Causal bootstrapping

Max A. Little*,†, Reham Badawy*

January 19, 2020

*School of Computer Science, University of Birmingham, UK
†MIT, Cambridge, MA, USA
First author contact: maxl@mit.edu

To draw scientifically meaningful conclusions and build reliable engineering models of quantitative phenomena, statistical models must take cause and effect into consideration (either implicitly or explicitly). This is particularly challenging when the relevant measurements are not obtained from controlled experimental (interventional) settings, so that cause and effect can be obscured by spurious, indirect influences. Modern predictive techniques from machine learning are capable of capturing high-dimensional, complex, nonlinear relationships between variables while relying on few parametric or probabilistic modelling assumptions. However, since these techniques are associational, applied to observational data they are prone to picking up spurious influences from non-experimental (observational) data, making their predictions unreliable. Techniques from causal inference, such as probabilistic causal diagrams and do-calculus, provide powerful (nonparametric) tools for drawing causal inferences from such observational data. However, these techniques are often incompatible with modern, nonparametric machine learning algorithms since they typically require explicit probabilistic models.

Here, we develop causal bootstrapping, a set of techniques for augmenting classical nonparametric bootstrap resampling with information about the causal relationship between variables. This makes it possible to resample observational data such that, if it is possible to identify an interventional relationship from that data, new data representing that relationship can be simulated from the original observational data. In this way, we can use modern machine learning algorithms unaltered to make statistically powerful, yet causally-robust, predictions. We develop several causal bootstrapping algorithms for drawing interventional inferences from observational data, for classification and regression problems, and demonstrate, using synthetic and real-world examples, the value of this approach.

1 Introduction

One of the main aims of the quantitative sciences is to produce models of observed phenomena in the world so that testable predictions can be made from these models. In the ideal case, it is possible to perform controlled experiments and measure the resulting change in variables of interest. Data obtained from controlled experiments can be used to produce models of the relationship between effects and their causes, for example, modelling the relationship between treating a medical issue by taking a drug (cause) and health status of that issue (effect), while controlling for age which can be a cause of both whether the drug is taken and health status [Pearl, 2009]. There are numerous

1This work partially funded by NIH grant UR-Udall Center, award number P50 NS108676.
situations where performing experiments is either physically impossible, unethical or just infeasible from a practical point of view. For example, we cannot modify the weather or prevent the population of a country from using water to determine the causal relationship between daily sunshine hours and domestic water usage, independent of atmospheric humidity which influences both cloud cover and the need for people to hydrate themselves.

Broadly speaking, there are two kinds of data about the world: experimental data obtained from controlled experiments, and observational data. In many sciences such as medicine and agriculture, the randomized controlled trial is the archetypal experiment used to test the effectiveness of a treatment [Matthews, 2006]. Well-developed statistical analysis of this data allows us to quantify the strength of the causal effect of the treatment on the outcome of interest. Whereas, in epidemiology and economics, data is almost entirely observational since experiments are usually impractical – a key question therefore for these mainly observational sciences is whether it is possible to nonetheless infer causes and their effects from the available data.

A variety of “tricks” for statistical analysis of such data have been developed to address this problem, among them so-called adjustment methods and instrumental variables. However, these tricks only work in special circumstances. Whether and how these tricks can be generalized to address a wider range of observational data raises important questions which have, over the last few decades, coalesced into the new discipline of causal inference. Arguably, the most systematic, complete and integrated work in this discipline uses the tools of (probabilistic) causal diagrams, do-calculus and other conceptual and analytical devices [Pearl, 2009].

Meanwhile, new forms of experimental and observational data have become usable due to advances in digital measurement, storage and processing hardware. For example, it is now possible to capture, store and process millions of digitized X-ray images recording the presentation of various medical conditions in the medical clinic. Digital measurements of patterns of human transport or online behaviour using devices such as smartphones, have also become available. This data is nearly all observational. As with data from “classical” observational epidemiological or ecological settings, it is generally infeasible (in terms of cost and/or logistics) to run controlled experiments to determine causal relationships in this setting. However, it differs from classical settings in that (1) the data is of enormous scale (on the order of billions of observations across thousands or millions of variables is not unusual), and (2) there are unknown, complex (nonlinear) rather than simple linear, relationships between these variables. Analyzing this kind of data to make reliable causal inferences is a challenge for traditional statistics but the discipline of statistical machine learning has emerged to take on some of these challenges. Machine learning predictors, such as kernel regression, random forests, support vector machines and deep learning, have been developed to learn high-dimensional, nonlinear statistical relationships between variables [Little, 2019].

