\epsilon}_j^T \hat{\epsilon}$ and $\beta_{HOLS}^j - \beta_{OLS}^j = \frac{1}{n} \hat{v}_j^T \epsilon$. The rest follows then trivially as $\hat{v}$ is fixed given $x$ and a Gaussian random variable multiplied by a fixed matrix is still Gaussian. Finally, note that

$$\frac{1}{n^2} \hat{v}_j^T \hat{v}_j = \left( \begin{pmatrix} P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j^3 \end{pmatrix}^\top - \hat{z}_j^3 \right) \hat{z}_j^3 \hat{z}_j^3 \top \left( \begin{pmatrix} P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j^3 \end{pmatrix}^\top - \hat{z}_j^3 \right) = \begin{pmatrix} \hat{z}_j^3 \top P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j \hat{z}_j^3 \top \hat{z}_j \end{pmatrix} \begin{pmatrix} \hat{z}_j^3 \top P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j \hat{z}_j^3 \top \hat{z}_j \end{pmatrix} \begin{pmatrix} \hat{z}_j^3 \top P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j \hat{z}_j^3 \top \hat{z}_j \end{pmatrix} \begin{pmatrix} \hat{z}_j^3 \top P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j \hat{z}_j^3 \top \hat{z}_j \end{pmatrix} \begin{pmatrix} \hat{z}_j^3 \top P_{-j}^\perp (\hat{z}_j^3) \\ \hat{z}_j \hat{z}_j^3 \top \hat{z}_j \end{pmatrix} = \frac{1}{n^2} \hat{v}_j^T \hat{v}_j,$$

which is the variance for a single predictor.

A.2 Proof of Theorem 2

Note that model (4) and (A2) imply that (B1) - (B3) hold for all $j$, i.e., $U' = \{1, \ldots, p\}$. Thus, we receive Theorem 2 for free by proving Theorem 3 and we receive Corollary 1 for free by proving Corollary 2.

A.3 Proof of Theorem 3

Note first that Assumptions (A1) and (A2) imply

$$\frac{1}{n} x_{-j}^T x_{-j} \overset{p}{\to} \Sigma_{x_{-j},-j} \implies n \left( x_{-j}^T x_{-j} \right)^{-1} \overset{p}{\to} (\Sigma_{x_{-j},-j})^{-1} \implies \left\| n \left( x_{-j}^T x_{-j} \right)^{-1} \right\| \overset{p}{\to} \left\| (\Sigma_{x_{-j},-j})^{-1} \right\| = O(1),$$

(18)
where we use invertibility and the continuous mapping theorem. In several occasions, we use bounds on multiplications with the projection matrix \( P_{-j} \), e.g.,

\[
\| z_j^T P_{-j} w_j \| = \left\| z_j^T x_{-j} \left( x_{-j}^T x_{-j} \right)^{-1} x_{-j}^T w_j \right\| \leq \left\| z_j^T x_{-j} \right\|_2 \left\| \left( x_{-j}^T x_{-j} \right)^{-1} \right\|_2 \left\| x_{-j}^T w_j \right\|_2
\]

\[
\leq \left\| z_j^T x_{-j} \right\|_1 \left\| \left( x_{-j}^T x_{-j} \right)^{-1} \right\|_2 \left\| x_{-j}^T w_j \right\|_1 = \sum_{k \neq j} \left\| z_j^T x_k \right\| \left\| \left( x_{-j}^T x_{-j} \right)^{-1} \right\|_2 \left\| x_k^T w_j \right\|
\]

\[
= O_p(\sqrt{n}) O_p\left( \frac{1}{n} \right) O_p(n).
\]

For the last equality, we used Chebyshev’s inequality, (18), and the LLN together with \( \mathbb{E}[Z_j X_k] = 0 \), \( \mathbb{E}\left[(Z_j X_k)^2\right] < \infty \) and \( \mathbb{E}[X_k W_j] = 0 \).

Theorem 3 consists of three parts. Consider \( \tilde{\beta}_{j}^{OLS} \).

\[
\frac{1}{n} \left| \tilde{z}_j^T \tilde{w}_j - z_j^T w_j \right| = \frac{1}{n} \left| z_j^T P_{-j}^\perp P_{-j} w_j - z_j^T w_j \right| = \frac{1}{n} \left| z_j^T P_{-j} w_j \right|
\]

\[
= \frac{1}{n} O_p(\sqrt{n}) O_p\left( \frac{1}{n} \right) O_p(n) = o_p\left( \frac{1}{\sqrt{n}} \right). \quad \text{Thus,}
\]

\[
\frac{1}{n} \tilde{z}_j^T \tilde{w}_j = \frac{1}{n} z_j^T w_j + o_p\left( \frac{1}{\sqrt{n}} \right) = \mathbb{E}[Z_j W_j] + o_p(1) + o_p\left( \frac{1}{\sqrt{n}} \right) = \mathbb{E}[Z_j W_j] + o_p(1).
\]

\[
\frac{1}{n} \tilde{z}_j^T \tilde{z}_j = \mathbb{E}[Z_j^2] + o_p\left( \frac{1}{\sqrt{n}} \right) \quad \text{follows analogously such that}
\]

\[
\tilde{\beta}_{j}^{OLS} = \frac{\mathbb{E}[Z_j W_j]}{\mathbb{E}[Z_j^2]} + o_p(1).
\]

For \( \hat{\beta}_{j}^{HOLS} \), we first consider some intermediate results.

\[
\| \hat{\gamma}_j - \gamma_j \|_2 = \left\| \left( x_{-j}^T x_{-j} \right)^{-1} x_{-j}^T z_j \right\| \leq \left\| \left( \frac{1}{n} x_{-j}^T x_{-j} \right)^{-1} \right\|_2 \left\| \frac{1}{n} x_{-j}^T z_j \right\|
\]

\[
= O_p(1) O_p\left( \frac{1}{\sqrt{n}} \right) = o_p\left( \frac{1}{\sqrt{n}} \right) \quad \text{such that}
\]

\[
\| \tilde{z}_j - z_j \|_\infty = \| x_{-j} (\gamma_j - \hat{\gamma}_j) \|_\infty \leq \| x_{-j} \|_\infty \| \hat{\gamma}_j - \gamma_j \|_1 \leq \| x_{-j} \|_\infty \sqrt{p} \| \hat{\gamma}_j - \gamma_j \|_2
\]

\[
= O_p(K) O_p\left( \frac{1}{\sqrt{n}} \right) = o_p\left( \frac{1}{\sqrt{n}} \right),
\]

using fixed \( p \). Note that we denote the bound on \( \| x_{-j} \|_\infty \) by \( K \). (A2) induces a worst-case bound of \( K = n^{1/6} \). This could be heavily improved for certain assumptions on the distribution of \( X \), e.g., \( K = \sqrt{\log(n)} \) for Gaussian data. To keep things more general, we will use generic \( K \) in the following. Further,

\[
\| \tilde{z}_j - z_j \|_2^2 = \left\| P_{-j}^\perp z_j - z_j \right\|_2^2 = \| P_{-j} z_j \|_2^2 = O_p(1) \quad \text{and analogously} \quad \| \tilde{w}_j - w_j \|_2^2 = o_p(n).
\]

We invoke the following identity

\[
(a^3 - b^3) = (a - b)^3 - 3a(a - b)^2 + 3a^2(a - b)
\]

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to find

\[
\| z_j^3 - \hat{z}_j^3 \|_2 \leq \left\| (z_j - \hat{z}_j)^3 \right\|_2 + 3 \left\| z_j \circ (z_j - \hat{z}_j)^2 \right\|_2 + 3 \left\| z_j^3 \circ (z_j - \hat{z}_j) \right\|_2 \\
\leq \left\| (z_j - \hat{z}_j)^2 \right\|_\infty \| z_j - \hat{z}_j \|_2 + 3 \| z_j \|_\infty \| z_j - \hat{z}_j \|_\infty \| z_j - \hat{z}_j \|_2 + 3 \| z_j^3 \|_\infty \| (z_j - \hat{z}_j) \|_2 \\
= O_p \left( \frac{K^2}{n} \right) + O_p \left( \frac{K^2}{\sqrt{n}} \right) + O_p (K^2) = O_p (K^2).
\]

(20)

With this at hand, we find

\[
\frac{1}{n} | (z_j^3)^\top w_j - (\hat{z}_j^3)^\top \hat{w}_j | = \frac{1}{n} \left| (z_j^3 - \hat{z}_j^3)^\top w_j + (\hat{z}_j^3 - z_j^3)^\top (w_j - \hat{w}_j) + (z_j^3)^\top (w_j - \hat{w}_j) \right| \\
\leq \frac{1}{n} \left( \left| (z_j^3 - \hat{z}_j^3)^\top w_j \right| + \left| (\hat{z}_j^3 - z_j^3)^\top (w_j - \hat{w}_j) \right| + \left| (z_j^3)^\top (w_j - \hat{w}_j) \right| \right) \\
\leq \frac{1}{n} \left( \| (z_j^3 - \hat{z}_j^3) \|_2 \| w_j \|_2 + \| (\hat{z}_j^3 - z_j^3) \|_2 \| (w_j - \hat{w}_j) \|_2 + \| (z_j^3) \|_2 \| (w_j - \hat{w}_j) \|_2 \right) \\
= \frac{1}{n} \left( O_p (K^2) o_p (\sqrt{n}) + O_p (K^2) o_p (\sqrt{n}) + o_p (\sqrt{n}) o_p (\sqrt{n}) \right) = o_p (1). \text{ Thus,} \\
\frac{1}{n} (z_j^3)^\top \hat{w}_j = \frac{1}{n} (z_j^3)^\top w_j + o_p (1) = \mathbb{E} [Z_j^3 W_j] + o_p (1). \\
\frac{1}{n} (z_j^3)^\top \hat{z}_j = \mathbb{E} [Z_j^4] + o_p \left( \frac{K^2}{\sqrt{n}} \right) \text{ follows analogously such that} \\
\hat{\beta}_j^{HOLS} = \frac{\mathbb{E} [Z_j^3 W_j]}{\mathbb{E} [Z_j^4]} = \frac{\mathbb{E} [Z_j^3 W_j]}{\mathbb{E} [Z_j^4]} + o_p (1).
\]

The last part of Theorem 3 considers the variance estimate (cf. (7)) and is implied by the following Lemma which is a more precise statement.

