Abstract

We analyze a family of methods for statistical causal inference from sample under the so-called Additive Noise Model. While most work on the subject has concentrated on establishing the soundness of the Additive Noise Model, the statistical consistency of the resulting inference methods has received little attention. We derive general conditions under which the given family of inference methods consistently infers the causal direction in a nonparametric setting.

1. Introduction

Drawing causal conclusions for a set of observed variables given a sample from their joint distribution is a fundamental problem in science. Conditional-independence-based methods (Pearl, 2000; Spirtes et al., 2000) estimate a set of directed acyclic graphs, all entailing the same conditional independences, from the data. However, these methods cannot distinguish between two graphs that entail the same set of conditional independences, the so-called Markov equivalent graphs. Consider for example the case of only two observed dependent random variables. Conditional-independence-based methods can not recover the causal graph since $X \rightarrow Y$ and $Y \rightarrow X$ are Markov equivalent. An elegant basis for causal graphs is the framework of structural causal models (SCMs) (Pearl, 2000), where every observable is a function of its parents and an unobserved independent noise term. This allows us to formulate an assumption on function classes which lets us infer the causal direction in two-variable case.

A special case of SCMs is the Causal Additive Noise Model (CAM) (Shimizu et al., 2006; Hoyer et al., 2009; Tillman et al., 2009; Peters et al., 2011a;b) which is given as follows: given two random variables $X$ and $Y$, $X$ is assumed to cause $Y$ if (i) $Y$ can be obtained as a function of $X$ plus a noise term independent of $X$, but (ii) $X$ cannot be obtained as a function of $Y$ plus independent noise, then we infer that $X$ causes $Y$. In this case, where (i) and (ii) hold simultaneously, the CAM is termed identifiable.

Initial work on the CAM focused on establishing its theoretical soundness, i.e. understanding the class of distributions $P_{X,Y}$ for which the CAM is identifiable, i.e. for which (i) and (ii) hold simultaneously. Early work by (Shimizu et al., 2006) showed that the CAM is identifiable when the functional relationship $Y = f(X) + \eta$ is linear, provided the independent noise $\eta$ is not Gaussian. Later, Hoyer et al. (2009), Zhang & Hyvärinen (2009) and Peters et al. (2011a) showed that the CAM is identifiable more generally even if $f$ is nonlinear, the main technical requirements being that the marginals $P_{X}$ and $P_{\eta}$ are absolutely continuous on $\mathbb{R}$, with $P_{\eta}$ having support $\mathbb{R}$. Note that Zhang & Hyvärinen (2009) also introduces a generalization of the CAM termed post-nonlinear models. Further work by Peters et al. (2011b) showed how to reduce causal inference for a network of multiple variables under the CAM to the case of two variables $X$ and $Y$ discussed so far, by properly extending the conditions (i) and (ii) to conditional distributions instead of marginals. Thus, the soundness of the CAM being established by these various works, the next natural question is to understand the statistical behavior of the resulting estimation procedures on finite samples.
Current insights into this last question are mostly empirical. Various works (Shimizu et al., 2006; Hoyer et al., 2009; Peters et al., 2011a) have successfully validated procedures based on the CAM (outlined in Section 1.1 below) on a mix of artificial and real-world datasets where the causal structure to be inferred is clear. However, on the theoretical side, it remains unclear whether these procedures can infer causality from samples in general situations where the CAM is identifiable. In the particular case where the functional relation between \( X \) and \( Y \) is linear, Hyvärinen et al. (2008) proposed a successful method shown to be consistent. Two recent ArXived results, Bühlmann et al. (2013); Nowzohour & Bühlmann (2013), show the consistency of maximum log-likelihood approaches to causal inference under the multi-variable network extension of Peters et al. (2011b).

While consistency has been shown for particular procedures, in this paper we are rather interested in general conditions under which common approaches, with various algorithmic instantiations, are consistent. We derive both algorithmic and distributional conditions for statistical consistency in general situations where the CAM is identifiable. The present work focuses on the case of two real variables, allowing us to focus on the inherent difficulties of achieving consistency with the common algorithmic approaches. These difficulties, described in Section 1.2 have to do with estimating the degree of independence between noise and input, while the noise is itself estimated from the input and hence is inherently dependent on the input.

### 1.1. Inference Methods Under the Additive Noise Model

Causal inference methods under the Additive Noise Model typically follow the meta-procedure below. Assume \( f \) and \( g \) are the best functional fits under some risk, respectively \( Y \approx f(X) \) and \( X \approx g(Y) \):

Fit \( Y \) as a function \( f(X) \), obtain the residuals \( \eta_{Y,f} = Y - f(X) \), fit \( X \) as a function \( g(Y) \), obtain the residuals \( \eta_{X,g} = X - g(Y) \), decide \( X \rightarrow Y \) if \( \eta_{Y,f} \perp \perp X \) but \( \eta_{X,g} \not\perp \perp Y \), decide \( Y \rightarrow X \) if the reverse holds true, abstain otherwise.

Instantiations thus vary in the regression procedures employed for function fitting, and in the independence measures employed. Our analysis concerns procedures employing an entropy-based independence measure, which is cheaper than usual independence tests. These procedures vary in the regression and entropy estimators employed. They are presented in detail in Section 3.

### 1.2. Towards Consistency: Main Difficulties

Assume (i) and (ii) hold so that \( X \) causes \( Y \) under the CAM. We want to detect this from sufficiently large finite samples. This is consistency in a rough sense.

Establishing consistency of the above meta-procedure faces many subtle difficulties. The above outlined algorithmic approach consists of four interdependent statistical estimation tasks, namely two regression problems and two independence-tests. Considered separately, the consistency of such estimation tasks is well understood, but in the present context the success of the independence tests is contingent on successful regression.

The main difficulty is that although we are observing \( X \) and \( Y \), we are not observing the residuals \( \eta_{Y,f} \) and \( \eta_{X,g} \), but empirical approximations \( \eta_{Y,f,n} \) and \( \eta_{X,g,n} \) obtained by estimating \( f \) and \( g \) as \( f_n \) and \( g_n \) on a sample of size \( n \).

