Detecting non-causal artifacts in multivariate linear regression models

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Abstract

We consider linear models where $d$ potential causes $X_1, \ldots, X_d$ are correlated with one target quantity $Y$ and propose a method to infer whether the association is causal or whether it is an artifact caused by overfitting or hidden common causes. We employ the idea that in the former case the vector of regression coefficients has ‘generic’ orientation relative to the covariance matrix $\Sigma_{XX}$ of $X$. Using an ICA based model for confounding, we show that both confounding and overfitting yield regression vectors that concentrate mainly in the space of low eigenvalues of $\Sigma_{XX}$.

1 Introduction

Inferring causal relations from passive observations data has gained increasing interest in machine learning and statistics. Although reliable causal conclusions can only be drawn from interventional data, the idea of postulating assumptions that render causal inference from passive observations feasible becomes more and more accepted. In addition to the more ‘traditional’ causal Markov condition and causal faithfulness assumption Spirtes et al. (1993); Pearl (2000), researchers have also stated assumptions that render causal inference from passive observations feasible becomes more and more accepted. In addition to the more ‘traditional’ causal Markov condition and causal faithfulness assumption Spirtes et al. (1993); Pearl (2000), researchers have also stated assumptions that admit causal inference when no conditional statistical independences hold, e.g., Kano and Shimizu (2003); Sun et al. (2006); Hoyer et al. (2009); Zhang and Hyvärinen (2009); Blöbaum et al. (2017). Each of these method relies on idealized assumptions that rarely hold in practice; nevertheless they can be useful if the methods possess a degree of robustness regarding violation of model assumptions.

Mooij et al. (2016). In a similar vein, the present work considers a causal inference problem that becomes solvable only under an idealized model assumption that is certainly debatable. However, it illustrates that high-dimensional observations contain a kind of causal information that has not been employed so far.

We assume that we are given a scalar target variable $Y$ that is potentially influenced by a multi-dimensional predictor variable $X = (X_1, \ldots, X_d)$. Suppose that i.i.d. samples from $P_{X,Y}$ show that $X$ and $Y$ are significantly correlated, but it is unclear whether this is mainly due to the influence of $X$ on $Y$ or due to a common cause of $X$ and $Y$ (here we assume that prior knowledge excludes the case where $Y$ causally influences $X$, e.g., due to time order). $Y$ may, for instance, be a quantitative property of a material (e.g., electrical resistance) and $X_j$ some features describing its chemical and physical structure. In biology, $X$ and $Y$ could represent information about genotype and phenotype, respectively. Note that conditional independences allow to decide which of the variables $X_j$ influence $Y$, given that the association between $X$ and $Y$ is unconfounded. The question of unconfoundedness, which we address here, is therefore prior to the former problem.

Figure 1, left, visualizes the generic scenario that we consider throughout the paper, where the statistical dependencies between $X$ and $Y$ are due to the influence of $X$ on $Y$ and due to the common cause $Z$. It contains the purely confounded case (middle) as limiting case where the arrow from $X$ to $Y$ is arbitrarily weak. Likewise, the purely causal case is obtained when one of the arrows from $Z$ gets weak (right).

Our confounder detection is based on observing ‘non-generic’ relations between $P_X$ and $P_{Y|X}$ Janzing and
Schölkopf (2017). We thus follow the abstract principle of independent mechanisms Peters et al. (2017), stating that for the purely causal relation $X \rightarrow Y$ of two arbitrary variables variables $X, Y$, the marginal $P_X$ and the conditional $P_{Y|X}$ do not contain information about each other (where ‘information’ needs to be further specified). The present paper contains the following novel contributions:

- We allow for multi-dimensional confounders. In contrast, the entire analysis of Janzing and Schölkopf (2017) is restricted to the case of a one-dimensional confounder, and cannot be extended using the methods presented in that work.
- We show that the multivariate setting permits an analysis which is significantly simpler, and also the ‘dependencies’ between $P_X$ and $P_{Y|X}$ become simple.
- We derive a statistical test for non-confounding based on our model assumptions.
- We show that for our model, overfitting generates the same kind of dependences between $P_X$ and $P_{Y|X}$ as confounding. This suggests a subtle link between regularization and the correction of confounding. One may conjecture, for instance, that models with ‘independent’ $P_X$ and $P_{Y|X}$ have better chances to generalize to future data points as well as to related data sets from other domains (including interventional data), cf. also Schölkopf et al. (2012).

It may sound counter-intuitive that the multivariate case can be simpler than the scalar case, but our derivations are based on a certain notion of genericity of the multivariate confounder which does not necessarily hold for the scalar case, although our experiments will also include data with scalar confounding.