**Lemma 1.** Assume that the data follows the model (10) and that (A1) - (A2) hold. Then,

\[
\sqrt{n} \left( \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right) \xrightarrow{p} \sigma_3^2 \left( \frac{\mathbb{E} \left[ (\hat{z}_j^3)^2 \right]}{\mathbb{E} [Z_j^4]^2} - \frac{1}{\mathbb{E} [Z_j^4]} \right) \forall j.
\]

Note that we defined

\[
\sqrt{n} \left( \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right) := n \sqrt{n} \left( \hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS} \right).
\]

A.3.1 **Proof of Lemma 1**

For \( \hat{z}_j^3 \) and \( (\hat{z}_j^3)^\top (\hat{z}_j^3)^2 = (\hat{z}_j^3)^\top \hat{z}_j \), we have established convergence already. It remains to look at the other terms in (7), i.e., \( (\hat{z}_j^3)^\top P_{-j}^\perp (\hat{z}_j^3) \) and \( \sigma^2 \). We find

\[
\frac{1}{n} \left| (\hat{z}_j^3)^\top P_{-j}^\perp (\hat{z}_j^3) - (z_j^3)^\top P_{-j}^\perp (z_j^3) \right| = \frac{1}{n} \left| (\hat{z}_j^3 - z_j^3)^\top P_{-j}^\perp (\hat{z}_j^3 - z_j^3) + 2(z_j^3)^\top P_{-j}^\perp (\hat{z}_j^3 - z_j^3) \right|
\]

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fulfilling (B1) and (A4). Note that since we assume (A3), we can sharpen

\[ \frac{1}{n} \left| \frac{1}{n} \| z_j^3 - z_j^3 \|_2^2 + \frac{2}{n} \| z_j^3 \|_2^2 \right| = O_p \left( \frac{K^4}{n} \right) + O_p \left( \frac{K^2}{\sqrt{n}} \right) = O_p \left( \frac{K^2}{\sqrt{n}} \right), \]

and

\[ \frac{1}{n} \left| \frac{1}{n} \| z_j^3 \|_2^2 \right| = \frac{1}{n} \left| \frac{1}{n} \frac{1}{z_j^3} P_{-j} (z_j^3) - \frac{1}{n} \frac{1}{z_j^3} (z_j^3)^\top (z_j^3) \right| = \frac{1}{n} \left| \frac{1}{n} \frac{1}{z_j^3} P_{-j} (z_j^3) \right| \]

= \sigma_p(1) such that

\[ \frac{1}{n} \frac{1}{z_j^3} P_{-j} (z_j^3) = \frac{1}{n} \frac{1}{z_j^3} (z_j^3)^\top + \sigma_p(1) = \mathbb{E} \left[ (\tilde{z}_j^3)^2 \right] + \sigma_p(1). \]

This ensures convergence of the per variable error scaling. It remains to estimate the variance of $\tilde{\epsilon}$. Although the error is now only uncorrelated but not independent from $X$ (cf. (10)), the variance can still be estimated consistently using the standard formula. Let

\[ \hat{\epsilon} = y - x\beta^{OLS} = P_{-j} \tilde{\epsilon}, \]

which is used for variance estimation. We find

\[ \frac{1}{n-p} \hat{\epsilon}^\top - \epsilon^\top \tilde{\epsilon} = \frac{1}{n-p} \hat{\epsilon}^\top P_{-j} \tilde{\epsilon} = O_p \left( \frac{1}{n} \right) \sigma_p(n) \frac{1}{n} \sigma_p(n) = c_p(1) \]

such that

\[ \hat{\sigma}^2 = \frac{\| \hat{\epsilon} \|_2^2}{n-p} = \frac{\| \hat{\epsilon} \|_2^2}{n-p} + \sigma_p(1) = \mathbb{E} \left[ \hat{\epsilon}^2 \right] + \sigma_p(1). \]

### A.4 Proof of Theorem 4

We provide a supporting Lemma.

**Lemma 2.** Assume that the data follows the model (10) and that (A1) - (A3) hold. Let $j$ be some covariate with $\beta_j^{OLS} = \beta_j^{HOLS}$ for which (B1) and (A4) hold. Then,

\[ \frac{1}{n} \left( \tilde{z}_j^3 - \frac{1}{n} \tilde{z}_j^3 \right) \Rightarrow \mathcal{N} \left( 0, \text{Var} \left( \frac{\tilde{Z}_j^3 \tilde{\epsilon}}{\mathbb{E} \left[ Z_j^4 \right]} - \frac{Z_j \tilde{\epsilon}}{\mathbb{E} \left[ Z_j^2 \right]} \right) \right). \]

If (B2) and (B3) hold as well for $j$, this can be refined as

\[ \frac{1}{n} \left( \tilde{z}_j^{HOLS} - \frac{1}{n} \tilde{z}_j^{HOLS} \right) \Rightarrow \mathcal{N} \left( 0, \frac{\sigma_p^2(\tilde{\epsilon})}{\mathbb{E} \left[ Z_j^2 \right]^2} - \frac{1}{\mathbb{E} \left[ Z_j^2 \right]^2} \right). \]

Note that (A4) is implied by (B3). Theorem 4 follows from Lemmata 1 and 2 applying Slutsky’s theorem. Thus, it remains to prove Lemma 2.

#### A.4.1 Proof of Lemma 2

We look at the scaled estimates $\sqrt{n} \hat{z}_j^{OLS}$ and $\sqrt{n} \tilde{z}_j^{HOLS}$ for some variable with $\beta_j^{OLS} = \beta_j^{HOLS}$ fulfilling (B1) and (A4). Note that since we assume (A3) we can sharpen $\left| x_k^\top w_j \right| = O_p(\sqrt{n})$ instead of just $O_p(n)$.

\[ \sqrt{n} \hat{z}_j^{OLS} = \frac{1}{n} \tilde{z}_j^3 \tilde{z}_j = \frac{1}{n} \tilde{z}_j^3 \tilde{z}_j + O_p(1) \]

and

\[ \sqrt{n} \tilde{z}_j^{HOLS} = \frac{1}{n} \tilde{z}_j^3 \tilde{z}_j = \frac{1}{n} \tilde{z}_j^3 \tilde{z}_j + O_p(1) \]

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In the second to last inequality, we use (B1). In short, using a derivation as in (19) and (A3), we know \( \|w_j\| = \sqrt{n}\beta_j^{OLS} + \frac{1}{n}z_j^\top x_j + \mathcal{O}_p(1/\sqrt{n}) \). Therefore, we take a closer look at the numerator.

\[
\sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top P_{-j}^\top \hat{\mathbf{e}} - \left( z_j^3 \right)^\top P_{-j}^\top \hat{\mathbf{e}} \leq \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top \mathcal{O}_p(1) + \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top P_{-j}^\top \hat{\mathbf{e}} \leq \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top \mathcal{O}_p(1) + \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top \mathcal{O}_p(1) = \mathcal{O}_p(1).
\]

In the second to last inequality, we use [B1]. In short, \( \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top P_{-j}^\top \hat{\mathbf{e}} - \left( z_j^3 \right)^\top P_{-j}^\top \hat{\mathbf{e}} \leq \mathcal{O}_p(1) \) such that

\[
\sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top P_{-j}^\top \hat{\mathbf{e}} - \left( z_j^3 \right)^\top P_{-j}^\top \hat{\mathbf{e}} \leq \mathcal{O}_p(1) + \mathcal{O}_p(1) + \mathcal{O}_p(1) = \mathcal{O}_p(1).
\]

This leads to

\[
\sqrt{n}\beta_j^{HOLS} = \sqrt{n}\frac{1}{n}\left( z_j^2 \right)^\top \mathbf{w}_j = \sqrt{n}\beta_j^{OLS} + \frac{1}{n}z_j^\top \mathcal{O}_p(1) = \sqrt{n}\beta_j^{OLS} + \frac{1}{n}z_j^\top \mathcal{O}_p(1) = \sqrt{n}\beta_j^{OLS} + \frac{1}{n}z_j^\top \mathcal{O}_p(1).
\]
Combining the results for $\sqrt{n} \hat{\beta}_{OLS}^j$ and $\sqrt{n} \hat{\beta}_{HOLS}^j$, we find

$$\sqrt{n} \left( \hat{\beta}_{HOLS}^j - \hat{\beta}_{OLS}^j \right) = \sqrt{n} \frac{1}{n} \left( \frac{\hat{\beta}_j^3}{E[Z_j]} - \frac{\beta_j^3}{Z_j^2} \right) \tilde{e} + o_p(1).$$  \hspace{1cm} (22)

Since the first term is a scaled sum of i.i.d. random variables, we can apply the CLT to it

$$\sqrt{n} \frac{1}{n} \left( \frac{\hat{\beta}_j^3}{E[Z_j]} - \frac{\beta_j^3}{Z_j^2} \right) \tilde{e} \xrightarrow{D} N \left( 0, \text{Var} \left( \frac{\hat{\beta}_j^3}{E[Z_j]} - \frac{\beta_j^3}{Z_j^2} \right) \right).$$  \hspace{1cm} (23)

Note that $E \left[ \hat{\beta}_j^3 \tilde{e} \right] = 0$ as $\beta_{OLS}^j = \beta_{HOLS}^j$. Combining (22) and (23) leads to the first statement in Lemma 2. Applying the independence relationship induced by (B2) and (B3), the second statement follows trivially.

A.5 Proof of Theorem 5

From (22), we know $\sqrt{n} \frac{1}{n} v_j^\top \tilde{e} - v_j^\top \tilde{e} \xrightarrow{p} 0$ for all $j \in U'$ under the given assumptions. For fixed dimensions, we can easily make this statement multivariate, i.e., $\sqrt{n} \frac{1}{n} \|v_j^\top \tilde{e} - v_j^\top \tilde{e}\| \xrightarrow{p} 0$. Therefore, we inspect $v_j^\top \tilde{e}$ in the following. Note that this is a (scaled) sum of mean 0 i.i.d random vectors. Obviously, this enables the multivariate CLT such that

$$\sqrt{n} \frac{1}{n} v_j^\top \tilde{e} \xrightarrow{D} N \left( 0, \text{E} \left[ v_j^\top \tilde{e} v_j^\top \tilde{e} \right] \right) = N \left( 0, \sigma^2 \text{E} \left[ V_j V_j^\top \right] \right),$$

which implies the first part of Theorem 5. For the second part, note

$$\frac{1}{n} v_j^\top \tilde{e}_j = \frac{1}{n} \left( P_{-j}^\perp \left( \hat{z}_j^3 \right) - \hat{z}_j \right) \left( P_{-k}^\perp \left( \hat{z}_k^3 \right) - \hat{z}_k \right)^\top \approx \frac{1}{n} \left( P_{-j} \left( \hat{z}_j^3 \right) \right) \left( P_{-k} \left( \hat{z}_k^3 \right) \right)^\top \tilde{e}_j - \frac{1}{n} \hat{z}_j^\top \hat{z}_k \frac{1}{n} \hat{z}_k^\top \tilde{e}_j - \frac{1}{n} \hat{z}_j^\top \frac{1}{n} \hat{z}_k \frac{1}{n} \hat{z}_k^\top \tilde{e}_j + \frac{1}{n} \hat{z}_j \frac{1}{n} \hat{z}_k \frac{1}{n} \hat{z}_k \frac{1}{n} \hat{z}_k^\top \tilde{e}_j$$

For each of the denominator terms, convergence has been established already. For the numerator terms, we can apply (19), (20), and $\| \hat{z}_j - z_j \|_2 = o_p(1)$.