For now, consider just detecting that \( \eta_{Y,f} \) is unknown, is independent from \( X \). A good estimator \( f_n \) will ensure that \( f_n \) and \( f \) are close, usually in an \( L_2 \) sense (i.e. \( \mathbb{E}[f_n(X) - f(X)]^2 \approx 0 \)). Hence \( \eta_{Y,f,n} \) is close to \( \eta_{Y,f} \), but unfortunately this does not imply that \( \eta_{Y,f,n} \perp X \) if \( \eta_{Y,f} \perp X \). In fact it is easy to construct r.v.’s \( A, B, C \) such that \( A \perp B, |B - C| < \epsilon \), for arbitrary \( \epsilon \), but \( C \not\perp A \). Thus, the estimate \( \eta_{Y,f,n} \) might be close to \( \eta_{Y,f} \), yet it might still appear dependent on \( X \) even if \( \eta_{Y,f} \) is not. Complicating matters further, \( \eta_{Y,f} \) and \( \eta_{Y,f} \) would only be close in an average sense (instead of close for every value of \( X \)) since \( f_n \) and \( f \) are typically only close in an average sense (e.g. close in \( L_2 \)).

Now consider the full causal discovery, i.e. consider also detecting that \( \eta_{X,g} \) depends on \( Y \). To achieve consistency, the independence test employed must detect more dependence between \( \eta_{X,g,n} \) and \( Y \) than between \( \eta_{Y,f,n} \) and \( X \). This will depend on how the particular independence test is influenced by errors in the particular regression procedures employed, and the relative rates at which these various procedures converge.

As previously mentioned, we will consider a family of independence-tests based on comparing sums of entropies. We will handle the above difficulties and derive conditions for consistency by first understanding how the various estimated entropies converge as a function of regression convergence (\( L_2 \) convergence).

We do not consider the question of finite-sample convergence rates for causal estimation under the CAM. In fact, it is not even clear whether it is generally possible to establish such rates. This is because it is generally possible that the Bayes best fits \( f(x) = \mathbb{E}[Y|x] \) is smooth while \( g(y) = \mathbb{E}[X|y] \) is not even continuous; yet it is well known that without smoothness or similar structural conditions, ar-
The Causal Additive Noise Model is captured as follows:

\[
P(\eta | X) \triangleq \frac{p(\eta | X)}{p(X)}
\]

By the chain rule of differential entropy we have

\[
H(X,Z) = H(X) + H(Z | X) = H(X) + H(\eta | f(X))
\]

Proof. By the chain rule of differential entropy we have

\[
H(X,Z) = H(X) + H(Z | X) = H(X) + H(\eta | f(X))
\]

\[
= H(X) + H(\eta | f(X)) - I(\eta | f(X), X)
\]

Equate the two r.h.s above and rearrange. \qed

Note that whenever \( \eta, f, X \) have \( I(\eta | f, X) = 0 \),

Therefore, by the above lemma, if \( \eta, f, X \) then \( C_{X,Y} \triangleq H(X) + H(\eta | f) \) is smaller than \( C_{Y,X} \triangleq H(Y) + H(\eta | g) \).

This yields a measure of independence which is relatively cheap to estimate. In particular the test depends only on the marginal distributions of the r.v.'s \( X, Y \) and functional

residuals, and does not involve estimating joint distributions or conditionals, as is implicit in most independence
tests. We analyze a family of procedures based on this idea. This family is given in the next subsection.

2. Preliminaries

2.1. Setup and Notation

We let \( H \) and \( I \) denote respectively differential entropy, and mutual information (Cover et al., 1994). Given a density \( p \)
we will at times use the (abuse of) notation \( H(p) \) when a
r.v. is unspecified.

The distribution of a r.v. \( Z \) is denoted \( P_Z \), and its density when it exists is denoted \( p_Z \).

Throughout the analysis we will be concerned with residuals from regression fits. We use the following notation.

Definition 1. For a function \( f : \mathbb{R} \rightarrow \mathbb{R} \), we consider either of the residuals: \( \tau_{Y,f} \triangleq Y - f(X) \) and \( \tau_{X,f} \triangleq X - f(Y) \).

The Causal Additive Noise Model is captured as follows:

Definition 2 (CAM). Given r.v.'s \( X, Y \), a function \( f : \mathbb{R} \rightarrow \mathbb{R} \) and a r.v. \( \eta \), we write \( X \rightarrow Y \) if the following holds:

1. \( P_{X,Y} \) is generated as \( X \sim P_X \), and \( Y = f(X) + \eta \), where the noise r.v. \( \eta \) has 0 mean and \( \eta \perp X \);
2. for any \( g : \mathbb{R} \rightarrow \mathbb{R} \), \( \tau_{X,g} \triangleq X - g(Y) \) depends on \( Y \).

We write \( X \rightarrow Y \) when \( f \) and \( \eta \) are clear from context.

3. Causal Inference Procedures

3.1. Main Intuition

Lemma 1. Consider any absolutely continuous joint-distribution \( P_{X,Y} \) on \( X, Y \in \mathbb{R} \). For any two functions \( f, g : \mathbb{R} \rightarrow \mathbb{R} \) we have

\[
H(X) + H(\eta_Y | f) = H(Y) + H(\eta_X | g)
\]

where the noise r.v. \( \eta \) has 0 mean and \( \eta \perp X \); for any two functions \( f, g : \mathbb{R} \rightarrow \mathbb{R} \) we have

\[
H(X) + H(\eta | f(X)) = H(Y) + H(\eta | g(Y))
\]

\[
- I(\eta_X | f(X), X) \}

Proof. By the chain rule of differential entropy we have

\[
H(X,Y) = H(X) + H(Y | X) = H(X) + H(\eta_Y | f(X))
\]

\[
= H(X) + H(\eta_Y | f(X)) - I(\eta_Y | f(X), X)
\]

Similarly

\[
H(X,Y) = H(Y) + H(\eta_X | g(Y)) - I(\eta_X | g(Y), Y)
\]

The analysis in this paper is carried with respect to the \( L_2, p_X \) and \( L_2, p_Y \) functional norms defined as follows.

Definition 3. For \( f : \mathbb{R} \rightarrow \mathbb{R} \), and a measure \( \mu \) on \( \mathbb{R} \), the \( L_2, \mu \) norm is given as \( \| f \|_{L_2, \mu} = (\int f(t)^2 \, d\mu(t))^{1/2} \).

We assume the internal procedures \( f_n, g_n, H_n \) have the following consistency properties.