2 Model for confounding with uncorrelated sources

Our model for the influence of the high-dimensional common cause $Z$ on both $X$ and $Y$ is inspired by Independent Component Analysis (ICA) Hyvärinen et al. (2001). Let $Z$ consist of $\ell \geq d$ independent sources $Z_1, \ldots, Z_\ell$, each having unit variance. They influence $X$ via a mixing matrix $M$ and $Y$ via a mixing vector $c$, as shown in Figure 2. Explicitly, the structural equations relating $Z, X, Y$ thus read:

\[
X = MZ \quad (1)
\]
\[
Y = a^TX + c^TZ. \quad (2)
\]

where $M$ is a $d \times \ell$ matrix and $a$ are $c$ are vectors in $\mathbb{R}^d$ and $\mathbb{R}^\ell$, respectively. The model induces the following correlations of the observed variables $X$ and $Y$:

\[
\Sigma_{XX} = MIM^T = MM^T \quad (3)
\]
\[
\Sigma_{XY} = MM^Ta + Mc, \quad (4)
\]

where $I$ denotes the identity matrix. While $a$ describes the causal influence of $X$ on $Y$, formally regressing $Y$ on $X$ yields

\[
a' := \Sigma_{XX}^{-1}\Sigma_{XY} = a + M^{-T}c, \quad (5)
\]

\[1\]In contrast to ICA, however, it is actually enough that the sources are uncorrelated.
where $M^{-T}$ denotes the transpose of the pseudoinverse of $M$. The vector $a'$ describes how the distribution of $Y$ is shifted when one observes $X$ has attained a particular $d$-tuple, while $a$ describes how it changes when $X$ is set to some $d$-tuple by an intervention. In Pearl’s language Pearl (2000), $a'$ vs. $a$ describe the difference between $p(y|x)$ and $p(y|do(x))$ for our particular linear model. Janzing and Schölkopf (2017) define the strength of confounding by

$$
\beta := \frac{\|a' - a\|^2}{\|a\|^2 + \|a' - a\|^2} \in [0, 1],
$$

where $M$ is the transpose of the pseudoinverse of $M$. The vector $a'$ describes how the distribution of $Y$ is shifted when one observes $X$ has attained a particular $d$-tuple, while $a$ describes how it changes when $X$ is set to some $d$-tuple by an intervention. In Pearl’s language Pearl (2000), $a'$ vs. $a$ describe the difference between $p(y|x)$ and $p(y|do(x))$ for our particular linear model. Janzing and Schölkopf (2017) define the strength of confounding by

$$
\beta := \frac{\|a' - a\|^2}{\|a\|^2 + \|a' - a\|^2} \in [0, 1],
$$

which is $0$ for the purely causal case $a' = a$ and $1$ for the purely confounded case $a = 0$, which is already a nice property. To further justify this definition, they argue that the vectors $a$ and $a' - a = M^{-T}c$ are close to orthogonal in high dimensions if $a$ is drawn independently from $M^{-T}c$ from a rotation-invariant distribution. Thus, the denominator is close to $\|a'\|^2$ and $\beta$ is the fraction of squared length of $a'$ that can be attributed to the confounder. Following Janzing and Schölkopf (2017) we define the estimation of $\beta$ from $P_{X,Y}$ as our crucial task.

The essential assumption that we add now is that the vectors $c$ and $a$ are randomly drawn from a rotation-invariant prior. One can already guess from (5) what kind of ‘non-generic’ relation the vector $a'$ then satisfies together with $\Sigma_{XX}$: whenever $a'$ is dominated by the confounding term $M^{-T}c$ it tends to be mainly located in the eigenspaces of $\Sigma_{XX}$ corresponding to small eigenvalues. The formal analysis is detailed below, but intuitively speaking, multiplication with $M^{-T}$ amplifies the components corresponding to small singular values of $M$ and thus to small eigenvalues of $\Sigma_{XX} = MM^T$.

To formally explore this idea we first introduce the following generating model for $a$ and $c$ and hence for $a'$:

**Definition 1** (ICA based confounding model). First sample each component of $a$ from a Gaussian with zero mean and standard deviation $\sigma_a$, then sample each component of $c$ from a Gaussian with standard deviation $\sigma_c$. Compute $a'$ as in (5), where $M$ is some given $d \times \ell$-matrix.

Together with $M$, the parameters $\sigma_a$ and $\sigma_c$ determine the expected value of $\beta$, but actually only their ratio matters because $\beta$ depends only on the relative squared lengths of vectors.