$$\frac{1}{n} \left| \left( \hat{z}_j^3 \right) \right|^\top P_{-j}^\perp P_{-k}^\perp (\hat{z}_j^3 - z_j^3)^\top P_{-j}^\perp P_{-k}^\perp \left( \hat{z}_k^3 \right) \left| \right| \approx \frac{1}{n} \left| \left( \hat{z}_j^3 - z_j^3 \right) \left( P_{-j}^\perp P_{-k}^\perp (\hat{z}_j^3 - z_j^3) \right) + \left( z_j^3 \right) \left( P_{-j}^\perp P_{-k}^\perp (\hat{z}_j^3 - z_j^3) \right) + \left( \hat{z}_j - z_j \right) \left( P_{-j}^\perp P_{-k}^\perp (\hat{z}_j^3 - z_j^3) \right) \right| \right.$$
\[1/n \| P_{-j}^{\top} (\hat{\beta}_j^3 - \hat{\beta}_k^3) \|_2 \| P_{-k}^{\top} (\hat{\beta}_k^3) \|_2 \]
\[\leq 1/n \| (\hat{\beta}_j^3 - \hat{\beta}_j^3) \|_2 \| (\hat{\beta}_k^3 - \hat{\beta}_k^3) \|_2 + 1/n \| (\hat{\beta}_j^3 - \hat{\beta}_j^3) \|_2 \| (\hat{\beta}_k^3 - \hat{\beta}_k^3) \|_2 \| \hat{\beta}_k^3 \|_2 = O_p \left( \frac{K^2}{\sqrt{n}} \right) = O_p(1)\]
\[1/n \| (\hat{\beta}_j^3)^{\top} P_{-j} - P_{-k} (\hat{\beta}_k^3) \|_2 \]
\[\leq 1/n \| (\hat{\beta}_j^3)^{\top} P_{-j} - P_{-k} (\hat{\beta}_k^3) \|_2 + 1/n \| (\hat{\beta}_j^3)^{\top} P_{-k} (\hat{\beta}_k^3) \|_2 + 1/n \| (\hat{\beta}_j^3)^{\top} P_{-j} (\hat{\beta}_k^3) \|_2 \leq O_p(1) \text{ such that } \]
\[(\hat{\beta}_j^3)^{\top} P_{-j} P_{-k} (\hat{\beta}_k^3) = (\hat{\beta}_j^3)^{\top} (\hat{\beta}_k^3) + O_p(1) = E \left[ \hat{\beta}_j^3 \hat{\beta}_k^3 \right] + O_p(1)\]

The other terms follow in a very similar fashion such that Slutsky’s theorem leads to

\[1/n \hat{\nu}_j \hat{\nu}_k = E[V_j V_k] + O_p(1)\]

For fixed \( p \), this can be directly made multidimensional which proves the theorem’s statement.

### A.5.1 Proof of Corollary 2

Consider \( S \) as given in Step 7 of Algorithm 1. Using the second part of Theorem 5 and a consistent estimate of \( \delta \), we have

\[\sqrt{n} S_{U'} \overset{D}{\to} N\left(0, \sigma^2 \mathbb{E} \left[ V_{U'} V_{U'}^{\top} \right] \right)\]

Let \( S^* \sim N\left(0, \sigma^2 \mathbb{E} \left[ V_{U'} V_{U'}^{\top} \right] \right) \) and denote the cumulative density function (CDF) of its maximum absolute value by \( F^* \). Denote the CDF of \( \sqrt{n} \left\| \hat{\beta}_{U'}^{HOLS} - \hat{\beta}_{U'}^{OLS} \right\|_\infty \) by \( F_n \). Let \( q \) be the quantile function and \( \hat{q} \) the estimated quantile function using \( s^1, \ldots, s^{n_{sim}} \). Then,

\[\lim_{n \to \infty} \lim_{n_{sim} \to \infty} P(\exists j \in U' \text{ such that } H_{0,j} \text{ is rejected}) = \lim_{n \to \infty} \lim_{n_{sim} \to \infty} P \left( \left\| \hat{\beta}_{U'}^{HOLS} - \hat{\beta}_{U'}^{OLS} \right\|_\infty > \hat{q}_{1-\alpha}(\|S\|_\infty) \right) \]
\[\leq \lim_{n \to \infty} \lim_{n_{sim} \to \infty} P \left( \left\| \hat{\beta}_{U'}^{HOLS} - \hat{\beta}_{U'}^{OLS} \right\|_\infty > \hat{q}_{1-\alpha}(\|S\|_\infty) \right) = 1 - \lim_{n \to \infty} \lim_{n_{sim} \to \infty} F_n(\hat{q}_{1-\alpha}(\|S\|_\infty)) \]
\[= 1 - \lim_{n \to \infty} \lim_{n_{sim} \to \infty} F^*(\hat{q}_{1-\alpha}(\|S\|_\infty)) = 1 - \lim_{n \to \infty} F^*(q_{1-\alpha}(\|S\|_\infty)) = 1 - F^*(q_{1-\alpha}(\|S\|_\infty)) = \alpha\]

For the equality between the second and third line, note that \( F_n \to F \) using Theorem 5 and the continuous mapping theorem. As the maximum of several Gaussian random variables has a continuous CDF, this convergence is uniform such the convergence also holds at \( \hat{q}_{1-\alpha}(\|S\|_\infty) \) which is not constant in \( n \) and \( n_{sim} \). For the convergence of empirical quantiles, see, e.g., the discussion in [van der Vaart 2000](#) Chapter 21).
A.6 Proof of Theorem 6

We provide the supporting lemmata. Theorem 6 follows directly by combining these.

**Lemma 3.** Assume that the data follows the model (10) and that (A1) - (A2) hold. Let \( j \not\in U \).

Then,

\[
P[|s_j| \geq \tau_n] \geq P[|\beta_j^{HOLS} - \beta_j^{OLS}| \geq \tau_n | \mathcal{O}_p(1/\sqrt{n})] + |\mathcal{O}_p(1)|.
\]

This probability can be ensured to approach 1 if we chose \( \tau_n = \mathcal{O}(\sqrt{n}) \). Under this condition, we find \( \lim_{n \to \infty} P[\hat{U} \subseteq U] = 1 \). Notably, we assume \( |\beta_j^{HOLS} - \beta_j^{OLS}| \) to be constant, i.e., we deal with a fixed alternative. We further remark that we could use a constant significance level \( \alpha_n = \alpha \) to receive just the first convergence in (15).

Let us now turn to variables for which \( H_{0,j} \) holds true. In order to reuse our convergence results from Section 3.1, we have to additionally invoke (A3), (B1) and (A4).

**Lemma 4.** Assume that the data follows the model (10) and that (A1) - (A3) hold. Let \( j \) be some covariate in \( U \) for which (B1) and (A4) hold. Then,

\[
P[|s_j| \geq \tau_n] \leq \mathbb{E} \left[ \left( \frac{\tilde{Z}_j^3}{\mathbb{E}[Z_j^4]} - \frac{Z_j}{\mathbb{E}[Z_j^2]} \right) \mathcal{O}_p(1) / (\tau_n |\mathcal{O}_p(1)/2|^2) \right] + \mathbb{P}[|\mathcal{O}_p(1)| \geq \tau_n/2].
\]

Either term vanishes if we choose \( 1/\tau_n = \mathcal{O}(1) \). Thus, as long as \( \tau_n \) grows at any rate, we receive \( \lim_{n \to \infty} P[\hat{U} \supseteq U] = 1 \).

A.6.1 Proof of Lemma 3

From Theorem 3, we know

\[
\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}) = \sqrt{n}(\beta_j^{HOLS} - \beta_j^{OLS}) + \mathcal{O}_p(\sqrt{n})
\]

\[
\hat{\text{Var}}(\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS})) = \mathcal{O}_p(1).
\]

Thus, we have

\[
|s_j| = \left| \frac{\sqrt{n}(\beta_j^{HOLS} - \beta_j^{OLS})}{\mathcal{O}_p(1)} \right| + \mathcal{O}_p(\sqrt{n}) \geq \left| \frac{\sqrt{n}(\beta_j^{HOLS} - \beta_j^{OLS})}{\mathcal{O}_p(1)} \right| - |\mathcal{O}_p(\sqrt{n})|
\]

\[
P[|s_j| \geq \tau_n] \geq P \left[ \left| \frac{\sqrt{n}(\beta_j^{HOLS} - \beta_j^{OLS})}{\mathcal{O}_p(1)} \right| \geq \tau_n + |\mathcal{O}_p(\sqrt{n})| \right] = P \left[ |\beta_j^{HOLS} - \beta_j^{OLS}| \geq \tau_n |\mathcal{O}_p(1/\sqrt{n})| + |\mathcal{O}_p(1)| \right].
\]

A.6.2 Proof of Lemma 4

For variables fulfilling (B1) we know from (22) and Theorem 3

\[
\sqrt{n}(\hat{\beta}_j^{HOLS} - \hat{\beta}_j^{OLS}) = \sqrt{n} \frac{1}{n} \left( \frac{\tilde{Z}_j^3}{\mathbb{E}[Z_j^4]} - \frac{Z_j}{\mathbb{E}[Z_j^2]} \right) \mathbf{\tilde{\epsilon}} + \mathcal{O}_p(1).
\]
\[
\text{Var}
\left( \sqrt{n} \left( \hat{\beta}_j^{\text{HOLS}} - \hat{\beta}_j^{\text{OLS}} \right) \right) = O_p(1).
\]

This yields
\[
|s_j| = \left| \sqrt{n} \frac{1}{n O_p(1)} \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \right| ^T \tilde{\epsilon} + O_p(1)
\]
\[
\leq \left| \sqrt{n} \frac{1}{n O_p(1)} \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \right| ^T \tilde{\epsilon} + |O_p(1)|
\]
\[
P(|s_j| \geq \tau_n) \leq P \left[ \left| \sqrt{n} \frac{1}{n O_p(1)} \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \right| ^T \tilde{\epsilon} + |O_p(1)| \geq \tau_n \right]
\]
\[
\leq P \left[ \left| \sqrt{n} \frac{1}{n O_p(1)} \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \right| ^T \tilde{\epsilon} \geq \tau_n / 2 \right] + P(|O_p(1)| \geq \tau_n / 2)
\]
\[
\leq P \left[ \left| \sqrt{n} \frac{1}{n} \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \right| ^T \tilde{\epsilon} \geq \tau_n |O_p(1)| / 2 \right] + P(|O_p(1)| \geq \tau_n / 2)
\]
\[
\leq \mathbb{E} \left[ \left( \frac{\tilde{z}_j^3}{E[\tilde{z}_j^4]} - \frac{z_j}{E[Z_j^2]} \right) \tilde{\epsilon} \right]^2 / (\tau_n |O_p(1)| / 2)^2 + P(|O_p(1)| \geq \tau_n / 2),
\]

where the last step follows from Chebyshev’s inequality, assuming the second moment exists (cf. \((A4)\)).

### A.7 Proof of Theorem 8

From the definitions in \((17)\), we see that \(\beta_j = \beta^*_j\) iff \(\left( \omega_{N,M} \omega_{M,M}^{-1} \right) \omega^*_N \right) = 0\). We can inspect this further
\[
\left( \omega_{N,M} \omega_{M,M}^{-1} \right) \beta^*_N = \left( \omega_{M,M}^{-1} \right) \omega_{M,M} \omega_{M,M}^{-1} \beta^*_N = \left( \omega_{M,M}^{-1} \right) \sum_{k \in N} \omega_{M,M} \beta^*_k = \sum_{k \in N} \left( \omega_{M,M}^{-1} \right) \omega_{M,M} \beta^*_k.
\]

For some variable \(k \in N\), we have
\[
\mathbb{E} \left[ \omega_{M,M} \Psi_M (\omega_{M,M} \Psi_M) ^T \right] = \omega_{M,M} \Sigma \Psi_M \omega_{M,M} ^T, \quad \text{and}
\]
\[
\mathbb{E} \left[ \omega_{M,M} \Psi_M (\omega_{M,M} \Psi_M) ^T \right] = \omega_{M,M} \Sigma \Psi_M \omega_{M,M} ^T. \quad \text{Thus,}
\]
\[
\mathbb{E} \left[ \omega_{M,M} \Psi_M (\omega_{M,M} \Psi_M) ^T \right] ^{-1} \mathbb{E} \left[ \omega_{M,M} \Psi_M (\omega_{M,M} \Psi_M) ^T \right] = \left( \omega_{M,M}^{-1} \right) \omega_{M,M} ^T
\]
is the regression parameter of the regression \(\omega_{M,M} \Psi_M\) versus \(\omega_{M,M} \Psi_M\). Naturally, \(\omega_{M,M} \Psi_M\) can be perfectly recovered by a linear combination of \(\omega_{M,M} \Psi_M\) using only \(k\)’s nearest ancestors in \(M\), say, \(PA^M(k)\). Thus, \(\left( \omega_{M,M}^{-1} \right) \omega_{M,M} = 0\) if \(j \notin PA^M(k)\). Extending this argument to all \(k \in N\) the theorem’s statement follows.
A.8 Proof of Theorem 9

We provide some supporting lemmata.