Assumption 1. The internal procedures are consistent:

- Suppose \( \mathbb{E} Y^2 < \infty \). Let \( f(x) \triangleq \mathbb{E}[Y|x] \). Then
  \( \| f_n - f \|_{2, p_X} \rightarrow 0 \).

- Suppose \( \mathbb{E} X^2 < \infty \). Let \( g(y) \triangleq \mathbb{E}[X|y] \). Then
  \( \| g_n - g \|_{2, p_Y} \rightarrow 0 \).

- Suppose \( Z \) has bounded variance, and has continuous density \( p_Z \) such that \( \exists \tau, C > 0, \alpha > 1, \forall |t| > T, p_Z(t) \leq C |t|^{-\alpha} \).

Many common nonparametric regression procedures (e.g. kernel, k-NN, Kernel-SVM, spline regressors) are consistent in the above sense (Györfi et al., 2002). Also the consistency of a variety of entropy estimators (e.g. plug-in entropy estimators) is well established (Beirlant et al., 1997).
4. Technical overview of results

We consider the following two versions of the above meta-procedure. The analysis (Section 5) is divided accordingly.

Definition 4 (Decoupled-estimation). $f_n$ and $g_n$ are learned on half of the sample $\{(X_i, Y_i)\}_{i=1}^n$, and the $H_n(\eta_f, f_n)$ and $H_n(\eta_g, g_n)$ are learned on the other half of the sample (w.l.o.g. assume $n$ is even). $H_n(X)$ and $H_n(Y)$ could be learned on either half or on the entire sample.

Definition 5 (Coupled-estimation). All $f_n$, $g_n$ and entropies $H_n$ are learned on the entire sample $\{(X_i, Y_i)\}_{i=1}^n$.

Our most general consistency result (Theorem 1, Section 5.1) concerns decoupled-estimation. By decoupling regression and entropy estimations, we reduce the potential of overfitting, during entropy estimation, the generalization error of regression. This generalization error could be large if the regression algorithms are too rich (e.g. ERM over large functional classes). Our simulations show that, when the regression algorithm is too rich, the variance of the causal inference is large for coupled-estimation but remains low for decoupled-estimation (Fig. 1(a)). By decreasing the richness of the class (simulated by increasing the kernel bandwidth for a kernel regressor) the source of variance shifts to the sample size, and coupled-estimation (which estimates everything on a larger sample) becomes the better procedure and tends to converge faster (Fig. 1(b)).

For the consistency result of Theorem 1 we make no assumption on the richness of the regression algorithms, but simply assume that they converge in $L_2$ (Assumption 1). The main technicality is to then show that entropies of residuals are locally continuous relative to the $L_2$ metric in both causal and anticausal directions.

For coupled-estimation, the main difficulty is the following. Even though the entropy estimators are consistent for a fixed distribution, the distribution of the residuals change with $f_n$ and $g_n$, thus with every random sample (this problem is alleviated by decoupling the estimation). However, if the richness of the regression algorithms is controlled, in other words if the set of potential $f_n$ and $g_n$ is not too rich, then the entropy estimate for residuals might converge. We show in Theorem 2 (Section 5.2) that if we employ kernel regressors with properly chosen bandwidths, and kernel-based entropy estimators with sufficiently smooth kernels, then the resulting method is consistent for causal inference.

Both consistency results of Theorem 1 and Theorem 2 rely on tail assumptions on the additive noise $\eta$ (where $X \overset{f,\eta}{\rightarrow} Y$). We assume an exponentially decreasing tail for the more difficult case of coupled-estimation, but need only a mild assumption of polynomially decreasing tail in the case of decoupled-estimation. Note that it is common to assume that $\eta$ has Gaussian tail, and our assumptions are milder in that respect.
Interestingly, our analysis for Theorem 1 suggests that convergence of causal inference is likely faster if the noise $\eta$ has faster decreasing tail (see Lemma 3). This is verified in our simulations where we vary the tail of $\eta$ (Fig. 1(c)).

5. Analysis

5.1. Consistency for Decoupled-estimation

In this section we establish a general consistency result for the meta-procedure above. The main technicality consists of relating differential entropy of residuals to the $L_2$-norms of residuals (i.e. to the error made in function estimation). We henceforth let $\Sigma$ denote the Lebesque measure.

The analysis in this section uses the following polynomial tail assumption on $\eta$. We note that Assumption 2 satisfies the identifiability conditions of (Zhang & Hyvärinen, 2009).

Assumption 2 (Tail). $P_{X,Y}$ is generated as follows: $X \xrightarrow{f} Y$ for some bounded function $f$, with bounded derivative on $\mathbb{R}$. $P_X$ has bounded support, and both $P_X$ and $P_\eta$ have densities $p_X, p_\eta$ with bounded derivatives on $\mathbb{R}$. Furthermore, we assume $\eta$ has bounded variance, and $p_\eta$ satisfies, for some $T > 0$, $C > 0$, and $\alpha > 1$:

$$\forall |t| > T, \quad p_\eta(t) \leq C |t|^{-\alpha},$$

Note that, since the unknown target functions are assumed bounded, any consistent regressor can be appropriately truncated while maintaining consistency. We therefore have the following technical assumption on the regressors.

Assumption 3. The regression procedures return bounded functions: $\lim_{n \to \infty} \max \{\|f_n(t)\|_\infty, \|g_n(t)\|_\infty\} < \infty$.

Theorem 1 (General consistency for decoupled-estimation). Suppose $X \xrightarrow{f,\eta} Y$ for some $f, \eta$, and $P_{X,Y}$ satisfies the tail Assumption 2. Suppose $f_n, g_n, H_n$ are consistent procedures satisfying Assumption 1 and 3. Let the meta-algorithm be decoupled as in Definition 4.

Then the probability of correctly deciding $X \to Y$ goes to 1 as $n \to \infty$.

To prove the theorem, we have to understand how the estimated entropies converge as a function of the $L_2$ error in regression estimation. We will proceed by bounding the distance between the densities $p_{f_{Y,f}}$ and $p_{f_{Y,f'}}$ of the residuals of functions $f$ and $f'$ in terms of the $L_2$ distance between $f$ and $f'$ (Lemma 3); this will then be used to bound the difference in the entropy of such residuals.

Given Assumption 2, the following lemma establishes some useful properties of the distribution $P_{X,Y}$ and of the distribution of certain residuals. It is easy to verify that under our assumptions, all distributions under consideration in the lemma are absolutely continuous.