**3 Estimating the ratio of $\sigma_a$ and $\sigma_c$**

We now describe how to infer the ratio of $\sigma_a$ and $\sigma_c$ as an intermediate step for inferring $\beta$. We could infer both parameters by maximizing the likelihood of $a'$ given our generating model in Definition 1 if we knew $M$ and $\ell$. Unfortunately, we only know $MM^T = \Sigma_{XX}$ and $d$. However, we can construct an equivalent generating model for $a'$ that contains only these observed elements:

**Definition 2** (alternative generating model for $a'$). Generate $b \in \mathbb{R}^d$ by drawing each component from a standard Gaussian. Set

$$
a' := \sqrt{\sigma_a^2 I + \sigma_c^2 \Sigma_{XX}} b.
$$

**Theorem 1** (equivalence of models). The model in Definition 2 generates vectors $a'$ with the same distribution as in Definition 1.

**Proof.** First define the $d \times (d + \ell)$-matrix

$$
K_{\sigma_a, \sigma_c} := \begin{pmatrix} \sigma_a I & \sigma_c M^{-T} \end{pmatrix}.
$$

We can then rewrite $a'$ in Definition 1 as

$$
a' = K_{\sigma_a, \sigma_c} b',
$$

with

$$
b' := \begin{pmatrix} a/\sigma_a \\
\sigma_a/c/\sigma_c \end{pmatrix}.
$$

Let

$$
K_{\sigma_a, \sigma_c} = \sqrt{K_{\sigma_a, \sigma_c} K_{\sigma_a, \sigma_c}^T} V_{\sigma_a, \sigma_c}
$$

be the right polar decomposition of $K_{\sigma_a, \sigma_c}$, where $V_{\sigma_a, \sigma_c}$ is a partial isometry from $\mathbb{R}^{d + \ell}$ to $\mathbb{R}^d$. It can be written as

$$
V_{\sigma_a, \sigma_c} = W_{\sigma_a, \sigma_c} Q,
$$

where $W_{\sigma_a, \sigma_c}$ is an orthogonal $d \times d$-matrix and $Q : \mathbb{R}^{d + \ell} \rightarrow \mathbb{R}^d$ is the projection that annihilates the last $\ell$ components of a vector. We then get

$$
a' = \sqrt{K_{\sigma_a, \sigma_c} K_{\sigma_a, \sigma_c}^T} W_{\sigma_a, \sigma_c} Q b'.
$$

Since the $d + \ell$ entries of $b'$ are drawn from independent standard Gaussians, the $d$ entries of $Q b'$ are also standard.
Gaussians. This distribution of entries is invariant under orthogonal maps, hence the entries of
\[ b := W_{\sigma_a, \sigma_e} Q b' \]
are also independent standard Gaussians. We have
\[ \sqrt{K_{\sigma_a, \sigma_e} K^T_{\sigma_a, \sigma_e}} = \sqrt{\sigma_a^2 I + \sigma_e^2 \Sigma^{-1}}. \]
Hence,
\[ a' = \sqrt{\sigma_a^2 I + \sigma_e^2 \Sigma^{-1}} b. \]

Note that the length of \( a' \) is irrelevant for \( \beta \). We thus consider \( a'/\|a'\| \) and infer only the quotient \( \theta := \sigma_e^2 / \sigma_a^2 \).

We therefore introduce the matrix
\[ R_\theta := I + \theta \Sigma^{-1}, \]
and conclude that our generating models for \( a' \) induces a distribution for the directions \( a'/\|a'\| \) that is the image of the uniform distribution on the unit sphere (i.e. the Haar measure for the orthogonal group) under the map
\[ b \mapsto \sqrt{R_\theta} b / \| \sqrt{R_\theta} b \|. \]

To compute this distribution, we use the following result shown in the appendix:

**Lemma 1** (distributions of directions induced by a matrix). Let \( A \) be an invertible real-valued \( d \times d \)-matrix. Define the map \( \Phi : S^{d-1} \to S^{d-1} \) by
\[ \Phi(v) := \frac{1}{\| Av \|} Av. \]
Then the image of the uniform distribution on \( S^{d-1} \) under \( \Phi \) has the following density with respect to the uniform distribution:
\[ p(\tilde{v}) = \frac{1}{\det(A) \| A^{-1} \tilde{v} \|} \] (8)

We now apply Lemma 1 to \( A := \sqrt{R_\theta} \) as defined by (7) and obtain
\[ p_\theta(\tilde{v}) = \frac{1}{\det \sqrt{R_\theta} \| \sqrt{R_\theta}^{-1} \tilde{v} \|} \] (9)

Using
\[ |\det \sqrt{R_\theta}| = \sqrt{|\det R_\theta|} \]
we can rewrite (9) as
\[ p_\theta(\tilde{v}) = \frac{1}{\sqrt{|\det R_\theta|} \| (1 + \theta \Sigma^{-1})^{-1} \tilde{v} \|^d}, \]
which proves the following theorem:

**Theorem 2** (density of directions). The generating model in Definition 1 generates vectors \( a' \) whose distribution of unit vectors \( \hat{v} := a'/\|a'\| \) has the following log density with respect to the uniform distribution on the sphere:
\[ \log p_\theta(\tilde{v}) = \frac{1}{2} \left[ \log \det R_\theta - d \log \| (1 + \theta \Sigma^{-1})^{-1} \tilde{v} \| \right]. \] (10)