**Lemma 5.** Assume that the data follows the model (16) without hidden variables. Then,

\[ Z_j = \delta_{j,j} \Psi_j + \sum_{k \in \text{CH}(j)} \delta_{j,k} \Psi_k \quad j = 1, \ldots, p \]

for an appropriate set of parameters. Further, the support of \( \gamma_j \) (cf. (5)) is restricted to \( j \)'s Markov boundary.

Thus, only the “noise” of \( j \) itself or its children remains in \( Z_j \).

Now, consider the best regression of \( Z_j^3 \) versus \( X_{-j} \) as defined in (8). We get an analogous result for the residuum \( \tilde{Z}_j^3 \).

**Lemma 6.** Assume that the data follows the model (16) without hidden variables. Then,

\[ \tilde{Z}_j^3 = Z_j^3 + \tilde{\delta}_{j,j} \Psi_j + \sum_{k \in \text{CH}(j)} \tilde{\delta}_{j,k} \Psi_k \quad j = 1, \ldots, p \]

for an appropriate set of parameters. Further, the support of \( \tilde{\gamma}_j \) (cf. (8)) is restricted to \( j \)'s Markov boundary.

Finally, we inspect the regression of \( \Psi_k \) versus \( X_M \) for some \( k \in N \). With a slight abuse of notation, define

\[ Z_k := \Psi_k - X_M^\top \beta^k, \text{ where } \beta^k := \arg\min_{b \in \mathbb{R}} \mathbb{E} \left[ \left( \Psi_k - X_M^\top b \right)^2 \right] = \mathbb{E} \left[ X_M X_M^\top \right]^{-1} \mathbb{E} [X_M \Psi_k]. \tag{24} \]

**Lemma 7.** Assume that the data follows the model (16). Let \( X_M \) and \( X_N \) be the observed and the hidden variables, where \( k \in N \). Then,

\[ Z_k = \sum_{l \in N} \delta_{k,l} \Psi_l + \sum_{m \in \text{CH}_N} \delta_{k,m} \Psi_m, \text{ where } \text{CH}_N = \left( \bigcup_{l \in N} \text{CH}(l) \right) \setminus N, \]

for an appropriate set of parameters. Further, the support of \( \beta^k \) is restricted to the union of the hidden variables’ Markov boundaries.

As \( \tilde{\mathcal{E}} \) is a linear combination of these \( Z_k \) and the independent \( \mathcal{E} \), we can combine Lemmata 5 and 6 and 7 to find \( Z_j \perp \tilde{\mathcal{E}} \) and \( \tilde{Z}_j^3 \perp \tilde{\mathcal{E}} \) for some variable \( j \) outside the hidden variables’ Markov boundaries. Furthermore, \( \beta^{\text{OLS}} - \beta \) is a linear combination of the \( \beta^k \) for \( k \in N \) such that outside the hidden variables’ Markov boundaries the two parameters are equal as claimed.

To check (B1), split \( X_k \) into a part consisting of \( \Psi_j \) and \( \Psi_l \forall l \in \text{CH}_j \), say \( X_{k,1} \), independent from \( \tilde{\mathcal{E}} \), and the remainder, say \( X_{k,2} \), independent from \( Z_j \). Then, we find

\[
\mathbb{E} \left[ Z_j^2 X_{k,1} \tilde{\mathcal{E}} \right] = \mathbb{E} \left[ Z_j^2 X_{k,1} \tilde{\mathcal{E}} \right] + \mathbb{E} \left[ Z_j^2 X_{k,2} \tilde{\mathcal{E}} \right] = \mathbb{E} \left[ Z_j^2 X_{k,1} \right] \mathbb{E} \left[ \tilde{\mathcal{E}} \right] + \mathbb{E} \left[ Z_j^2 \right] \mathbb{E} \left[ X_{k,2} \tilde{\mathcal{E}} \right]
\]

\[
= \mathbb{E} \left[ Z_j^2 \right] \mathbb{E} \left[ X_{k,2} \tilde{\mathcal{E}} \right] = \mathbb{E} \left[ Z_j^2 \right] \left( \mathbb{E} \left[ X_k \tilde{\mathcal{E}} \right] - \mathbb{E} \left[ X_{k,1} \tilde{\mathcal{E}} \right] \right) = 0.
\]
A.8.1 Proof of Lemma 5

Recall the representation
\[ Z_j = \delta_{j,j} \Psi_j + \sum_{k \in \text{CH}(j)} \delta_{j,k} \Psi_k. \]  

(25)

Assume first only the noise terms \( \Psi_j \) and \( \Psi_k \) \( \forall k \in \text{CH}(j) \) exist, while all the other terms are set to 0. Call the variables in this construction \( X'_k \) and the residuum \( Z'_j \). Obviously, \( Z'_j \) has a representation as in (25). Now by the definition of least squares, \( Z'_j \) and \( Z_j \) always have the smallest possible variance in their given model. If we add more independent noise terms to the model, the variance cannot decrease. Therefore, it holds \( \text{Var}(Z_j) \geq \text{Var}(Z'_j) \). Thus, if there exists a parameter such that \( X_j - \gamma^T X_k = Z'_j \), it must be optimal such that \( Z_j = Z'_j \). Let now \( \gamma = -\delta_j \). Then, we have

\[
X_j - \sum_{k \neq j} \gamma_k X_k = X_j + \sum_{k \in \text{CH}(j)} \delta_{j,k} X_k = X_j + \sum_{k \in \text{CH}(j)} \delta_{j,k} \left( \Psi_k + \theta_{k,j} X_j + \sum_{l \in \text{PA}(k) \setminus j} \theta_{k,l} X_l \right)
\]

\[
= X_j \left( 1 + \sum_{k \in \text{CH}(j)} \delta_{j,k} \theta_{k,j} \right) + \sum_{k \in \text{CH}(j)} \delta_{j,k} \Psi_k + \sum_{k \in \text{CH}(j)} \delta_{j,k} \sum_{l \in \text{PA}(k) \setminus j} \theta_{k,l} X_l.
\]

Now adjust \( \gamma \) by

- \( \forall l \in \text{PA}(j) \) adding \( \left( 1 + \sum_{k \in \text{CH}(j)} \delta_{j,k} \theta_{k,j} \right) \theta_{j,l} \) to \( \gamma_l \)

- \( \forall k \in \text{CH}(j), \forall l \in \text{PA}(k) \setminus j \) adding \( \delta_{j,k} \theta_{k,l} \) to \( \gamma_l \)

This leads to

\[
X_j - \sum_{k \neq j} \gamma_k X_k = \Psi_j \left( 1 + \sum_{k \in \text{CH}(j)} \delta_{j,k} \theta_{k,j} \right) + \sum_{k \in \text{CH}(j)} \delta_{j,k} \Psi_k.
\]

This is almost the optimal \( Z'_j \) as in (25). It remains to argue that the term in the bracket equals \( \delta_{j,j} \). For this, note that the weighted sum of terms that include \( \Psi_k \) in the construction of \( Z'_j \) must be exactly \( \delta_{j,k} \). These terms can occur from adding a multiple of either \( k \) itself or of descendants thereof (that are children of \( j \) as well). These descendants have “inherited” the same multiple of \( \Psi_k \) as of \( \theta_{k,j} \Psi_j \). Therefore, there is a net contribution of \( \delta_{j,k} \theta_{k,j} \Psi_j \) originating from variable \( k \). Applying this argument to each child, we receive the desired sum. Naturally, the 1 is the contribution from \( X'_j = \Psi_j \) itself.

Thus, we receive the desired construction of \( Z_j \). Further, we see that in this construction the support of \( \gamma_j \) is restricted to \( j \)'s parents, its children, and its children’s other parents, which is exactly the second part of the lemma.

A.8.2 Proof of Lemma 6

This follows using very similar arguments as in Section A.8.1 and is omitted here for simplicity.
We argue as before: Assume first only these variables are non-zero leading to an optimal residuum $Z_k'$. Naturally, $Z_k = \Psi_k - (\beta^k)\top X_M$ for some $\beta^k$. If we find a parameter such that $\Psi_k - (\beta^k)\top X_M = Z_k'$, it must be optimal as $\text{Var}(Z_k) \geq \text{Var}(Z_k')$. We now construct such a parameter. Start by $\beta^k = -\delta_k$.

\[
-(\beta^k)\top X_M = \sum_{m \in \text{CH}_N} \delta_{k,m}X_m = \sum_{m \in \text{CH}_N} \delta_{k,m}(\mathcal{E}_m + \omega_{m,N}\Psi_N)
\]

\[
= \sum_{l \in N} \Psi_l \sum_{m \in \text{CH}_N} \delta_{k,m}\omega_{m,l} + \sum_{m \in \text{CH}_N} \delta_{k,m}\mathcal{E}_m
\]

\[
= \sum_{l \in N} \Psi_l \sum_{m \in \text{CH}_N} \delta_{k,m}\omega_{m,l} + \sum_{m \in \text{CH}_N} \delta_{k,m}\left(\Psi_m + \sum_{r \in \text{PA}^M(m)} \theta_m'r\mathcal{E}_r\right)
\]

\[
= \sum_{l \in N} \Psi_l \sum_{m \in \text{CH}_N} \delta_{k,m}\left(\omega_{m,l} - \sum_{r \in \text{PA}^M(m)} \theta_m'r\omega_{l,r}\right) + \sum_{m \in \text{CH}_N} \delta_{k,m}\left(\Psi_m + \sum_{r \in \text{PA}^M(m)} \theta_m'rX_r\right),
\]

where we have used the fact that $\mathcal{E}_X$ follows a linear SEM as well for some suitable set of parameters $\theta_m'r$. Now adjust $\beta^k$ by

- $\forall m \in \text{CH}_N, \forall r \in \text{PA}^M(m)$ adding $\delta_{k,m}\theta_m'r$ to $\beta^k$.

This leads to

\[
\Psi_k - (\beta^k)\top X_M = \Psi_k + \sum_{l \in N} \Psi_l \sum_{m \in \text{CH}_N} \delta_{k,m}\left(\omega_{m,l} - \sum_{r \in \text{PA}^M(m)} \theta_m'r\omega_{l,r}\right) + \sum_{m \in \text{CH}_N} \delta_{k,m}\Psi_m,
\]

which is as in (26). It remains to argue that the coefficient for $\Psi_l$ equals $\delta_{k,l}$. Note that $\forall m \in \text{CH}_N$ there is a net contribution of $\delta_{k,m}\Psi_m$ coming from a weighted sum of $m$ and its descendants. There must be an according net contribution of all other parts that $X'_m$ does not inherit from its parents (in $M$). These must be multiples of $\Psi_l$ for $l \in N$. If $\omega_{l,r} \neq 0$, there is already a multiple of $\Psi_l$ in $X'_r$. Thus, $X'_m$ inherits $\theta_m'r\omega_{l,r}$ from $X'_r$. Extending this argument to all parents, a total of $\sum_{r \in \text{PA}^M(m)} \theta_m'r\omega_{l,r}$ is inherited. The remainder, i.e., $\omega_{m,l} - \sum_{r \in \text{PA}^M(m)} \theta_m'r\omega_{l,r}$ must then originate from $X'_m$, itself and there is a contribution of $\delta_{k,m}$ times this remainder times $\Psi_l$. As this holds $\forall m \in \text{CH}_N$, one can add all contributions leading to the desired sum.