Lemma 2 (Properties of induced densities). Suppose $P_{X,Y}$ satisfies Assumption 2 for some $f, \eta$, and $\alpha > 1$. We then have the following: (i) $p_{X,Y}$ has a bounded gradient on $\mathbb{R}^2$, (ii) consider functions $f', g : \mathbb{R} \to \mathbb{R}$ and suppose $\sup |f'|$ and $\sup |g|$ are at most $T_0$ for some $T_0$; then there exists $T' > 0$ depending on $T_0$, and $C' > 0$ such that $\forall |t| > T'$

$$\left\{ p_{X,Y}(\cdot,t), p_{X,Y}(\cdot,t'), p_{\eta_{f'},f}(t), p_{\eta_{g},f}(t) \right\} \leq C' |t|^{-\alpha}.$$

In particular, the above holds for $g(y) \triangleq \mathbb{E}[X | Y = y]$.

The next lemma relates the density of residuals to the $L_2$ distance between functions. Notice, as discussed in Section 4, that the Lemma suggests that the densities of residuals converge faster the sharper the tails of the noise $\eta$: the larger $\alpha$, the sharper the bounds are in terms of the $L_2$ distance between functions.

Lemma 3 (Density of residuals w.r.t. $L_2$ distance). Suppose the joint distribution $P_{X,Y}$ satisfies Assumption 2 for some $f, \eta$ and $\alpha > 1$. Let $g(y) \triangleq \mathbb{E}[X | Y = y]$. Consider functions $f', g' : \mathbb{R} \to \mathbb{R}$. There exist a constant $C''$ such that for $\|f - f'\|_{L_2}$ and (respectively) $\|g - g'\|_{L_2}$ sufficiently small,

$$\sup_{t \in \mathbb{R}} |p_{f_{Y,f}}(t) - p_{f_{Y,f'}}(t)| \leq C'' \left( \|f' - f\|_{L_2}^{\alpha-1/2\alpha} \right),$$

$$\sup_{t \in \mathbb{R}} |p_{\eta_{g,f}}(t) - p_{\eta_{g,f'}}(t)| \leq C'' \left( \|g' - g\|_{L_2}^{\alpha-1/2\alpha} \right).$$

Proof. We start by bounding the difference between $p_{f_{Y,f}}(t)$ and $p_{f_{Y,f'}}(t)$. We note that the same ideas can be used to bound the difference between $p_{\eta_{g,f}}(t)$ and $p_{\eta_{g,f'}}(t)$, since $X$ and $Y$ are interchangeable in the analysis from this point on. This is because what follows does not depend on how $P_{X,Y}$ is generated, just on the properties of the induced distributions as stated in Lemma 2.

We will partition the space $\mathbb{R}$ as follows. First, let $\mathbb{R}_\tau$ denote the set $\{x : |f(x) - f'(x)| > \sqrt{\|f - f'\|_{L_2}^2} \}$. We define the following interval $\mathcal{U} \subset \mathbb{R}$: let $T'$ be defined as in Lemma 2, and $\tau > T'$; we have $\mathcal{U} \triangleq [-\tau, \tau]$.

For any $t \in \mathbb{R}$ we have by writing residual densities in terms of the joint $p_{X,Y}$ (as in the proof of Lemma 2 in
To bound the first term (2), let \( y_x \) denote either of \( t + f'(x) \) or \( t + f(x) \), we have by Lemma 2 that
\[
\int_{\mathbb{R}}^\infty p_{X,Y}(x, y_x) \, dx \leq \int_{\tau}^\infty C' x^{\alpha} \, dx \leq \frac{C'}{\alpha - 1} t^{-(\alpha - 1)},
\]
so that the first term (2) is at most \( 2 \frac{C'}{\alpha - 1} t^{-(\alpha - 1)} \).

To bound the second term (3) we recall that \( p_{X,Y} \) has a bounded gradient on \( \mathbb{R}^2 \) (Lemma 2). Therefore there exists \( C_0 \) such that for every \( x, y, \epsilon \in \mathbb{R} \), \( p_{X,Y}(x, y + \epsilon) \) differs from \( p_{X,Y}(x, y) \) by at most \( C_0 \cdot |\epsilon| \). It follows that the second term (3) is at most
\[
\int_{U \setminus \mathbb{R}^2} C_0 |f'(x) - f(x)| \, dx \leq 2\tau \cdot C_0 \sqrt{\|f - f'\|_{2, P_X}}.
\]

The third term (4) is equal to
\[
\left| P \left( X \in \mathbb{R}^2, Y = t + f'(X) \right) - P \left( X \in \mathbb{R}^2, Y = t + f(X) \right) \right| \leq P_X(\mathbb{R}^2).
\]

We next bound \( P_X(\mathbb{R}^2) \) while noting that \( \|f - f'\|_{2, P_X} \) could be \( 0 \). Let \( \epsilon > \|f - f'\|_{2, P_X} \). By Markov’s inequality,
\[
P_X \left\{ |f(X) - f'(X)| > \sqrt{\epsilon} \right\} \leq \frac{\|f - f'\|_{1, P_X}}{\sqrt{\epsilon}} \leq \frac{\|f - f'\|_{2, P_X}}{\sqrt{\epsilon}}.
\]

Thus, consider a sequence of \( \epsilon \rightarrow \|f - f'\|_{2, P_X} \), by Fatou’s lemma we have \( P_X(\mathbb{R}^2) \leq \sqrt{\|f - f'\|_{2, P_X}} \).

Combining the above analysis we have that
\[
\left| p_{\eta, \eta'}(t) - \eta(t) \right| \leq 2 \frac{C'}{\alpha - 1} t^{-(\alpha - 1)}
+ (1 + 2\tau \cdot C_0) \sqrt{\|f - f'\|_{2, P_X}}.
\]

Now, for \( \|f - f'\|_{2, P_X} \) sufficiently small, we can pick \( \tau = O \left( \|f - f'\|_{2, P_X} \right)^{-1/2\alpha} \) to get the result.

As previously noted we can use the same ideas as above to similarly bound \( \left| p_{\eta, \eta'}(t) - \eta(t) \right| \) for all \( t \in \mathbb{R} \). It suffices to interchange \( X \) and \( Y \) in the above analysis.