While these machine learning predictors can have extremely high accuracy, the major drawback is their complete “blindness” to causal structure. This is because they find associational relationships, not causal ones. For example, empirical evidence points to these predictors easily exploiting spurious associations in observational data [Zech et al., 2018, Chyzyk et al., 2018, Kaufman et al., 2012, Neto et al., 2019, Neto, 2018]. Thus, these machine learning methods cannot learn causal (interventional) relationships from observational data (at least not without special adaptations). It would therefore be valuable to somehow co-opt the predictive power of these machine learning algorithms, meanwhile, ensuring they can make interventional predictions from the available observational data, without having to make special adaptations to these algorithms.

Here, we introduce a simple method to achieve this. We augment the classical bootstrap resampling method [Efron and Tibshirani, 1994] with information from the causal diagram generating the observational data. This leads to a simple weighted bootstrap which can be used to generate new data faithful to an interventional distribution of interest. Any standard, complex nonlinear machine learning predictor can then be applied to the new data to construct interventional predictors, rather than associational predictors. This method is applicable to most interventional distributions which can be derived from observational causal models using the rules of do-calculus, according to the general
identification algorithm of Shpitser and Pearl [2008].

We develop several bootstrap algorithms for common causal inference scenarios including general back-door and front-door deconfounding, tailored to supervised classification or regression machine learning methods. We demonstrate the effectiveness of this technique for synthetic data and real-world, practical causal inference problems.

2 Methods

First we introduce some notation. Labels such as \( X, Y, U, W \) and \( Z \) refer to random variables and their realizations, \( x, y, u, w \) and \( z \). These have sample spaces \( \Omega_X, \Omega_Y, \) and so on. Multidimensional variables are bold, e.g. \( \mathbf{X} \) and \( \mathbf{x} \), and \( x_n \) is the \( n \)-th observation of the variable \( x \). For the set of variables \( \mathcal{S} = \{x, y, u, w\} \), the shorthand \( f(z, \mathcal{S}) \) refers to \( f(z, x, y, u, w) \), and \( \mathcal{S}_n \) refers to tuple of observations \((x_n, y_n, u_n, w_n)\). The notation \( \int g(z, \mathcal{S}) \, d\mathcal{S} \) refers to the marginalization of the variables \( \mathcal{S} \) from \( g \). A causal graph, which is a directed acyclic graphical (DAG) model with vertices \( \mathcal{V} \) being a set of random variables, indicates the conditional independence relationships between the variables.

The edges in the graph capture dependencies, e.g. \( U \leftarrow Y \rightarrow X \) encodes that both \( U \) and \( X \) depend upon \( Y \), but \( Y \) does not depend upon either. The set-valued function \( \mathcal{P} : \mathcal{V} \rightarrow 2^\mathcal{V} \) gives the set of \textit{parent} variables for \( U \), e.g. if \( \mathcal{P}(u) = \{v, w, z\} \), then \( f(u|\mathcal{P}(u)) = f(u|v, w, z) \), representing these relationships.

Our approach uses nonparametric estimates of interventional distributions, and manipulates them analytically to produce a simple expression capturing the causal relationship of interest, from which interventional samples can be simulated from the observational data. We make use of nonparametric \textit{kernel density estimates} (KDE) obtained from joint and marginal \textit{reproducing kernel Hilbert space} (RKHS) functions \( K[\cdot] \), to illustrate:

\[
\hat{f}(x, y) = \frac{1}{N} \sum_{n \in \mathcal{N}} K(x - x_n) K(y - y_n) \tag{1}
\]

\[
\hat{f}(x) = \frac{1}{N} \sum_{n \in \mathcal{N}} K(x - x_n) \tag{2}
\]

where \( \mathcal{N} = \{1, 2, \ldots, N\} \) is the set of indices of the sample data for the random variables \( X, Y \). Note that the kernels for \( X \) and \( Y \) can generally be distinct. Simplifying these KDEs to relies on two basic mathematical devices. The first is the \textit{reproducing property} [Berlinet and Thomas-Agnan, 2011]:

\[
\langle f, K[x, \cdot] \rangle = \int f(x') \, K(x - x') \, dx' = f(x) \tag{3}
\]