Thus, we have established that $Z_k = Z_k'$ such that $Z_k$ and $\beta^k$ must be optimal. We also see that the support of $\beta^k$ is restricted to $\text{CH}_N$ and $\bigcup_{m \in \text{CH}_N} \text{PA}^M(m)$, which is exactly the hidden variables’ Markov boundary.
A.9 Proof of Theorem 10

To find $\beta_f,\text{OLS}$, we invoke the representation $XY = \omega \Psi$, which we can do since it follows to model (16). Then, we apply the definition of least squares. For ease of notation, we omit the superscript $Y$ in the following.

$$\beta_f,\text{OLS} = E\left[XX^\top \right]^{-1} E[Xf(Y)] = (\omega^{-1})^\top E\left[\Psi \Psi^\top \right]^{-1} \omega^{-1} E[\Psi f(Y)]$$

$$= (\omega^{-1})^\top \text{diag}\left(\frac{1}{E[\Psi_1^2]}, \ldots, \frac{1}{E[\Psi_p^2]}\right) E[\Psi f(Y)] = (\omega^{-1})^\top \left(\frac{E[\Psi_1 f(Y)]}{E[\Psi_1^2]}, \ldots, \frac{E[\Psi_p f(Y)]}{E[\Psi_p^2]}\right)^\top$$

Naturally, for all $k \notin (\text{AN}(0) \cup 0)$ we have $\Psi_k \perp Y$ such that $E[\Psi_k f(Y)] = 0$. Further, $\omega_{kl}^{-1} = 0$ if $k \notin (\text{DE}(l) \cup l)$. Thus,

$$\beta_{\text{OLS}}^l = \sum_{k} \omega_{kl}^{-1} \frac{E[\Psi_k f(Y)]}{E[\Psi_k^2]} = \sum_{k \in (\text{DE}(l) \cup l)} \omega_{kl}^{-1} \frac{E[\Psi_k f(Y)]}{E[\Psi_k^2]} = \sum_{k \in ((\text{DE}(l) \cup l) \cap (\text{AN}(0) \cup 0))} \omega_{kl}^{-1} \frac{E[\Psi_k f(Y)]}{E[\Psi_k^2]}$$

such that $\beta_{\text{OLS}}^l = 0$ if $(\text{DE}(l) \cup l) \cap (\text{AN}(0) \cup 0) = \emptyset$, i.e., if $l$ is not an ancestor of 0.

A.10 Proof of Theorem 11

We can reuse the convergence results for $\hat{\beta}_j^{f,\text{OLS}}$ from the proof of Lemma 2. Thus,

$$\sqrt{n}\hat{\beta}_j^{f,\text{OLS}} = \sqrt{n}\beta_j^{f,\text{OLS}} + \frac{\sqrt{n-1}}{n} \hat{\epsilon}_j \frac{1}{Z_j^2} + O_p\left(1/\sqrt{n}\right).$$

The middle term is a (scaled) sum of i.i.d. mean zero random variables to which we can apply the CLT. As long as both the variance

$$\frac{E}{\mathbb{E}}\left[\frac{(Z_j\hat{\epsilon}_j)^2}{Z_j^2}\right]$$

as well as the estimate

$$\frac{\hat{\sigma}^2}{\frac{1}{n} \hat{\epsilon}_j \hat{Z}_j}$$

stay bounded, we can perfectly distinguish between variables with $\beta_j^{f,\text{OLS}} = 0$ and those with $\beta_j^{f,\text{OLS}} \neq 0$, using a threshold on the absolute $z$-statistics that grows in $n$ but slower than $\sqrt{n}$. The variance is controlled using the assumptions, while as for the estimate we use the results from Theorem 3.

For the suggested two-step procedure, we find the following result.

**Corollary 3.** Assume that the data $XY$ follows the model (16), $H_0$ induced by (4) holds true using $X_{\text{AN}^*(0)}$ as predictors, (A1) to (A2) hold, and $E\left[(X_j f(Y))^2\right] < \infty \ \forall j$. Let $H_{0,j}$ be tested first using significance level $\alpha_n$ and $H_0$ for predictors $X_{\tilde{\text{AN}}(0)}$ be tested second significance level $\alpha$. We can find a decreasing sequence $\alpha_n$ such that

$$\lim_{n \to \infty} P\left[\tilde{\text{AN}}(0) = \text{AN}^*(0) \cap H_0 \text{ is accepted for } \tilde{\text{AN}}(0)\right] \geq 1 - \alpha.$$

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A.10.1 Proof of Corollary

\[
\lim_{n \to \infty} P[\hat{A}N(0) = AN^*(0) \cap H_0 \text{ is accepted for } \hat{A}N] = \\
1 - \lim_{n \to \infty} P[\hat{A}N(0) \neq AN^*(0) \cup H_0 \text{ is rejected for } AN^*] \\
= 1 - \lim_{n \to \infty} P[\hat{A}N(0) \neq AN^*(0)] \\
= 1 - \lim_{n \to \infty} P[H_0 \text{ is rejected for } AN^*] = 1 - \alpha
\]

In the last inequality, we use Theorems 11 and 2.

B Theory for the high-dimensional extension

We provide additional details on the high-dimensional extension including proofs of the main results.

The difference between \( \hat{\beta}_{j}^{OLS} \) and \( \hat{\beta}_{j}^{HOLS} \) can be written as

\[
\sqrt{n}\left(\hat{\beta}_{j}^{HOLS} - \hat{\beta}_{j}^{OLS}\right) = \sqrt{n}\left(\frac{\hat{z}_{j}^3}{\hat{z}_{j}}\right)^{\top} \frac{x_{-j}/n}{x_j/n} \left(\beta_{-j} - \hat{\beta}_{-j}\right) - \sqrt{n}\left(\frac{\hat{z}_{j}^3}{\hat{z}_{j}}\right)^{\top} \frac{x_{-j}/n}{x_j/n} \left(\beta_{-j} - \hat{\beta}_{-j}\right) + \\
\left(\frac{\hat{z}_{j}^3}{\hat{z}_{j}}\right)^{\top} \frac{1}{\sqrt{n}} - \hat{z}_{j}^3/n \frac{1}{\sqrt{n}} \frac{x_{-j}/n}{x_j/n} \hat{z}_{j}^3/n \frac{1}{\sqrt{n}} \frac{x_{-j}/n}{x_j/n} \epsilon = \Delta_{j}^{HOLS} - \Delta_{j}^{OLS} + \sqrt{n}\frac{1}{n}\hat{v}_{j}^{\top} \epsilon
\]

Thus, it consists of two bias terms and an error term, whose variance we can estimate. In the following, we inspect the terms in (27) assuming model (4) to justify Algorithm 2 and Theorem 12. \( \Delta_{j}^{OLS} \) is under control under certain conditions as discussed in (van de Geer et al., 2014). For \( \Delta_{j}^{HOLS} \) as well as the error scaling, we invoke our extra assumptions.

We consider the bias term.

Lemma 8. Assume that the data follows the model (4) with sub-Gaussian \( \mathcal{E} \) and that (C1) - (C3) and (C5) - (C6) hold (\( \forall j \)). Let \( \hat{\beta} \) come from Lasso regression with \( \lambda \asymp \sqrt{\log(p)/n} \), \( \hat{z}_{j} \) from nodewise Lasso regression using \( \lambda_{j} \asymp \sqrt{\log(p)/n} \), and \( \hat{z}_{j}^3 \) from nodewise Lasso regression of \( \hat{z}_{j}^3 \) versus \( x_{-j} \) using \( \tilde{\lambda}_{j} \asymp \max\left\{ \log(p)^{5/2}n^{-1/2}, s_{j}^{2}\log(p)^{5/2}n^{-3/2}, s_{j}\log(p)^{2}n^{-1}, \sqrt{s_{j}}\log(p)n^{-1/2}\right\} \). Use the definitions in (27). Then,

\[
\|\Delta^{HOLS}\|_{\infty} = o_p(1) \quad \text{and} \quad \|\Delta^{OLS}\|_{\infty} = o_p(1).
\]

Thus, under suitable assumptions, the bias vanishes. In order to get powerful tests, we want the variance of the error term to stay bounded. For asymptotically valid tests, we must ensure that the estimated standard deviation is of higher order of magnitude than the bias term.
Lemma 9. Assume that the data follows the model (4) with sub-Gaussian \( \mathcal{E} \) and that (C1), (C2), (C4) and (C6) hold (\( \forall j \)). Let \( \hat{\beta} \) come from Lasso regression with \( \lambda \approx \sqrt{\log(p)/n} \), \( \hat{z}_j \) from nodewise Lasso regression using \( \lambda_j \approx \sqrt{\log(p)/n} \), and \( \tilde{z}_j^3 \) from nodewise Lasso regression of \( \hat{z}_j^3 \) versus \( x_j \) using \( \tilde{\lambda}_j \approx \max \left\{ \log(p)/5 - 1/2, s^2_j \log(p)/5 - 3/2, s_j \log(p)/n - 1, \sqrt{s_j \log(p)/n} \right\} \). Use the definitions in (27). Then,

\[
\frac{1}{n} \hat{v}_j^\top \hat{v}_j \overset{p}{\to} \mathbb{E}[V_j^2]
\]

uniformly in \( j \).

where \( V_j = \frac{\tilde{Z}_j^3 - Z_j}{\mathbb{E}[Z_j^3] - \mathbb{E}[Z_j^2]} \).

Note that the sub-Gaussian assumption ensures \( \mathbb{E}[V_j^2] < \infty \), while as \( \mathbb{E}[V_j^2] > 0 \) if \( \mathbb{E}\left(\tilde{Z}_j^3\right)^2 \mathbb{E}[Z_j^2] > \mathbb{E}[Z_j^4]^2 \), which always holds if \( \tilde{Z}_j^3 \) is not a linear function of \( Z_j \). Thus, the estimate of the standard error approaches a bounded positive constant, enabling asymptotically valid \( z \)-tests.

In (C3) we have joint conditions on the different sparsity levels \( s \) and \( s_j \). Thus, the larger the one is, the more restrictive the assumption on the other is. Let us consider some specific cases, namely, \( s \approx s_j \), \( s_j \) maximal according to (C4), and \( s \) maximal according to (C2).

For \( s \approx s_j \), we need \( s \approx s_j = \mathcal{O}\left(\frac{n^{1/3}}{\log(p)}\right) \).

For \( s_j = \mathcal{O}\left(\frac{n^{3/5}}{\log(p)}\right) \), we need \( s = \mathcal{O}\left(\frac{n^{1/5}}{\log(p)}\right) \).

For \( s = \mathcal{O}\left(\frac{n^{1/2}}{\log(p)^3}\right) \), we need \( s_j = \mathcal{O}\left(\log(p)^3\right) \).