**Lemma 4.** Let \( p_1, p_2 \) be two densities such that there exist \( T, C > 1 \) and \( \alpha > 1 \), for all \( |t| > T \), \( \max_{x \in [2]} p_1(t) < C |t|^{-\alpha} \). Suppose \( \sup_{t \in \mathbb{R}} |p_1(t) - p_2(t)| < \epsilon \) for some \( \epsilon < \min \{ 1/T^2, 1/(3e) \} \) satisfying the further condition: \( \forall t > 1/\sqrt{\epsilon}, t^{(\alpha - 1)/2} > \ln t \). We then have for \( \epsilon \) sufficiently small
\[
|H(p_1) - H(p_2)| \leq 18\sqrt{\epsilon} \ln(1/3e) + \frac{4C\alpha}{\alpha - 1} e^{(\alpha - 1)/4}.
\]

**Proof.** For simplicity of notation in what follows, let \( \mathcal{U} \triangleq [\tau, \infty) \) and let \( \mathcal{U}_2 \triangleq \{ t \in \mathcal{U}, p_2(t) > 2\epsilon \} \). Define \( \gamma(u) = -u \ln u \) for \( u > 0 \), and \( \gamma(0) = 0 \). We will use the fact that for the function \( \gamma(\cdot) \) is increasing on \( [0, 1/\epsilon] \). We have
\[
\int_{\mathcal{U}} \gamma(p_1(t)) \, dt + \int_{\mathcal{U}_2} \gamma(p_1(t)) \, dt 
+ \int_{\mathcal{U} \setminus \mathcal{U}_2} \gamma(p_1(t)) \, dt
\leq \int_{\mathcal{U}} \gamma(p_1(t)) \, dt + \int_{\mathcal{U}_2} p_1(t) \ln \frac{1}{p_1(t)} \, dt
+ \Sigma (\mathcal{U} \setminus \mathcal{U}_2) \cdot \gamma(3\epsilon),
\]

since for \( t \in \mathcal{U} \setminus \mathcal{U}_2 \), we have \( p_1(t) \leq p_2(t) + \epsilon \leq 3\epsilon \leq 1/\epsilon \).

To bound the first term of (5), notice that
\[
\int_{\tau}^\infty \gamma(p_1(t)) \, dt \leq \int_{\tau}^\infty C t^{-\alpha} \ln(C t^{-\alpha}) \, dt
\leq \int_{\tau}^\infty C t^{-\alpha} \ln t \, dt
\leq \int_{\tau}^\infty C t^{-\alpha} \ln t \, dt
\leq \frac{2C\alpha}{\alpha - 1} e^{(\alpha - 1)/2},
\]

hence we have \( \int_{\mathcal{U} \setminus \mathcal{U}_2} \gamma(p_1(t)) \, dt \leq 2C\alpha e^{(\alpha - 1)/2} \), for \( C', \alpha' > 0 \).
Next we bound the second term of (5) as follows:

\[ \int_{U_{2>}} p_1(t) \ln \frac{1}{p_1(t)} dt \]

\[ \leq \int_{U_{2>}} (p_2(t) + \epsilon) \ln \frac{1}{p_2(t) - \epsilon} dt \]

\[ = \int_{U_{2>}} p_2(t) \ln \frac{1}{p_2(t)(1 - \epsilon/p_2(t))} dt \]

\[ + \int_{U_{2>}} \epsilon \ln \frac{1}{p_2(t) - \epsilon} dt \]

\[ \leq H(p_2) + \int_{U_{2>}} p_2(t) \ln \frac{1}{1 - \epsilon/p_2(t)} dt \]

\[ + \int_{U_{2>}} \epsilon \ln \frac{1}{\epsilon} dt \]

\[ \leq H(p_2) + \int_{U_{2>}} p_2(t) \ln(1 + 2\epsilon/p_2(t)) dt \]

\[ + \Sigma (U_{2>}) \cdot \epsilon \leq H(p_2) + 2\Sigma (U_{2>}) \cdot \epsilon. \]

Combining all the above, we have

\[ H(p_1) \leq H(p_2) + 3\Sigma (U) \cdot \epsilon + C'\epsilon^{-\alpha'} \]

\[ = H(p_2) + 18\sqrt{c} \ln(1/3\epsilon) + C'\epsilon^{\alpha'/2}. \]

Notice that \( p_1 \) and \( p_2 \) are interchangeable in the above argument. The result therefore follows.

We are now ready to prove the main theorem.

**Proof of Theorem 1**

Let \( f(x) \triangleq \mathbb{E}[Y|x] \) and \( g(y) \triangleq \mathbb{E}[X|y] \). By Lemma 1,

\[ H(X) + H(\eta_Y,f) + 8\epsilon < H(Y) + H(\eta_X,g), \quad (6) \]

for some \( \epsilon > 0 \).

Thus we detect the right direction \( X \rightarrow Y \) if all quantities (a) \( |H_n(\eta_{Y,f_n}) - H(\eta_{Y,f})| \), (b) \( |H_n(\eta_{X,g_n}) - H(\eta_{X,g})| \), (c) \( |H_n(X) - H(X)| \), and (d) \( |H_n(Y) - H(Y)| \), are at most \( \epsilon \).

By assumption, (c) and (d) both tend to 0 in probability. The quantities (a) and (b) are handled as follows. We only show the argument for (a), as the argument for (b) is the same. We have:

\[ |H_n(\eta_{Y,f_n}) - H(\eta_{Y,f})| \leq |H_n(\eta_{Y,f_n}) - H(\eta_{Y,f_n})| \]

\[ + |H(\eta_{Y,f_n}) - H(\eta_{Y,f})|. \]

Now \( H_n(\eta_{Y,f_n}) \) is consistent for \( f_n \) fixed (it easy to check that \( P_{\eta_{Y,f_n}} \) satisfies the necessary conditions provided \( f_n \) is bounded) and \( f_n \) is learned on an independent sample from \( H_n \), we have \( |H_n(\eta_{Y,f_n}) - H(\eta_{Y,f_n})| \xrightarrow{P} 0 \).

By Lemma 3, convergence of \( f_n \) i.e. \( \|f_n - f\|_{2,P_X} \xrightarrow{P} 0 \) implies \( \sup_t |p_{\eta_{Y,f_n}}(t) - p_{\eta_{Y,f}}(t)| \xrightarrow{P} 0 \); this in turn implies by Lemma 4 that \( |H(\eta_{Y,f_n}) - H(\eta_{Y,f})| \xrightarrow{P} 0 \).