Given sufficiently many samples \( a' \) generated with the same \( \theta \), we can certainly infer \( \theta \) by maximizing (10). Remarkably, we can infer the loglikelihood already from a single instance for large \( d \) under appropriate conditions:

**Theorem 3** (concentration of measure). Let \( \tilde{v} \) be drawn from \( p_\theta \). Then for sufficiently small \( \epsilon \) we have
\[ \left| \log p_\theta(\tilde{v}) - \frac{1}{2} \left[ \log \det R_\theta - \log \left( \frac{\tau(R_\theta, R_\theta^{-1})}{\tau(R_\theta')} \right) \right] \right| \leq \epsilon \]
with probability at least
\[ 1 - \frac{1}{d^2} \left( \frac{\tau(R_\theta^2 R_\theta^{-2})}{\tau(R_\theta R_\theta')} + \frac{\tau(R_\theta^2)}{\tau(R_\theta')^2} \right), \]
where \( \tau() := \frac{1}{d} \text{tr}() \) denotes the renormalized trace.

The proof can be found in the appendix. Whenever one assumes a limit for \( d \to \infty \) in which the expressions with \( \tau \) converge\(^\ddagger\), the error thus tends to zero. Intuitively speaking, the reason is that drawing one vector from \( p_\theta \) in dimension \( d \) can be reduced to drawing \( d \) independent coefficients with respect to an appropriate basis, which finally reduces the problem to the usual law of large numbers.

\(^\ddagger\)This holds, for instance, for any sequence \( \Sigma^{(d)} \) for which the eigenvalues have a uniform positive lower bound \( b \) and the distribution of eigenvalues converges weakly to some measure \( \mu \). Then, \( \tau(f(\Sigma^{(d)})) \) converges to \( \int fd\mu \) for any bounded continuous function \( f : [b, \infty) \to \mathbb{R} \) by definition of weak convergence.
4 Estimating confounding strength $\beta$

To infer $\beta$ (which we defined as our crucial task) from $\theta$ we need some approximations that hold for large $d$. First we use $||a||^2/d \approx \sigma_a^2$ which is justified by the law of large numbers. Moreover we can estimate the length of $M^{-T}c$ using the trace of the concentration matrix of $X$:

$$\frac{1}{d} ||a' - a||^2 = \frac{1}{d} ||M^{-T}c||^2 = \frac{1}{d} (c, M^{-1}M^{-T}c) \approx \sigma_c \tau(M^{-1}M^{-T}) = \sigma_c \tau(M^{-T}M^{-1}) = \sigma_c \tau(\Sigma_{XX}^{-1})$$

where the approximation uses also the law of large numbers since we can generate $c$ by drawing its coefficients with respect to the eigenbasis of $M^{-1}M^{-T}$ from independent Gaussians of standard deviation $\sigma_c$. Thus we obtain

$$\beta \approx \frac{\tau(\Sigma_{XX}^{-1}) \sigma_a^2}{\tau(\Sigma_{XX}^{-1}) \sigma_c^2 + \sigma_a^2} = \frac{\tau(\Sigma_{XX}^{-1}) \theta}{\tau(\Sigma_{XX}^{-1}) \theta + 1}. \quad (11)$$

Putting everything together, we obtain the following procedure for estimating $\beta$ from $(X, Y)$ samples:

1. Compute the empirical covariance matrices $\hat{\Sigma}_{XX}$ and $\hat{\Sigma}_{XY}$.
2. Estimate $a'$ via
   $$\hat{a}' := \hat{\Sigma}_{XX}^{-1} \hat{\Sigma}_{XY}.$$
3. Infer $\theta$ via maximizing the likelihood $\log p_\theta(\hat{a}'/||\hat{a}'||)$ defined by (10).
4. Compute $\beta$ from the estimated value of $\theta$ via (11).

Here we have neglected finite sample issues completely. We will discuss them in section 6.

5 Test for non-confounding

To test the null hypothesis $\theta = 0$, that is $a' = a$, we define the test statistics (applied to a single instance $\tilde{v} = a'/||a'||$)

$$T(\tilde{v}) := \frac{1}{\sqrt{d}} \left\{ (\tilde{v}, \Sigma_{XX}^{-1}\tilde{v}) - \tau(\Sigma_{XX}^{-1}) \right\}. \quad (12)$$

One can easily show that its expectation is zero when $\tilde{v}$ is drawn uniformly at random from the unit sphere, which we assumed for the unconfounded case. Intuitively, the definition of $T$ is motivated by the idea to detect overpopulation of eigenspaces with small eigenvalues, which we expect for confounding. As a further justification, we observed that $T$ coincides, up to a scaling factor, with the score function

$$\frac{\partial \log p_\theta(\tilde{v})}{\partial \theta},$$

at $\theta = 0$. This is a natural candidate for detecting changes of $\theta$ because score functions occur in the construction of optimal estimators whenever there exist unbiased estimators attaining the Cramér Rao bound Cramér (1946).