Note that if \( \tilde{\lambda}_j \) is chosen optimally with respect to \( s_j \), (C5) is actually the same as (C2) and (C3) such that there is no extra assumption on \( s \) that one has to invoke. In (C6) we have joint conditions on the different sparsity levels \( s_j \) and \( \tilde{s}_j \). Thus, the larger the one is, the more restrictive the assumption on the other is. Let us consider some specific cases, namely, \( s_j \approx \tilde{s}_j \), \( s_j \) maximal according to (C4) and \( \tilde{s}_j \) maximal according to (C6).

For \( s_j \approx \tilde{s}_j \), we need \( s_j \approx \tilde{s}_j = \mathcal{O}\left(\frac{n^{1/2}}{\log(p)}\right) \).

For \( s_j = \mathcal{O}\left(\frac{n^{3/5}}{\log(p)}\right) \), we need \( \tilde{s}_j = \mathcal{O}\left(\frac{n^{2/5}}{\log(p)}\right) \).

For \( \tilde{s}_j = \mathcal{O}\left(\frac{n}{\log(p)^5}\right) \), we need \( s_j = \mathcal{O}\left(\log(p)^3\right) \).
Naturally, $s_j$ and $\tilde{s}_j$ are to some extent related. In a linear SEM, the support of $\gamma_j$ and the support of $\tilde{\gamma}_j$ always lie within $j$’s Markov boundary as we argue in Section 4.2. For completely arbitrary setups, it is typically even all of the blanket. Thus, $s_j = \tilde{s}_j$ would then be usual, except for “sink” nodes, such that the first case appears to be most interesting. Furthermore, if $E \left[ Z_j^3 X_{-j} \right] = 0 \; \forall j$, it holds $\tilde{s}_j = 0$ and (C6) is automatically fulfilled.

B.1 Proof of Lemma 8

Following the proofs in van de Geer et al. (2014), the assumptions are sufficient to claim

$$\| \Delta^{OLS} \|_\infty = O_p(1), \quad \| \hat{\beta} - \beta \|_1 = O_p(s\lambda), \quad \frac{1}{n} \| x (\hat{\beta} - \beta) \|_2^2 = O_p(s^2\lambda^2),$$

$$\| \hat{\gamma}_j - \gamma_j \|_1 = O_p(s_j \lambda_j) \; \forall j \quad \text{and} \quad \frac{1}{n} \| x_{-j} (\hat{\gamma}_j - \gamma_j) \|_2^2 = O_p(s_j \lambda_j^2) \; \forall j.$$  

We now turn to $\| \Delta^{HOLS} \|_\infty$. To control this, we want to ensure that

$$\left[ \left( \hat{\beta}_j^3 \right)^T X_{-j} (\beta_{-j} - \hat{\beta}_{-j}) \right] / n = O_p(1/\sqrt{n}) \quad \text{and} \quad \left( \hat{\beta}_j^3 \right)^T x_j / n = E \left[ Z_j^4 \right] + O_p(1). \quad \quad (29)$$

Note that we always have $\| \left( \hat{\beta}_j^3 \right)^T x_{-j} \|_\infty / n = \hat{\lambda}_j$. Thus, the first goal in (29) is fulfilled using (C2) and (C3). Further,

$$\hat{\beta}_j^3 = z_j^3 + (\hat{z}_j^3 - z_j^3) = x_{-j} \hat{\gamma}_j + \hat{z}_j^3 + (\hat{z}_j^3 - z_j^3).$$

From standard Lasso theory (cf. Bühlmann and van de Geer (2011)), we know that the order of which we should choose the tuning parameter $\lambda_j$ is dependent on the bound for

$$\frac{1}{n} \| x_{-j} (\hat{z}_j^3 + (\hat{z}_j^3 - z_j^3)) \|_\infty \leq \frac{1}{n} \| x_{-j} \hat{z}_j^3 \|_\infty + \frac{1}{n} \| x_{-j} (\hat{z}_j^3 - z_j^3) \|_\infty \leq \frac{1}{n} \| x_{-j} \hat{z}_j^3 \|_\infty + \frac{1}{n} \| x_{-j} \|_\infty \| \hat{z}_j^3 - z_j^3 \|_1.$$  

For the first term,

$$E \left[ \max_j \left( \left( \hat{z}_j^3 \right)^T x_{-j} \right) \right] = E \left[ \max_{j,k \neq j} \left( \hat{z}_j^3 \right)^T x_k \right] = E \left[ \max_{j,k \neq j} \sum_{i=1}^n \hat{z}_{ij}^3 x_{ik} \right] = E \left[ \max_{j,k \neq j} \sum_{i=1}^n \hat{z}_{ij}^3 x_{ik} - E \left[ \hat{z}_{ij}^3 x_{ik} \right] \right].$$

We maximise over $j$ as well to receive results uniformly in $j$. In the last equality, we use $E \left[ \hat{z}_{ij}^3 x_{ik} \right] = E \left[ \hat{z}_j^3 X_k \right] = 0$.

All the terms of the type $\hat{z}_{ij}^3 x_{ik}$ can be viewed as different functions of the vector $(x_{i1} \ldots x_{ip} \; \hat{z}_{i1}^3 \ldots \hat{z}_{ip}^3)^T$. In total, these are $p(p-1)$ functions. For these, we can apply the Nemirovski moment inequality from Lemma 14.24 in Bühlmann and van de Geer (2011), which yields

$$E \max_{j,k} \left| \sum_{i=1}^n \hat{z}_{ij}^3 x_{ik} - E \left[ \hat{z}_{ij}^3 x_{ik} \right] \right| \leq (8 \log(2p(p-1)))^{1/2} E \left[ \max_{j,k} \left( \hat{z}_{ij}^3 x_{ik} \right)^2 \right]^{1/2} \leq (8 \log(2p(p-1)))^{1/2} E \left[ \sum_{i=1}^n \max_{j,k} (\hat{z}_j^3)^2 x_{ik}^2 \right]^{1/2} = (8 \log(2p(p-1)))^{1/2} E \left[ \max_{j,k} (\hat{z}_j^3)^2 X_k^2 \right]^{1/2}. $$

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\[
\leq (8 \log(2p(p-1))n)^{1/2} \mathbb{E}\left[ \max_k X_k^8 \right]^{1/2}.
\]

In the last expression, we simplify the notation and let \( k \in \{1, \ldots, 2p\} \) with \( X_{p+j} = \left( \tilde{Z}_j^3 \right)^{1/3} \). We aim to bound the last expectation term, for which we use the sub-Gaussian assumption.

\[
\mathbb{E}\left[ \max_k X_k^8 \right] = \int_0^\infty \mathbb{P}\left( \max_k X_k^8 > t \right) dt = \int_0^\infty \mathbb{P}\left( \max_k |X_k| > t^{1/8} \right) dt
\]

\[
\leq \int_0^\infty \min \left\{ 1, \sum_k \mathbb{P}\left( |X_k| > t^{1/8} \right) \right\} dt \leq \int_0^\infty \min \left\{ 1, 2p \max_k \mathbb{P}\left( |X_k| > t^{1/8} \right) \right\} dt
\]

\[
\leq \int_0^\infty \min \left\{ 1, 4p \max_k \exp\left( -\frac{t^{1/4}}{2\sigma_k^2} \right) \right\} dt \leq \int_0^a \min \left\{ 1, 4p \exp\left( -\frac{t^{1/4}}{2\sigma^2_{\max}} \right) \right\} dt
\]

\[
= a + p \exp\left( -\frac{a^{1/4}}{2\sigma^2_{\max}} \right) \text{poly}(a) = a + \exp\left( -\frac{a^{1/4}}{2\sigma^2_{\max}} + (\log(p)) \right) \text{poly}(a)
\]

This holds for any positive integration bound \( a \). If we choose \( a > 16\sigma^8_{\max} \log(p)^4 \), the second term will vanish as \( p \to \infty \) leading to

\[
\mathbb{E}\left[ \max_k X_k^8 \right] \leq \mathcal{O}\left( \log(p)^4 \right)
\]

such that

\[
\frac{1}{n} \left\| \left( \tilde{Z}_j^3 \right)^{\top} x_{-j} \right\|_\infty \leq \frac{1}{n} \left( \tilde{Z}_j^3 \right)^{\top} x_{-j} \leq \frac{1}{n} \left\| \left( \tilde{Z}_j^3 - z_j^3 \right)^{\top} x_{-j} \right\|_\infty \leq \mathcal{O}_p\left( \sqrt{\log(p)} \right)
\]

from the sub-Gaussian assumption.

Thus,

\[
\frac{1}{n} \left\| \tilde{Z}_j^3 - z_j^3 \right\|_1 = \frac{1}{n} \left\| (\tilde{Z}_j - z_j)^3 + 3z_j \odot (\tilde{Z}_j - z_j)^2 + 3z_j^2 \odot (\tilde{Z}_j - z_j) \right\|_1
\]

\[
\leq \frac{1}{n} \left\| (\tilde{Z}_j - z_j)^3 \right\|_1 + \frac{3}{n} \left\| z_j \odot (\tilde{Z}_j - z_j)^2 \right\|_1 + \frac{3}{n} \left\| z_j^2 \odot (\tilde{Z}_j - z_j) \right\|_1
\]

\[
\leq \frac{1}{n} \left\| \tilde{Z}_j - z_j \right\|_\infty \left( \frac{1}{n} \left\| z_j \right\|_\infty + \frac{3}{n} \left\| z_j \right\|_\infty \right) + \frac{3}{n} \left\| z_j^2 \right\|_\infty \left( \frac{1}{n} \left\| z_j \right\|_\infty + \frac{3}{n} \left\| z_j \right\|_\infty \right)
\]

\[
\leq \frac{1}{n} \left\| \tilde{Z}_j - z_j \right\|_\infty \left( \frac{1}{n} \left\| z_j \right\|_\infty + \frac{3}{n} \left\| z_j \right\|_\infty \right) + \frac{3}{n} \left\| z_j \right\|_\infty \left( \frac{1}{n} \left\| z_j \right\|_\infty + \frac{3}{n} \left\| z_j \right\|_\infty \right)
\]

\[
= \mathcal{O}_p\left( \sqrt{\log(p)} s_j^2 \lambda_j \right) + \mathcal{O}_p\left( \sqrt{\log(p)} s_j \lambda_j \right) + \mathcal{O}_p\left( \sqrt{s_j^2} \right).
\]
In summary,
\[
\frac{1}{n} \left\| x_{-j} (\tilde{z}_j^3 + (\hat{z}_j^3 - z_j^3)) \right\|_\infty = O_p \left( \log(p)^{5/2} n^{-1/2} + \log(p) s_j^2 \lambda_j^3 + \log(p) s_j \lambda_j^2 + \sqrt{\log(p) s_j^2} \right).
\]
If we choose \(\tilde{\lambda}_j\) of this order (as we do in the statement of Lemma 8), we have
\[
\left\| \hat{\gamma}_j - \hat{\gamma}_j \right\|_1 = O_p(\tilde{\lambda}_j) \quad \text{and} \quad \frac{1}{n} \left\| x_{-j} (\hat{\gamma}_j - \hat{\gamma}_j) \right\|_2^2 = O_p(\tilde{\lambda}_j^2).
\]
For \(\left( \tilde{z}_j^3 \right)^T x_j\), we use the decomposition
\[
\tilde{z}_j^3 = z_j^3 - x_{-j} \hat{\gamma}_j = z_j^3 + (\hat{z}_j^3 - z_j^3) - x_{-j} \hat{\gamma}_j + x_{-j} (\hat{\gamma}_j - \hat{\gamma}_j) = \tilde{z}_j^3 + (\hat{z}_j^3 - z_j^3) + x_{-j} (\hat{\gamma}_j - \hat{\gamma}_j).
\]
Thus,
\[
\frac{1}{n} \left\| \left( \tilde{z}_j^3 \right)^T x_j - (\hat{z}_j^3)^T x_j \right\| = \frac{1}{n} \left\| \left( \tilde{z}_j^3 - z_j^3 \right)^T x_j + \left( \hat{\gamma}_j - \hat{\gamma}_j \right)^T x_{-j} x_j \right\|
\leq \frac{1}{n} \left\| \tilde{z}_j^3 - z_j^3 \right\| \left\| x_j \right\|_\infty + \frac{1}{n} \left\| x_{-j} (\hat{\gamma}_j - \hat{\gamma}_j) \right\|_2 \left\| x_j \right\|_2
= O_p \left( \log(p) s_j^2 \lambda_j^3 + \log(p) s_j \lambda_j^2 + \sqrt{\log(p) s_j^2} \right) + O_p \left( \sqrt{\tilde{\lambda}_j^2} \right),
\]
which is \(o_p(1)\) by assumption. This leads to
\[
\frac{1}{n} \left( \tilde{z}_j^3 \right)^T x_j = (\hat{z}_j^3)^T x_j + o_p(1) = E \left[ \tilde{Z}_j^3 X_j \right] + o_p(1).
\]