Thus all quantities (a)-(d) are at most \( \epsilon \) with probability going to 1. \( \square \)

### 5.2. Coupled Regression and Residual-entropy Estimation

Here we consider a coupled version of the meta-algorithm where \( f_n \) and \( g_n \) are kernel regressors. This is described in the next subsection.

#### 5.2.1. Kernel instantiation of the meta-algorithm

**Regression:** Although any kernel that is 0 outside a bounded region will work for the regression, we focus here (for simplicity) on the particular case where \( f_n \) and \( g_n \) are box-kernel regressors defined as follows (interchange \( X \) and \( Y \) to obtain \( g_n(y) \)):

\[ f_n(x) = \frac{1}{n_{x,h}} \sum_{i=1}^{n} Y_i 1(|X_i - x| < h), \quad (7) \]

where \( n_{x,h} = |i : |X_i - x| < h| \), for a bandwidth \( h \).

**Entropy estimation:** Given a sequence \( \epsilon = \{\epsilon_i\}_{i=1}^{n} \), and a bandwidth \( \sigma \), define \( p_{n,\epsilon} \) as follows:

\[ p_{n,\epsilon}(t) = \frac{1}{n} \sum_{i=1}^{n} K \left( \frac{\epsilon_i - t}{\sigma} \right), \]

where \( \int K(u) du = 1 \) and \( \left| \frac{d}{du} K(u) \right| < \infty \).

Let \( \epsilon_{Y,i} = Y_i - f_n(X_i) \) and \( \epsilon_{X,i} = X_i - g_n(Y_i) \). The residual entropy estimators are defined as:

\[ H_n(\eta_{Y,f_n}) \triangleq H(p_{n,\epsilon_Y}) \] and \( H_n(\eta_{X,g_n}) \triangleq H(p_{n,\epsilon_X}) \).

#### 5.2.2. Consistency result for coupled-estimation

We abuse notation and use \( h \) and \( \sigma \) to denote the bandwidth parameters used to estimate either \( f_n \) and \( H_n(\eta_{Y,f_n}) \), or \( g_n \) and \( H_n(\eta_{X,g_n}) \). We make the distinction clear whenever needed.

The consistency result depends on the following quantities bounded in Lemma 5.

**Definition 6** (Expected average excess risk). Define \( R_n(f_n) \triangleq \mathbb{E}[\frac{1}{n} \sum_{i=1}^{n} |f_n(X_i) - f(X_i)|] \) and similarly \( R_n(g_n) \triangleq \mathbb{E}[\frac{1}{n} \sum_{i=1}^{n} |g_n(Y_i) - g(Y_i)|] \).
We assume in this section that the noise $\eta$ has exponentially decreasing tail:

**Definition 7.** A r.v. $Z$ has **exponentially decreasing tail** if there exists $C, C' > 0$ such that for all $t > 0$, $\Pr(|Z - E[Z]| > t) \leq Ce^{-C't}$.

The following consistency theorem hinges on properly choosing the bandwidths parameters $h$ and $\sigma$. Essentially we want to choose $h$ such that regression estimation is consistent, and we want to choose $\sigma$ so as not to overfit regression error. If the bandwidth $\sigma$ is too small relative to regression error (captured by $R_n$), then the entropy estimator (for the residual entropy) is only fitting this error. The conditions on $\sigma$ in the Theorem are mainly to ensure that $\sigma$ is not too small relative to regression error $R_n$.

**Theorem 2** (Coupled estimation). Suppose $X \overset{f,n}{\sim} Y$ for some $f, \eta$, and suppose $P_{X,Y}$ satisfies Assumption 2, and $\eta$ has exponentially decreasing tail. Let $f_n, g_n$, and $H_n$ be defined as in Section 5.2.1, and let both $H_n(X)$ and $H_n(Y)$ be consistent as in Assumption 1.

Suppose that:

(i) For learning $f_n$ and $H_n(\eta_{Y,f_n})$, we use $h = c_1n^{-\alpha}$ for some $c_1 > 0$ and $0 < \alpha < 1$, and $\sigma = c_2n^{-\beta}$ for some $c_2 > 0$ and $0 < \beta < \min\{(1 - \alpha)/4, \alpha/2\}$.

(ii) For learning $g_n$ and $H_n(\eta_{X,g_n})$, $h$ satisfies $h \to 0$ and $nh \to \infty$, and $\sigma$ satisfies $\sigma \to 0$, $n\sigma \to \infty$, and $\sigma = \Omega(R_n(g_n)^{-\gamma})$ for some $0 < \gamma < 1/2$.

Then the probability of correctly detecting $X \sim Y$ goes to 1 as $n \to \infty$.

The theorem relies on Lemma 5 which bounds the errors $R_n$ for both $f_n$ and $g_n$. Suppose $X \overset{f,n}{\sim} Y$, then if $f$ is smooth or continuously differentiable, $R_n(f_n) \to 0$, and in fact we can obtain finite rates of convergence for $R_n(f_n)$, thus yielding advice on setting $\sigma$. The second part of the Lemma corresponds to this situation.

However, as mentioned earlier in the paper introduction, a smooth $f$ does not ensure that $g(y) \triangleq g(X|y)$ is smooth or even continuous, so we do not have rates for $R_n(g_n)$. We can nonetheless show that $R_n(g_n)$ would generally converge to 0, which is sufficient for there to be proper settings for $\sigma$ (i.e. $\sigma$ larger than the error, but also tending to 0).

We note that the r.v.’s $X$ and $Y$ are interchangeable in this lemma since it does not assume $X$. The proof is given in the supplemental appendix.

**Lemma 5.** Let $f_n$ be defined as in (7). Let $f(x) \triangleq E[Y|x]$, $E[Y^2] < \infty$ and that $f$ is bounded; $h \to 0$ and $nh \to \infty$. Then $\frac{1}{n} \sum_{i=1}^{n} |f_n(X_i) - f(X_i)| \to 0$.

Suppose further (ii) that $P_X$ has bounded support and that $f$ is continuously differentiable; $h = c_1n^{-\alpha}$ for some $c_1 > 0$ and $0 < \alpha < 1$.

Then we have $\mathbb{E} \frac{1}{n} \sum_{i=1}^{n} |f_n(X_i) - f(X_i)| \leq c_2n^{-\beta}$, for $\beta \equiv \min\{(1 - \alpha)/2, \alpha\}$.