To derive a simple approximation for the null distribution of $T$ we think of $\tilde{v} = a'/||a'||$ as being generated by drawing its coefficients $a_j$ with respect to the eigenbasis of $\Sigma_{XX}^{-1}$ from $\mathcal{N}(0, 1/\sqrt{d})$ followed by renormalization:

$$T(\tilde{v}) = \frac{1}{\sqrt{d}} \left( \sum_{j=1}^{d} a_j^2 s_j - \tau(\Sigma_{XX}^{-1}) \right) \approx \frac{1}{\sqrt{d}} \left( \sum_{j=1}^{d} a_j^2 s_j - \tau(\Sigma_{XX}^{-1}) \right),$$

where $s_j$ denotes the eigenvalues of $sX^{-1}$. Already for moderate size of $d$, we can thus get a good approximation for the null distribution of $T$ by a weighted sum of squared Gaussian, i.e., it approximately follows a mixed $\chi^2$-distribution.

6 Overfitting

So far we have completely ignored finite sampling issues. High-dimensional regression requires regularization which could spoil our model assumptions, e.g., if they enforce sparsity which is not compatible with our rotation invariant prior on $a$. Therefore, the method should only be applied if the sample size is sufficiently high for the respective dimension (see section 7) to avoid overfitting. Remarkably, overfitting generates the sample kind of ‘dependences’ between the estimator of $a'$ and the estimator of $\Sigma_{XX}$ as confounding generated for the true objects $a'$ and $\Sigma_{XX}$ themselves.
To show this, assume that $Y$ is independent of $X$ and let $(x_1^j, \ldots, x_n^j, y^j)$ for $j = 1, \ldots, n$ be samples independently drawn from $P_X P_Y$, where $P_X$ is arbitrary and $P_Y$ is Gaussian. Define the matrix

$$
x := \left( x_1^j - \bar{x}_j \right)_{i=1, \ldots, n, j=1, \ldots, d},
$$

where $\bar{x}_j := \frac{1}{n} \sum_{i=1}^n x_i^j$ denotes the empirical average of the respective component. Likewise, define the vector $y := (y_1^j, \ldots, y_n^j)^T - \bar{y}(1, \ldots, 1)^T$. Then, we obtain $\Sigma_{XX} = x^T x$ and $\Sigma_{XY} = x^T y$ (where we have skipped the symbol $\hat{}$ for better readability). Since $y$ is the projection of $(y_1, \ldots, y_n)^T$ onto the orthogonal complement of $1 := (1, \ldots, 1)^T$, its distribution is isotropic in the $n - 1$-dimensional subspace defined by the orthogonal complement $1^\perp$ of 1. Let $V$ be an $(n - 1) \times n$ matrix that rotates $1^\perp$ onto $\mathbb{R}^{n-1}$. Then we may write

$$
\Sigma_{XX} = x^T V^T V x,
$$

because the image of $x$ is contained in the image of the projection $V^T V$. Moreover,

$$
\Sigma_{XY} = x^T V^T V y.
$$

To show the formal analogy to the mixing scenario above we now set $M := V x$ and $y' := V y$. Then we can write $\Sigma_{XX} = M^T M$ and $\Sigma_{XY} = M^T y'$, and thus obtain

$$
\hat{a} = M^{-T} y',
$$

where $y'$ is isotropically chosen from $R^{n-1}$. The generating model for $a$ thus coincides with the model above with $\ell = n - 1$ for the case of pure confounding.

Computing an unregularized regression for $X$ and $Y$ being independent thus yields a regression vector $\hat{a}'$ that is also mainly located in the low eigenvalue eigenspace of $\Sigma_{XX}$. We expect the same behavior if $X$ influences $Y$ without confounder when the sample size is so small that the observed correlations are dominated by statistical fluctuations rather than by the true causal influence.

On the one hand one may regret that confounding and overfitting becomes indistinguishable. On the other hand, the method thus provides an unified approach to detect that a regression vector $\hat{a}'$ does not show the true causal influence; either because $\hat{a}' \neq a'$ or because $a' \neq a$ due to confounding. There is a simple reason why both cases generate similar dependences between $\Sigma_{XX}$ and $\hat{a}'$: Whenever $\Sigma_{XY}$ is a vector that has been generated independently of $\Sigma_{XX}$, the vector $\Sigma_{XX}^{-1} \Sigma_{XY}$ tends to live mainly in the small eigenvalue subspace of $\Sigma_{XX}$. Only if $\Sigma_{XY}$ is not drawn independently of $\Sigma_{XX}$, for instance, because it is generated by $\Sigma_{XX} \hat{a}$ (where $a$ is drawn independently of $\Sigma_{XX}$), this overpopulation of small eigenvalues does not happen.