The last equality could be derived using the Nemirovski moment inequality in a very similar fashion. For the expectation, we have
\[
E \left[ \tilde{Z}_j^3 X_j \right] = E \left[ \tilde{Z}_j^3 \left( Z_j + \gamma_j^3 X_{-j} \right) \right] = E \left[ \tilde{Z}_j^3 Z_j \right] = E \left[ \left( Z_j^3 - \gamma_j^3 X_{-j} \right) Z_j \right] = E \left[ Z_j^4 \right]
\]
such that the second goal in (29) is fulfilled as well. As all these derivations hold uniformly in \(j\), \(|\Delta_{HOLS}^j| = o_p(1)\) implies \(\|\Delta_{HOLS}\| = o_p(1)\).

### B.2 Proof of Lemma 9

We analyse the error term in (27). From the proof of Lemma 8 as well as results in \cite{vandeGeerEtAl2014}, we know
\[
\left( \tilde{z}_j^3 \right)^T x_j / n = E [Z_j^4] + o_p(1), \quad \hat{z}_j^T x_j / n = E [Z_j^2] + o_p(1) \quad \text{and} \quad \|\tilde{z}_j\|_2^2 / n = E [Z_j^2] + o_p(1).
\]

For the remaining terms in \(\tilde{\psi}_j^T \tilde{\psi}_j / n\), we want to ensure
\[
\frac{1}{n} \left\| \tilde{z}_j^3 \right\|_2^2 = E \left[ \tilde{Z}_j^6 \right] + o_p(1) \quad \text{and} \quad \frac{1}{n} \left( \tilde{z}_j^3 \right)^T \tilde{z}_j = \|\tilde{z}_j\|_2^2 / n = [Z_j^4] + o_p(1).
\]
Using the Nemirovski equation in a similar fashion as before, we know
\[
\max_j \frac{1}{n} \sum_{i=1}^{n} z_{ij}^* - \mathbb{E}[Z_j^*] = O_p\left(\frac{\log(p)(r+1)/2}{n^{1/2}}\right).
\]
We assume this to be \(O_p(1) \forall r \leq 10\) and even \(O_p(1) \forall r \leq 6\) (which is implied by the first condition). We look at some intermediary results. Each difference is \(O_p(1)\) using the sparsity assumptions.
\[
\frac{1}{n} \left\| z_j^4 \circ \hat{z}_j^4 - z_j^4 \right\|_1 = \frac{1}{n} \left\| z_j^4 \circ (\hat{z}_j^2 - z_j^2) \right\|_1 = \frac{1}{n} \left\| z_j^2 \circ \left( (\hat{z}_j - z_j)^2 + 2z_j \circ (\hat{z}_j - z_j) \right) \right\|_1
\leq \frac{1}{n} \left\| z_j^2 \right\|_\infty \left\| \hat{z}_j - z_j \right\|_2^2 + \frac{2}{n} \left\| z_j^2 \right\|_2 \left\| \hat{z}_j - z_j \right\|_2 = O_p\left(\log(p)s_j \lambda_j^2\right) + O_p\left(\sqrt{s_j \lambda_j^2}\right).
\]
This implies \(\frac{1}{n} \left\| z_j^2 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| z_j \circ \hat{z}_j \right\|_2^2 = O_p(1)\). With this, we can refine our result in a stepwise fashion:
\[
\frac{1}{n} \left\| z_j^4 \circ \hat{z}_j^4 - z_j^4 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| z_j^4 \circ (\hat{z}_j^2 - z_j^2) \right\|_1 = \frac{1}{n} \left\| z_j^2 \circ \hat{z}_j^2 \circ \left( (\hat{z}_j - z_j)^2 + 2z_j \circ (\hat{z}_j - z_j) \right) \right\|_1
\leq \frac{1}{n} \left\| z_j^2 \right\|_\infty \left\| \hat{z}_j - z_j \right\|_2^2 + \frac{2}{n} \left\| z_j \right\|_\infty \left\| \hat{z}_j \right\|_\infty \left\| z_j^2 \hat{z}_j \right\|_2 \left\| \hat{z}_j - z_j \right\|_2 = O_p\left(\log(p)^2 s_j \lambda_j^2\right) + O_p\left(\log(p)(1 + s_j \lambda_j)\sqrt{s_j \lambda_j^2}\right)
\]
such that \(\frac{1}{n} \left\| z_j^2 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| z_j \circ \hat{z}_j \right\|_2^2 = O_p(1)\).
\[
\frac{1}{n} \left\| \hat{z}_j^4 - z_j^4 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| \hat{z}_j^4 \circ (\hat{z}_j^2 - z_j^2) \right\|_1 = \frac{1}{n} \left\| \hat{z}_j^2 \circ \hat{z}_j^2 \circ \left( (\hat{z}_j - z_j)^2 + 2z_j \circ (\hat{z}_j - z_j) \right) \right\|_1
\leq \frac{1}{n} \left\| \hat{z}_j^2 \right\|_\infty \left\| \hat{z}_j - z_j \right\|_2^2 + \frac{2}{n} \left\| z_j \right\|_\infty \left\| \hat{z}_j \right\|_\infty \left\| z_j^2 \hat{z}_j \right\|_2 \left\| \hat{z}_j - z_j \right\|_2 = O_p\left(\log(p)^2 (1 + s_j^4 \lambda_j^4) s_j \lambda_j^2\right) + O_p\left(\log(p)(1 + s_j \lambda_j)^2\sqrt{s_j \lambda_j^2}\right)
\]
such that \(\frac{1}{n} \left\| \hat{z}_j^2 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| z_j \circ \hat{z}_j \right\|_2^2 = O_p(1)\).
Finally, it follows
\[
\frac{1}{n} \left\| z_j^3 \circ \hat{z}_j^3 - z_j^4 \circ \hat{z}_j^2 \right\|_1 = \frac{1}{n} \left\| z_j^3 \circ \hat{z}_j^2 \circ (\hat{z}_j - z_j) \right\|_1 = \frac{1}{n} \left\| z_j^2 \circ \hat{z}_j^2 \circ \hat{z}_j \circ (\hat{z}_j - z_j) \right\|_1
\leq \frac{1}{n} \left\| z_j^2 \right\|_\infty \left\| \hat{z}_j \right\|_\infty \left\| z_j^2 \hat{z}_j \right\|_2 \left\| \hat{z}_j - z_j \right\|_2 = O_p\left(\log(p)^2 \sqrt{s_j \lambda_j^2}\right) \text{ such that}
\]
\[
\frac{1}{n} \left\| \hat{z}_j^3 - z_j^3 \circ \hat{z}_j^2 \right\|_2 = \frac{1}{n} \left\| \hat{z}_j^3 - z_j^3 \right\|_2 \leq \frac{1}{n} \left\| \hat{z}_j^3 \circ (\hat{z}_j - z_j) \left\|_1 \leq \frac{1}{n} \left\| \hat{z}_j^3 \circ \hat{z}_j \circ z_j \right\|_1 \leq \frac{1}{n} \left\| \hat{z}_j^3 \circ \hat{z}_j \right\|_2 \left\| z_j \right\|_\infty \left\| \hat{z}_j - z_j \right\|_2 + \frac{1}{n} \left\| \hat{z}_j^3 \circ \hat{z}_j \right\|_2 \left\| \hat{z}_j - z_j \right\|_2
\leq O_p\left(\log(p)^2 (1 + s_j^4 \lambda_j^4) s_j \lambda_j^2\right) + O_p\left(\log(p)(1 + s_j^2 \lambda_j^2)^2\sqrt{s_j \lambda_j^2}\right) = O_p(1),
\]
This can now be applied to find the desired convergence.

\[
\frac{1}{n} \left| \left( \hat{z}_j^3 \right)^\top z_j - \left( \hat{z}_j^3 \right)^\top z_j \right| = \frac{1}{n} \left| \left( \hat{z}_j^3 \right)^\top (\hat{z}_j - z_j) + \left( \hat{z}_j^3 - z_j \right)^\top z_j + \left( \hat{z}_j^3 - z_j \right)^\top (\hat{z}_j - z_j) \right| \\
\leq \frac{1}{n} \left\| \hat{z}_j \right\|_2 \left\| z_j - z_j \right\|_2 + \frac{1}{n} \left\| \hat{z}_j^3 - z_j \right\|_2 \left\| z_j \right\|_2 + \frac{1}{n} \left\| \hat{z}_j^3 - z_j \right\|_2 \left\| z_j - z_j \right\|_2 + \frac{1}{n} \left\| z_j \right\|_2 \left\| x_j \left( \hat{y}_j - \hat{y}_j \right) \right\|_2 + \frac{1}{n} \left\| x_j \left( \hat{y}_j - \hat{y}_j \right) \right\|_2 \left\| z_j - z_j \right\|_2.
\]

All these terms have already been bounded. Thus, we do not need any further assumptions to claim

\[
\frac{1}{n} \left( \hat{z}_j^3 \right)^\top z_j = \frac{1}{n} \left( \hat{z}_j^3 \right)^\top z_j + \sigma_p(1) = \mathbb{E} \left[ \hat{Z}_j^3 Z_j \right] + \sigma_p(1) = \mathbb{E} \left[ Z_j^3 \right] + \sigma_p(1).
\]