Here, \( f(x) \) is some distribution function, and the integral computes a marginal distribution function. Using this property, we analytically solve the marginal integral by replacing occurrences of the variable \( x \), with evaluations of the distribution \( f(x_n) \) at the realization \( x_n \). The second property is the linearity of integration allowing us to swap integrals with summations.

Through such analytical manipulations, the “heart” of our approach involves simple \textit{weighted} interventional KDEs:

\[
\hat{f}(x|do(y)) \approx \sum_{n \in \mathcal{N}} K(x - x_n) \, w_n \tag{4}
\]

where \( 0 < w_n < \infty \) is some real-valued weighting vector. Sampling from this equation is straightforward; we draw some \( i \in \mathcal{N} \) with probability proportional to \( w_i \), then draw a value \( x \) from the kernel function \( K \) centered on \( x_i \). Furthermore, if we replace the kernel \( K \) in this equation with the Dirac delta function (for continuous \( X \)), then the value \( x = x_i \), without the need to sample from the kernel.

This is the basis of the \textit{bootstrap} [Efron and Tibshirani, 1994], which motivates the description of sampling from models like (4) as \textit{causal bootstrapping}.

Here we illustrate briefly an application of these ideas to supervised machine learning. Consider that we want to learn the nonlinear relationship \( Y, X \). Here, \( Y \) is a univariate \textit{prediction target} variable
Figure 1: Using causal bootstrapping to construct an interventional machine learning predictor for digit recognition when the observational data is confounded. The “brightness-MNIST” problem has variables where $U$ is the image brightness, $X$ are the pixels and $Y$ is the target digit label, (“2” vs. “6”). (a) In the observational data, brightness $U$ is a confounder since it is a common cause of the target and the image data, $Y \leftarrow U \rightarrow X$. Therefore, it is highly correlated with the digit label $Y$, in which case, any standard supervised classifier trained on this data has a high risk of simply using the brightness to predict the digit. (b) When the digit label and brightness are independent (which would be the case in an experiment where the digit label is controlled) then there is no advantage to using the brightness information to make a digit label prediction. However, in practice, the observational training data may be confounded as in (a). Back-door (Algorithm 1) or (when there is a mediator) front-door causal bootstrapping (Algorithm 2) can be used to simulate the controlled experiment (b), on which a classifier which correctly solves the problem of digit label recognition, can be trained. Random forest classification accuracy trained on confounded data (a) reaches 96% out-of-sample, but tested on non-confounded data (b) collapses to near chance, 58%. By contrast, training on causal bootstrapped data achieves greater than 90% tested out-of-sample and similar accuracy on (b). See Table 1 for details.
and \( \mathbf{X} \) is a high-dimensional feature variable. However, there is a variable \( U \) which introduces the confounding path \( Y \leftarrow U \rightarrow \mathbf{X} \) (Figure 2a). This means we cannot, from the training data pairs \( \mathcal{D} = (\mathbf{x}_n, y_n), n \in \mathcal{N}, \) learn the causal relationship which would have been obtained by measuring the training data under an experiment whereby we control \( Y \) independent of \( U \). This is because the data was generated from \( f (\mathbf{x} | y) \) which is not the same as \( f (\mathbf{x} | \text{do}(y)) \) due to the confounding path. If the resulting predictor, trained on \( (\mathbf{x}_n, y_n) \) were to be used in a situation in which there was no confounding, we cannot expect it to make reliable predictions. However, if we have also measured \( u_n \), we can resample a new, deconfounded set of training data \( \mathcal{D}^* \) by causal bootstrapping from (4) using the weights:

\[
w_n = \frac{K [y_n - y]}{N \hat{f} (y | u_n)}
\]

where \( K = 1 \), the discrete Kronecker delta, in the classification case where where the sample space \( Y \in \Omega_Y \) is discrete, or \( K \) is some suitable kernel in the (univariate) regression case where \( \Omega_Y = \mathbb{R} \) is continuous. The conditional \( \hat{f} (y | u) \) can obtained using any suitable density estimator (we suggest using KDEs for their simplicity). In the classification setting where \( Y, U \) are both discrete, this method is parameter-free, and thus the only source of additional error in this bootstrap procedure over and above those sources in the original data, is due to bootstrap resampling variability alone.