## 7 Experiments with simulated data

The code and the data sets for all experiments are available at http://webdav.tuebingen.mpg.de/causality/. We generated models as follows:

1. We have drawn $n$ samples of each $Z_1, \ldots, Z_\ell$ as independent standard Gaussians
2. We have drawn the entries of $M$ by independent standard Gaussians
3. We have drawn the parameters $\sigma_a, \sigma_c$ from the uniform distribution on $[0, 1]$
4. We have drawn each coefficient of $a \in \mathbb{R}^d$ and $c \in \mathbb{R}^\ell$ from Gaussians of standard deviation $\sigma_a$ and $\sigma_c$, respectively.
5. We computed samples $(X, Y)$ via the structural equations $X = M Z$ and $Y = a^T X + c^T Z$.

Knowing the above parameters, we can easily compute the exact confounding strength using

$$
\beta = \frac{\|M^{-T} c\|^2}{\|a\|^2 + \|M^{-T} c\|^2}.
$$

### 7.1 Estimating $\beta$

We have estimated $\beta$ as described at the end of section 4 for $d = \ell = 10, 20, 50, 100$ with sample size 10,000. The scatter plots in Figure 3 show the relation between the true values $\beta$ and the estimated values $\hat{\beta}$. One can see that $\beta$ and $\hat{\beta}$ are clearly correlated and that the performance increases (although slowly) for higher dimension. The estimation is reasonably good in the regions where $\beta$ is close to 0 or 1, which suggests that one should rather trust in the qualitative statement about whether there is confounding or not than in the exact value of $\beta$. 


Since our theory has shown that $\ell$ is completely irrelevant in our idealized scenario provided that it is not smaller than $d$ (see the generating model in Definition 2) it would be pointless to explore the case $\ell > d$ here.

### 7.2 Test for non-confounding

For the simulated data described above we have applied the test for unconfoundedness described in section 5 by drawing 1000 samples from the null distribution of $T$ and comparing them to the observed value $T(\hat{\alpha}/||\hat{\alpha}||)$. Figure 4 visualizes the joint distribution of p-values with $\beta$.

One can see that for $\beta > 0.5$ the p-values begin to be mostly close to zero. Figure 5 shows how the fraction of rejections increases when $\beta$ increases for the two cases where the confidence level $\alpha$ is set to 0.1 (left) or 0.05 (right). Here we have chosen a one-sided test because confounding increases $T$ due to the overpopulation of subspaces with small eigenvalues of $\Sigma_{XX}$. The results show that for those confidence levels unconfoundedness is mostly rejected for models with $\beta > 0.6$.

![Graphs showing p-values for different values of $\beta$](image)

**Figure 4:** p-values obtained in the test for non-confounding for different values of the confounding parameters $\beta$. It can be seen that the p-values get close to zero when $\beta$ tends to 1.

### 7.3 Overfitting

We generated $d + 1$-tuples of $X, Y$ by first drawing $X$ via a random mixing matrix and then $Y$ by $Y = \alpha^T X + E$,
Figure 5: Fraction of rejections when the confidence is chosen to be 0.1 (top) and 0.05 (bottom) for different values of $\beta$ in 5000 runs.

where $E$ is $\mathcal{N}(0, 1)$ distributed and $\mathbf{a}$ is a random vector whose entries are randomly drawn from $\mathcal{N}(0, 1)$.

Figure 6 shows the distribution of p-values of the test for unconfoundedness for different sample sizes $n$. As one can see, for $n = 20$ one gets mostly small p-values although the model is actually unconfounded (in agreement with our theoretical insights saying that overfitting yields the same type of untypical regression vectors as confounding). For $n = 100$ and $n = 1000$, small p-values are still over-represented and only for $n = 10,000$ the distribution of p-values is close to uniform. This suggests that dimension 10 already requires sample sizes of the order 10,000 if one wants to avoid too many false rejections (when focusing on confounding rather than on overfitting).

Figure 6: Distribution of p-values in the statistical test for unconfoundedness in a scenario without confounding.