We turn to the final term in the error scaling

\[
\frac{1}{n} \left( \hat{z}_j^3 \right)^\top \left( \hat{z}_j^3 \right) - \left( \hat{z}_j^3 \right)^\top \left( \hat{z}_j^3 \right) = \\
\frac{1}{n} \left[ 2 \left( \hat{z}_j^3 \right)^\top \left( \hat{z}_j^3 - z_j \right) + 2 \left( \hat{z}_j^3 \right)^\top x_j \left( \hat{y}_j - \hat{y}_j \right) + \left( \hat{z}_j^3 - z_j \right)^\top \left( \hat{z}_j^3 - z_j \right) + 2 \left( \hat{z}_j^3 - z_j \right)^\top x_j \left( \hat{y}_j - \hat{y}_j \right) \right] \\
\leq \frac{2}{n} \left\| \hat{z}_j \right\|_2 \left\| \hat{z}_j^3 - z_j \right\|_2 + \frac{2}{n} \left\| \hat{z}_j^3 \right\|_2 \left\| \hat{z}_j \right\|_2 + \frac{1}{n} \left\| \hat{z}_j^3 - z_j \right\|_2 \left\| z_j \right\|_2 + \frac{2}{n} \left\| \hat{z}_j^3 - z_j \right\|_2 \left\| x_j \left( \hat{y}_j - \hat{y}_j \right) \right\|_2 + \frac{1}{n} \left\| x_j \left( \hat{y}_j - \hat{y}_j \right) \right\|_2 \left\| z_j - z_j \right\|_2.
\]

Again, these are all terms that we have seen before such that we do not need any additional assumptions to claim

\[
\frac{1}{n} \left( \hat{z}_j^3 \right)^\top \left( \hat{z}_j^3 \right) = \frac{1}{n} \left( \hat{z}_j^3 \right)^\top \left( \hat{z}_j^3 \right) + \sigma_p(1) = \mathbb{E} \left[ \left( \hat{Z}_j^3 \right)^2 \right] + \sigma_p(1).
\]

Thus, we have shown convergence for all terms in \( \hat{v}_j^\top \hat{v}_j/n \). Finally, note that

\[
\mathbb{E} \left[ V_j^2 \right] = \mathbb{E} \left[ \left( \frac{\hat{z}_j^3}{\mathbb{E} \left[ Z_j^3 \right]} - \frac{Z_j}{\mathbb{E} \left[ Z_j^3 \right]} \right)^2 \right] = \frac{\mathbb{E} \left[ \left( \hat{Z}_j^3 \right)^2 \right]}{\mathbb{E} \left[ Z_j^4 \right]} - \frac{2 \mathbb{E} \left[ \hat{Z}_j^3 Z_j \right]}{\mathbb{E} \left[ Z_j^4 \right] \mathbb{E} \left[ Z_j^3 \right]} + \frac{\mathbb{E} \left[ Z_j^3 \right]^2}{\mathbb{E} \left[ Z_j^4 \right]^2} = \frac{\mathbb{E} \left[ \left( \hat{Z}_j^3 \right)^2 \right]}{\mathbb{E} \left[ Z_j^4 \right]} - \frac{1}{\mathbb{E} \left[ Z_j^3 \right]}
\]

such that convergence is towards \( \mathbb{E} \left[ V_j^2 \right] \) as claimed.

### B.3 Proof of Theorem 12

With Lemmata 8 and 9, we have already established that the bias terms vanish and the denominator converges. It remains to look at \( \hat{v}_j^\top \epsilon/\sqrt{n} \).

\[
\mathbb{E} \left[ (\hat{v}_j - v_j)^\top \epsilon/\sqrt{n} \right] = \mathbb{E} \left[ (\hat{v}_j - v_j)^\top \epsilon/\sqrt{n} | x \right] = \mathbb{E} \left[ (\hat{v}_j - v_j)^\top \epsilon/\sqrt{n} | x \right] = 0 \quad \text{and}
\]

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\[
\text{Var}\left((\hat{v}_j - v_j)^\top \epsilon / \sqrt{n}\right) = \mathbb{E}\left[\text{Var}\left((\hat{v}_j - v_j)^\top \epsilon / \sqrt{n}|x\right)\right] + \text{Var}\left(\mathbb{E}\left[(\hat{v}_j - v_j)^\top \epsilon / \sqrt{n}|x\right)\right)
\]
\[
= \sigma^2 \mathbb{E}\left[\|\hat{v}_j - v_j\|^2/n\right] + 0 = \mathcal{O}(1)
\]

The last equality uses the convergence rates from the proof of Lemma 9. By Chebyshev’s inequality and the CLT
\[
\hat{v}_j^\top \epsilon / \sqrt{n} \xrightarrow{p} v_j^\top \epsilon / \sqrt{n} \xrightarrow{D} N\left(0, \sigma^2 \mathbb{E}\left[V_j^2\right]\right)
\]
By Slutsky’s theorem, we can replace \( \sigma^2 \) with a consistent estimate such that the theorem’s statement follows.

C Additional simulation results

C.1 Global null with Gaussian error

We present here a simulation study to support the results in Section 2.2. It is very similar to the simulation example in Section 2.2.1 but with jointly Gaussian \( X \) and \( Y \). Otherwise, the setup is identical: The dimensionality of \( x \) is \( n = 100 \) and \( p = 30 \), it has a Toeplitz covariance matrix \( \Sigma_X \) with \( \Sigma_X_{ij} = r^{|i-j|} \) with \( r = 0.6 \). The coefficient vector \( \beta \) is 5-sparse, and the active predictors are \{1, 5, 10, 15, 20\}, each of which having a coefficient equal to 1. The random error \( E \) is Gaussian with a standard deviation of \( \sigma = 2 \).

In Figure 6, we plot the histogram and the empirical cumulative density function (ECDF) of the p-values obtained for all predictors in all simulation runs. From either plot, we see that the p-values follow the target distribution even closer than for non-Gaussian data. This is of course

![Histogram of p-values](image1)

![ECDF of p-values](image2)

Figure 6: Results for Gaussian design under the global null. On the left: histogram of p-values (unadjusted \( p_j \) as in Step 9 of Algorithm 1) over all \( p = 30 \) predictors. On the right: ECDF of these p-values. The grey dotted line corresponds to the desired uniform distribution.
non-surprising as the only approximation we make is in the use of \( \hat{\sigma} \) instead of the true \( \sigma = 2 \) to calculate the \( z \)-statistics.

### C.2 Confounding onto block-independent \( E_X \)

To simulate block-independent data, we make use of the Boston housing data, available in the R-package MASS (Venables and Ripley 2002). We use all but the variable \texttt{medv}, which is typically the response variable for regression. Then, we create two independent bootstrap samples and concatenate those such that we have two independent blocks forming the matrix \( \epsilon_X \). Before this bootstrap sampling, we make all variables have 0 mean and unit variance. We let \( H \) be a standard normal random variable and set \( X_1 = \mathcal{E}_{X_1} + H \) and \( X_7 = \mathcal{E}_{X_7} - H \). For the remaining variables, we let \( X_j = \mathcal{E}_{X_j} \). Finally, we set \( Y = H \) for simplicity. Thus, the first block is confounded with \( Y \), but the second is not.

We vary the sample size from 10\(^2\) to 10\(^6\), doing 200 simulation runs for each sample size. Thus, it is a “\( m \) out of \( n \)” bootstrap, where \( m \) can be smaller than \( n \) (for \( m = 10^2 \)) or larger (for the rest). In the remainder, we call the bootstrap sample size \( n \) to keep the notation consistent and as the size of the real Boston housing data is not of primary interest. On the left-hand side of Figure 7 we plot the average absolute \( z \)-statistics for a representative subset of the predictors. Notably, it is the same four predictors once from the first block and once from the second. As expected, this average grows as \( \sqrt{n} \) for variables in the confounded block, while it stays approximately constant for variables from the independent block. Further, we see that the two variables \( X_1 \) and \( X_7 \), which are directly confounded, are the easiest to detect as such. For only 10\(^2\) samples the multiplicity

![Figure 7: Confounding onto block independent \( E_X \). On the left: Average absolute \( z \)-statistics per covariate for different sample sizes. The dotted lines grow as \( \sqrt{n} \) and are fit to match perfectly at \( n = 10^5 \). On the right: Empirical probability (over 200 simulation runs) of perfectly recovering \( U \) (cf. (13)) for different sample sizes.](image-url)
corrected p-values for $X_1$ and $X_7$ lead to a rejection of the local null hypothesis in 78.5% respectively 46% of the simulation runs at level $\alpha = 0.05$. For some of the other variables in the confounded block, it takes many more samples to reliably reject the local null hypothesis. For $X_9$, the local null hypothesis is only rejected in 3% of the cases for $n = 10^4$ and only from $n = 10^5$ it is always rejected.

On the right-hand side, we show the empirical probability of perfectly recovering $U$, i.e., rejecting the null hypotheses for all variables from the first block and accepting it for those from the second block. We see that for $n = 10^5$ we are able to achieve this recovery with an empirical probability of 1, and, for $n = 10^6$, it is even possible for a larger range of thresholds. Comparing the two curves for $n = 10^5$ and $n = 10^6$, we see that they initially look very similar. This is as one would expect as the initial increase of the curve corresponds to reducing the type I error, which is independent of the sample size, assuming the CLT has kicked in sufficiently. The decrease of the curve depends on the z-statistics for the confounded variables, which we know to increase as $\sqrt{n}$. Thus, this decrease will appear later the larger $n$ gets.

In Figure 8, we analyse the partial recovery of $U$ as before. We see that for a sample size of $10^4$, for which perfect recovery is hardly achievable, we receive an average intersection size of 9.175 (out of 13) allowing for 10% probability of false inclusion. For lower sample sizes, there is not much that can be found under this constraint. In this setup, there is a confounding bias onto 13 OLS parameters with varying signal strength $|\beta^{OLS}_j - \beta_j|$. The two directly confounded variables
amount to 45.254% of the confounding signal. Thus, a remaining fraction of 54.746% appears to be particularly achievable. We see that we can do even better than that. Namely, for a sample size of $10^3$ we receive can get an empirical probability of 1 of including all variables of $U$ in $\hat{U}$ allowing for an average of 44.775% of the confounding signal. For $10^4$, we can go down to a remaining fraction of 17.597%.

### C.3 Global null in a high-dimensional setting

We revisit the simulation example from Section 2.2. We reuse the setup with the only exception that $p = 200 > n$. Thus, we add an extra 170 predictors that do not actually have any influence on $Y$.

To calculate $\hat{z}_j$, $\hat{w}_j$, and $\hat{\sigma}$ we use the default implementation of the debiased Lasso, available in the R-package hdi (Dezeure et al., 2015). To get the estimate $\hat{z}_j^3$ we run a second level of nodewise regression with cross-validated $\hat{\lambda}_j$. It shall be noted that all the estimated $\hat{\gamma}_j = 0$. Thus, $x_{-j}$ does not appear to contain strong enough information on $z_j^3$, at least for the given sample size.

Again, we look at all the obtained p-values and plot the histogram and the ECDF in Figure 9. We see some deviations from the uniform distribution. Especially, very low p-values become more unlikely. Thus, the procedure is a bit too conservative. This might be related to $\sigma$ being overestimated: the empirical average of $\hat{\sigma}^2$ is 1.35 and $\hat{\sigma} > \sigma$ occurred in 88.5% of the cases. However, when replacing the estimate with the true $\sigma$ the p-values become too liberal.

In summary, after increasing the number of predictors but keeping the sample size the same, the results deviate a bit more from the optimal distribution. Though, the behaviour is still fairly close to what one would aim for, supporting the benefit of our method.

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**Figure 9:** Results for non-Gaussian design under the global null for high-dimensional data. On the left: histogram of p-values (unadjusted $p_j$ as in Step 10 of Algorithm 2) over all $p = 200$ predictors. On the right: ECDF of these p-values. The grey dotted line corresponds to the desired uniform distribution.