We can now prove the theorem of this section.

**Proof of Theorem 2**

Let $\bar{e}_{Y,i} \triangleq Y_i - f(X_i)$ and $\bar{e}_{X,i} \triangleq X_i - g(Y_i)$. Note that, under our conditions on $\sigma$ both $H(p_{n,\bar{e}_Y})$ and $H(p_{n,\bar{e}_X})$ are respectively consistent estimators of $H(\eta_{Y,f}) \triangleq H(\eta)$ and $H(\eta_{X,g})$ (see e.g. (Beiriant et al., 1997)). For any two densities $p, p'$ we write $|p - p'|$ to denote $\sup_t |p(t) - p'(t)|$.

Given the assumption that $K$ has bounded derivative on $\mathbb{R}$, there exists a constant $c_K$ such that

$$|p_{n,\bar{e}_Y} - p_{n,\bar{e}_Y}| \leq \frac{c_K}{\sigma^2} \cdot \left(\frac{1}{n} \sum_{i=1}^{n} |f_n(X_i) - f(X_i)|\right),$$

$$\therefore \mathbb{E} |p_{n,\bar{e}_Y} - p_{n,\bar{e}_Y}|^{1/2} \leq \frac{\sqrt{c_K R_n(f_n)}}{\sigma},$$

$$|p_{n,\bar{e}_X} - p_{n,\bar{e}_X}| \leq \frac{c_K}{\sigma^2} \cdot \left(\frac{1}{n} \sum_{i=1}^{n} |g_n(Y_i) - g(Y_i)|\right),$$

$$\therefore \mathbb{E} |p_{n,\bar{e}_X} - p_{n,\bar{e}_X}|^{1/2} \leq \frac{\sqrt{c_K R_n(g_n)}}{\sigma}.$$
6. Final Remarks

We derived the first consistency results for an existing family of procedures for causal inference under the Additive Noise Model. We obtained mild algorithmic requirements, and various distributional tail conditions which guarantee consistency. The present work focuses on the case of two r.v.s \( X \) and \( Y \), which captures the inherent difficulties of consistency. We believe however that the insights developed should extend to the case of random vectors under corresponding tail conditions. The details however are left for future work.

Another interesting multivariate situation is that of a causal network of r.v.s. as in Peters et al. (2011b) discussed earlier. Extending our consistency results to this particular multivariate case would primarily consist of extending our distributional tail conditions to the tails of distributions resulting from conditioning on appropriate sets of variables in the network. This is however a non-trivial extension as it involves, e.g. for the convergence of conditional entropies, some additional integration steps that have to be carefully worked out.

A possible future direction of investigation is to understand under what conditions finite sample rates can be obtained for such procedures. For reasons explained earlier, we do not believe that this is possible without less general distributional assumptions.

References


A. Omitted figures from Section 4

Some additional experimental results were omitted in the main paper for space, and are given in Figure 3.

B. Omitted Proofs: Section 5.1

Proof of Lemma 2. Note that, by assumption, both \( p_X \) and \( p_Y \) are bounded. For any \( x, y \in \mathbb{R} \), we have

\[
p_{X,Y}(x, y) = p_X(x) \cdot p_{Y|x}(y) = p_X(x) \cdot p_Y(y - f(x)).
\]

(9)

Therefore \( \frac{d}{dx}p_{X,Y}(x, y) \) is given by

\[
\frac{d}{dx}p_X(x) \cdot p_Y(y - f(x)) - \frac{d}{dx}f(x) \cdot \frac{d}{dx}p_Y(y - f(x)).
\]

It is clear that \( \sup_{x,y} \frac{d}{dx}p_{X,Y}(x, y) < \infty \). Similarly \( \sup_{x,y} \frac{d}{dx}p_{X,Y}(x, y) < \infty \). Also, since \( p_Y \) is bounded, we have from (9) that for \( |t| \) sufficiently large, \( p_{X,Y}(t, y) = 0 \) independent of \( y \). Also, since \( f \) and \( p_X \) are bounded, we have, independent of \( x \), that for \( |t| \) sufficiently large, \( p_{X,Y}(x, t) < C't^{-\alpha} \) for some \( C' > 0 \).

Next the density of the residual \( \eta_{Y,f'} \) of a function \( f' \) is easily obtained as follows for any \( t \in \mathbb{R} \).

\[
p_{\eta_{Y,f'}}(t) = \int_{\mathbb{R}} p_X(x) \cdot p_{Y|x}(t + f'(x)) \, dx
\]

\[
= \int_{\mathbb{R}} p_X(x, y, t + f'(x)) \, dx
\]

\[
= \int_{\mathbb{R}} p_X(x) \cdot p_Y(t + f'(x) - f(x)) \, dx.
\]

(10)

Thus if \( f' \) is bounded, there exists \( T' > 0 \) such that for \( |t| > T' \),

\[
p_{\eta_{Y,f'}}(t) \leq C' |t|^{-\alpha} \cdot \int_{\mathbb{R}} p_X(x) \, dx = C' |t|^{-\alpha},
\]

where \( \alpha \) is the same as for the bound on \( p_Y \) from the assumption.

We have similarly for any function \( g \) that,

\[
p_{\eta_{X,g}}(t) = \int_{\mathbb{R}} p_Y(y) \cdot p_{X|Y}(t + g(y)) \, dy
\]

\[
= \int_{\mathbb{R}} p_X(t + g(y), y) \, dy.
\]

(11)

If \( g \) is bounded, then for \( t \) sufficiently large, \( p_X(t + g(y)) = 0 \) for all \( y \) so \( p_{\eta_{X,g}}(t) = 0 \).

C. Omitted Proofs: Section 5.2

We denote the random \( n \)-samples as \( X^n \triangleq \{X_i\}_1^n \) and \( Y^n \triangleq \{Y_i\}_1^n \), throughout this section.

We bound \( R_n(f_n) \) and \( R_n(g_n) \) in Lemma 5 which makes use of Lemma 6. We note that the r.v.'s \( X \) and \( Y \) are interchangeable in the two lemmas 5 and 6, since they do not assume \( X \rightarrow Y \).