**Algorithm 1** Back-door causal bootstrapping for supervised classification and regression.

**Input:** \( N \) samples \( \mathcal{D} = (\mathbf{x}_n, y_n, S), n \in \mathcal{N} = \{1, 2, \ldots, N\} \) from a graphical model, and samples from the back-door admissible variable set \( S \). The variables are: arbitrary multidimensional feature data (vector) \( \mathbf{X} \), prediction target \( Y \) and arbitrary adjustment set \( S \), with sample spaces \( \Omega_X, \Omega_Y \) and \( \Omega_S \).

**Output:** \( N \) deconfounded samples \( \mathcal{D}^* = (\mathbf{x}_m, y_m), m \in \mathcal{N} \) approximating samples from \( f (\mathbf{x} | \text{do}(y)) \).

1. Find empirical KDEs \( \hat{f} (y, S) \) and \( \hat{f} (S) \) from \( \mathcal{D} \) to compute \( \hat{f} (y | S) \).
2. For each \( n \in \mathcal{N} \):
3. Produce new sample \( \mathcal{D}^* = (\mathbf{x}_i, y_n) \), where index \( i \) is selected from \( \mathcal{N} \) with weights:

\[
w_i = \frac{K [y_i - y_n]}{N \hat{f} (y_n | S_i)}
\]

where \( K [\cdot] = 1 [\cdot] \) for classification, and a suitable kernel for regression.

In this way, we can co-opt any high-performance, predictive machine learning algorithm to learn the desired causal relationship from observational training data without the need to modify the machine learning algorithm, nor perform a separate, potentially logistically difficult, controlled experiment. See Figure (1) for an example of high-dimensional machine learning prediction from confounded digital image data, deconfounded using causal bootstrapping.

**2.1 Bootstrap weights for interventional distributions**

We now develop the theoretical justification for causal bootstrapping such as Algorithm 1. In causal inference problems, we often have an interventional distribution in the form:

\[
f (\mathbf{x} | \text{do}(y)) = \int f (\mathbf{x} | \mathcal{P} (\mathbf{x})) \prod_{v \in \mathcal{E}} f (v | \mathcal{P} (v)) d\mathcal{E}
\]

where \( \mathbf{X} \) is (primary) effect variable, \( Y \) is the intervention variable (prediction target), and \( \mathcal{E} = \mathcal{P} (\mathbf{x}) \setminus y \) are secondary effect variables which are marginalized out. This can be obtained by various
methods such as truncated factorization, back- or front-door deconfounding, or the general identification algorithm of Shpitser and Pearl [2008]. The causal bootstrapping weights in (4) to simulate from this distribution, given observational data, are given by:

$$w_n = \frac{1}{N} \times \begin{cases} K[y_n - y] \bar{w}_n & \text{if } y \in \mathcal{P}(x) \\ \bar{w}_n & \text{otherwise} \end{cases}$$  

(7)

$$\bar{w}_n = \prod_{v \in \mathcal{E}} \hat{f}(v|\mathcal{P}(v)) \bigg| \mathcal{V}_{\psi \in \mathcal{E}: u = u_n}$$  

(8)

In the second line, each occurrence of the $u \in \mathcal{E}$ is replaced with the realization $u_n$ from the observational data (note that $y \notin \mathcal{E}$ by construction of interventional distributions). For example, if $f(v|\mathcal{P}(v)) = f(v|x, z, y)$, then $f(v|\mathcal{P}(v)) = f(v|x_n, z_n, y)$ after replacement. The notation $\hat{f}$ refers to a (generally nonparametric) estimate of the true $f$. A proof of this is given in Appendix A: Proofs.