8 Experiments with real data

Since it is hard to get data where the confounding strength $\beta$ is known we can mostly only discuss plausibility except for the data set in the following section.
8.1 Data from an optical device

Janzing and Schölkopf (2017) describe an optical device where the causal structure and $\beta$ is known by construction. The variable $X$ is a low-resolution image ($3 \times 3$ pixel) shown on the screen of a laptop and $Y$ is the brightness measured by a photodiode at some distance in front of the screen. The image $X$ is generated by a webcam placed in front of a TV. As confounder $Z$ (which is one-dimensional following the assumptions of Janzing and Schölkopf (2017)), an LED in front of the photodiode and another LED in front of the webcam is controlled by a random noise. Since $Z$ is known, an approximation of $\beta'$ for $\beta$ can be directly computed from the observed covariances ($\beta \neq \beta'$ only due to finite sample issues). We first tried the 11 data sets with variable confounding and obtained the results displayed in Figure 7. The results are quite similar to those from Janzing and Schölkopf (2017) although the scenario matches the very specific one-dimensional confounding scenario there while our model is more general. Also here the results are qualitatively right ($\beta'$ and $\hat{\beta}$ are significantly correlated) but with a clear tendency to underestimate confounding, which has already been discussed by Janzing and Schölkopf (2017).

![Figure 7: True and estimated confounding strength for the optical device used by Janzing and Schölkopf (2017).](image)

We also tested the two data sets where one is purely confounded ($\beta = 1$) and one completely unconfounded ($\beta = 0$) and obtained $\hat{\beta} = 0.768$ and $\hat{\beta} = 0$, respectively.

8.2 Taste of wine

This dataset Lichman (2013) describes the dependence between the scores on the taste between 0 and 10 (given by human subjects) of red wine, and 11 different ingredients: $X_1$: fixed acidity, $X_2$: volatile acidity, $X_3$: citric acid, $X_4$: residual sugar, $X_5$: chlorides, $X_6$: free sulfur dioxide, $X_7$: total sulfur dioxide, $X_8$: density, $X_9$: pH, $X_{10}$: sulphates, $X_{11}$: alcohol. Taking the taste $Y$ as target variable we obtained $\hat{\beta} = 0$ (after we normalized all $X_j$ to unit variance since their scale where incompatible) which is plausible to some extent given that the crucial ingredients are considered in the data set.

After dropping alcohol, which one can easily check to have the most dominant influence on taste (given that the relation between the full variable $X$ and $Y$ has been unconfounded), we obtained $\hat{\beta} = 0.62$, which sounds sensible since the set of predictor variables is no longer sufficient. When we dropped one of then other $X_j$, we always obtained $\hat{\beta}$ zero or close to zero (in one case). Since the other variables influence the taste much weaker than $X_{11}$, the algorithm is not able to detect any significant confounding.

8.3 Data sets with shuffling the target variable

Here we describe a family of experiments where each single one cannot be assessed but one can discuss whether the collection of results seem sensible.

If a data set contains $d + 1$ correlated variables $X_1, \ldots, X_{d+1}$ we can take each $X_j$ as hypothetical target variable $Y$ and the remaining variables $X^{(j)} := (X_1, \ldots, X_{j-1}, X_{j+1}, \ldots, X_{d+1})$ as hypothetical causes. Although we do not know whether some of these $d + 1$ choices are purely causal in the sense that $X^{(j)}$ influences $Y^{(j)} := X_j$ without confounder, we know that not all of them are purely causal because not all the variables can be a sink node of the underlying causal DAG.

Since our model uses independent sources as in Independent Component Analysis (ICA) as basis it is natural to apply our method to data sets that have been used in the context of ICA, for instance data from Magnetoencephalographic Recordings (MEG) used by Vigário et al.\footnote{The data set is available at \url{http://research.ics.aalto.fi}.}
We first write \( s(t) := \Phi(s(t)) \) its image. Then we have
\[
\frac{d}{dt}\Phi(s(t)) = \langle \nabla g(As(t)), As'(t) \rangle As(t) + g(As(t))As'(t),
\]
with \( \nabla g(w) = -w/\|w\|^3 \). Hence we obtain
\[
\frac{d}{dt}\Phi(s(t)) = \frac{-1}{\|As(t)\|^3} \langle As(t), As'(t) \rangle As(t) + g(As(t))As'(t).
\]
(13)
Note that the matrix \( 1 - \tilde{s}(t)s(t)^T \) projects \( As'(t) \) onto the tangent space at \( \tilde{s}(t) \) and (14) describes the Jacobian \( D\Phi \) which maps between tangent spaces \( T_s(t) \) and \( T_{\tilde{s}(t)}(s(t)) \) and \( \tilde{s}(t) \), respectively. Let \( e_1, \ldots, e_{d-1} \) and \( \tilde{e}_1, \ldots, \tilde{e}_{d-1} \) be orthonormal bases of \( T_v \) and \( T_{\tilde{v}} \), respectively. If we set \( U_v := (e_1, \ldots, e_{d-1}) \) and \( U_{\tilde{v}} := (\tilde{e}_1, \ldots, \tilde{e}_{d-1}) \), the Jacobian with respect to these bases reads
\[
\overrightarrow{D}\Phi(v) := g(Av)U_v^T AU_v.
\]
We then have
\[
\det \overrightarrow{D}\Phi(v) = g(Av)^{d-1} \det(U_v^T AU_v).
\]
Multiplying the equation \( \tilde{v} = Av/\|Av\| \) with \( A^{-1} \) and taking the norm on both sides yields
\[
1/\|Av\| = \|A^{-1}\tilde{v}\|.
\]
(15)
We thus obtain
\[
p(\tilde{v}) = \left| \det \overrightarrow{D}\Phi(\Phi^{-1}(\tilde{v})) \right|^{-1} = \left( \|A^{-1}\tilde{v}\|^{d-1} |\det(U_{\tilde{v}}^T AU_v)| \right)^{-1} = \left( \|A^{-1}\tilde{v}\|^{d-1} |\det(A)\right)^{-1},
\]
(16)
with the abbreviation \( A' := U_v^T AU_v \). Let us now define the orthogonal \( d \times d \) matrices
\[
W_v := (U_v, v) \quad \text{and} \quad (U_{\tilde{v}}, \tilde{v}).
\]
Then we define $A' := W^T A W_v$, which implies $|\det(A')| = |\det(A)|$. $A'$ can be written as