Lemma 6 ([Gyorfi et al., 2002]). For any positive \( f : \mathbb{R} \rightarrow \mathbb{R} \) such that \( \mathbb{E} f < \infty \), there exists \( c_0 \) such that

\[
\mathbb{E} X,X^n \left\{ \frac{1}{n} \sum_{i=1}^n X_i \cdot |X_i - X| < h \cdot f(X_i) \right\} \leq c_0 \mathbb{E} f(X).
\]

Proof of Lemma 5. We simply have to show that

\[
\mathbb{E} \left\{ \frac{1}{n} \sum_{i=1}^n |f_n(X_i) - f(X_i)|^2 \right\} \xrightarrow{n \to \infty} 0 \text{ since by Hölder’s inequality and Jensen’s inequalities, for any } \phi_n(\cdot),
\]

\[
\mathbb{E} \left\{ \frac{1}{n} \sum_{i=1}^n |\phi_n(X_i)| \right\} \leq \mathbb{E} \left\{ \frac{1}{n} \sum_{i=1}^n |\phi_n(X_i)|^2 \right\} \leq \sqrt{\mathbb{E} \left\{ \frac{1}{n} \sum_{i=1}^n |\phi_n(X_i)|^2 \right\}}.
\]

For assumption (i), pick any \( \epsilon > 0 \). We will show that for \( n \) sufficiently large, the above expectation is at most \((7 + 3c_0)\epsilon\), where \( c_0 \) is as in Lemma 6. The further claim of assumption (ii) will be obtained along the way.

First condition on \( X^n \), fixing \( x = X_i \) for some \( X_i \), and taking expectation with respect to the randomness in \( Y^n \triangleq \{Y_i\}_1^n \). We have by a standard bias-variance decomposition (see e.g. ([Gyorfi et al., 2002])) that

\[
\mathbb{E} Y^n |X^n \{ f_n(x) - f(x) \}^2 \leq \frac{C}{n_{x,h}} + \frac{1}{n_{x,h}} \sum_{|X_j - x| < h} f(X_j) - f(x)^2 = A_x + B_x,
\]

(12)

for some \( C \) depending on the variance of \( Y \).

We start with a bound on the first term of (12). Pick an interval \( S \) such that \( P_X(\mathbb{R} \setminus S) < \epsilon \).

Consider an \( (h/2) \)-cover \( Z \) of \( S \) such that for every \( z \in S \), the interval \([z - h/2, z + h/2] \) is contained in \( S \). We can pick such a \( Z \) of size at most \( 2\Sigma(S)/h \). Note that for any \( x \in [z - h/2, z + h/2] \), \( n_{x,h} \geq n_{z,h/2} \triangleq n_{z,h} \).
\[\{X_i : |z - X_i| < h/2\}\]. We then have
\[
\frac{1}{n} \sum_{i=1}^{n} A_{X_i} = \frac{1}{n} \sum_{i=1}^{n} \frac{C}{n_{X_i,h}} \left(1_{\{X_i \in S\}} + 1_{\{X_i \notin S\}}\right)
\]
\[
\leq \frac{1}{n} \sum_{j=1}^{n} \frac{C}{n_{X_j,h}} 1_{\{X_j \in S\}} + \frac{1}{n} \sum_{i=1}^{n} 1_{\{X_i \notin S\}}
\]
\[
\leq \frac{1}{n} \sum_{z \in Z} C \cdot n_{z,h/2} + \frac{1}{n} \sum_{i=1}^{n} 1_{\{X_i \notin S\}}.
\]
Therefore by taking expectation over \(X^n\) and letting \(nh\) sufficiently large, we have
\[
\mathbb{E} \frac{1}{n} \sum_{i=1}^{n} A_{X_i} \leq \frac{2C \cdot \Sigma(S)}{nh} + P_X(\mathbb{R} \setminus S) \leq 2\epsilon.
\]

Under assumption (ii), pick \(S\) larger than the support of \(P_X\), we have by the same equation above that for large \(n\)
\[
\mathbb{E} \frac{1}{n} \sum_{i=1}^{n} A_{X_i} \leq \frac{2C \cdot \Sigma(S)}{nh} = \frac{2C \cdot \Sigma(S)}{c_1 n^{1-\alpha}}.
\]

We now turn to the second term of (12). Under assumption (ii) the function \(f\) is Lipschitz continuous and we therefore have for some constant \(c_f\) that \(A_x \leq c_f h^2 = c_f c_1 n^{-2\alpha}\). Combining with the bound on \(A_x\) gives the result for assumption (i).

For assumption (i) we proceed as follows. It is well known that bounded uniformly continuous functions are dense in \(L_{2,P_X}\) for any \(P_X\). Therefore let \(\tilde{f}\) be a bounded uniformly continuous function such that \(\|\tilde{f} - f\|_{2,P_X} < \sqrt{\epsilon}\). Since \(h = h(n) \to 0\), we have \(\sup_{|x'| < h} |\tilde{f}(x) - \tilde{f}(x')| < \epsilon\) for \(n\) sufficiently large. The second term of the r.h.s. of the above equation (12) can then be bounded as follows. If \(n_{x,h} = 1\), then \(B_x = 0\). Otherwise, if \(n_{x,h} > 1\), we have
\[
B_x \leq \frac{3}{n_{x,h}} \sum_{|x_j - x| < h} \left( |f(x_j) - \tilde{f}(x_j)|^2 + |\tilde{f}(x_j) - f(x_j)|^2\right)
\]
\[
\leq 3\epsilon + \frac{3}{n_{x,h}} \sum_{|x_j - x| < h} \left|f(x_j) - \tilde{f}(x_j)\right|^2
\]
\[
\leq 3\epsilon + \left(\frac{3}{n_{x,h}} + 1\right) \left|\tilde{f}(x) - f(x)\right|
\]
\[
\leq 3\epsilon + \left(\frac{3}{n_{x,h}} + 1\right) \sum_{|x_j - x| < h, x_j \neq x} \left|f(x_j) - \tilde{f}(x_j)\right|^2.
\]
Therefore taking expectation over \(X^n\), and applying Lemma 6 to the second term above for \(x = X_i\), we have
\[
\mathbb{E} B_{X_i} \leq 3\epsilon + 2\mathbb{E} X \left|\tilde{f}(X) - f(X)\right|^2
\]
\[
+ 3c_0 \mathbb{E} X \left|\tilde{f}(X) - f(X)\right|^2 = (5 + 3c_0)\epsilon,
\]
so that \(\mathbb{E} \frac{1}{n} \sum_i B_{X_i} \leq (5 + 3c_0)\epsilon\). \(\square\)