$$A' = \begin{pmatrix} \tilde{A} & 0 \\ w & \|A v\|^2 \end{pmatrix},$$

where $w$ is some $1 \times (d - 1)$-matrix and $\tilde{A} := U^T A U_v$. Hence we obtain

$$\det(A') = \det(\tilde{A}) |A v\| = \frac{\det(\tilde{A})}{\|A^{-1} \tilde{v}\|^d},$$

where we have used also (15). We can thus rewrite (16) as

$$p(\tilde{v}) = \frac{1}{|\det(A)||A^{-1} \tilde{v}|^d}$$

### 10.2 Proof of Theorem 3

By definition, $p_{\theta'}$ is obtained by applying the map $\sqrt{R_{\theta}}$ to vectors drawn from a rotation invariant distribution with renormalizing it later. Without loss of generality, let $R_{\theta}$ be diagonal with eigenvalues $f_j(\theta)$. Let $v$ be generated by drawing each entry $v_j$ from $N(0, 1)$. We can then compute the entries of $\tilde{v}$ by

$$\tilde{v}_j := \frac{1}{\sum_{i=1}^d f_j(\theta')} \sqrt{|f_j(\theta')|} v_j.$$

Rewriting (10) in terms of $v_j$ instead of $\tilde{v}$ yields

$$\log p_{\theta}(\tilde{v}) = -\frac{1}{2} \left\{ \log \frac{1}{d} \sum_{j=1}^d f_j(\theta')f_j(\theta)^{-1} v_j^2 \right\}$$

$$- \log \frac{1}{d} \sum_{j=1}^d f_j(\theta')v_j^2 \right\} + \log \det R_{\theta}.$$

Due to Chebychev’s inequality we have

$$\left| \frac{1}{d} \sum_{j=1}^d f_j(\theta')f_j(\theta)^{-1} v_j^2 - \tau(R_{\theta} R_{\theta}^{-1}) \right| \leq \delta,$$

with probability $1 - \frac{1}{d^2} \sum_{j=1}^d f_j(\theta')^2 f_j(\theta)^{-2} / \delta^2 = 1 - \frac{1}{d} \tau(R_{\theta} R_{\theta}^{-2}) / \delta^2$. Likewise,

$$\left| \frac{1}{d} \sum_{j=1}^d f_j(\theta')v_j^2 - \text{tr}(R_{\theta}) \right| \leq \delta,$$

with probability $1 - \frac{1}{d} \tau(R_{\theta} R_{\theta}^{-1}) / \delta^2$. To ensure that

$$\left| \log \frac{1}{d} \sum_{j=1}^d f_j(\theta')f_j(\theta)^{-1} v_j^2 - \log \tau(R_{\theta} R_{\theta}^{-1}) \right| \leq \epsilon,$$

we need to ensure that $\delta \leq \epsilon / \tau(R_{\theta} R_{\theta}^{-1}) - \delta$ which can be achieved by $\delta \leq \epsilon \tau(R_{\theta} R_{\theta}^{-1}) / 2$ for sufficiently small $\epsilon$. Likewise, we can achieve that

$$\left| \log \frac{1}{d} \sum_{j=1}^d f_j(\theta')v_j^2 - \log \tau(R_{\theta}) \right| \leq \epsilon,$$

if $\delta \leq \epsilon \tau(R_{\theta}) / 2$. Thus, both inequalities (17) and (18) together hold with probability at least

$$1 - \frac{4}{d^2} \left( \tau(R_{\theta} R_{\theta}^{-1}) + \frac{\tau(R_{\theta} R_{\theta}^{-2})}{\tau(R_{\theta})^2} \right).$$

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