As an example of the above, given a causal graphical model, the identification (ID) algorithm of Shpitser and Pearl [2008] can be used to determine whether any desired interventional distribution can be obtained from this model. If so, it produces the expression for the interventional distribution. Using this expression and the interventional formula (6)-(8), we can simplify this to a causal bootstrap (with the only restriction that $\mathcal{E} = \mathcal{P}(x) \setminus y$). As an example, Tikka and Karvanen [2017] derive the following formula for the causal effect of $Y$ on $X$ from the causal diagram of Figure 2c:

$$f(x|do(y)) = \int f(w) \int f(z|w, y) \int f(x|w, y', z) f(y'|w) dy' dz dw$$  

(9)

Following the above and applying RKHS estimators and then simplifying, leads to the following weighted KDE:

$$f(x|do(y)) \approx \frac{1}{N} \sum_{n \in \mathcal{N}} K[x_n - x] \frac{\hat{f}(z_n|w_n, y)}{f(z_n|w_n, y_n)}$$  

(10)

For a proof of this, see Appendix A: Proofs.

2.2 Choice of effect kernel

The choice of RKHS kernel function for the effect $X$ depends heavily on the sample spaces of the variables involved. For instance, if $\Omega_X$ is discrete, it makes sense to use the Kronecker delta $\mathbf{1}[x] = 1$ for $x = 0$, zero otherwise. For continuous sample spaces, the choice depends to a large extent on
computational or smoothness considerations; many kernels have bandwidth parameters which control the regularity of the KDE for the variable [Silverman, 1986].

We will also make use the Dirac delta function as a “kernel” for $X$; although this is not in an RKHS, it does satisfy the reproducing property, e.g. $\int f(x') \delta[x-x'] dx' = f(x)$ which is in fact all we need. Replacing $K = \delta$ in (4) leads to an even more tractable bootstrap model. To sample from this model, on having chosen $i$ as described above, it suffices to simply emit the sample $x_i$ (since all the mass of the estimator is concentrated on the point set $x_n$, $n \in N$). This is the basis of bootstrap resampling [Efron and Tibshirani, 1994].

Next, we develop the application of the theory above to several examples from causal inference, and derive associated causal bootstrapping algorithms.

2.3 Back-door causal bootstrap

A common situation encountered in practice is that of confounding where unwanted causal paths exist between the (prediction target) variable $Y$ and the observed feature data $X$, interfering with the direct causal path of interest relating $Y$ to $X$. It is possible to estimate the interventional distribution $f(x|do(y))$ if an admissible set of variables $S$, can be found [Pearl, 2009]. This set must satisfy the back-door criterion: (i) no variable in $S$ is a descendent of $Y$, and (ii) the variables $S$ block all causal paths with an arrow pointing to $Y$. Applying the rules of do-calculus shows that the interventional distribution can be obtained using:

$$f(x|do(y)) = \int f(x|y, S) f(S) dS$$

(11)

Now, using (7)-(8), we obtain the following back-door adjusted KDE:

$$f(x|do(y)) \approx \frac{1}{N} \sum_{n \in N} K[x - x_n] \frac{K[y_n - y]}{\hat{f}(y|S_n)}$$

(12)

A detailed derivation is given in Appendix A: Proofs. An interesting special admissible set are the direct parents of $Y$, that is, the variables upon which $Y$ depends immediately in the DAG [Pearl, 2009]. By definition they cannot be descendents of $Y$ (satisfying criterion (i)) and since all back-door paths must go through the incoming edges to $Y$, these can only originate in the direct parents of $Y$ (satisfying condition (ii)). Another example is shown in Figure 2a with a single back-door path blocked by the variable $U$. Selecting $K[x - x_n] = \delta[x - x_n]$, leads to the simple back-door causal bootstrap algorithm which is suitable for supervised classification and regression applications, Algorithm 1.

Note that in this algorithm, if $Y$ is discrete, rather than simulating a single intervention for each sample $y_n$ in $D$, we can usually simplify the computations by grouping together all simulated data that share the same value of $y$. If, for each $y \in \Omega_Y$ we simulate $\left\lfloor N \hat{f}(y) \right\rfloor$ samples with the same value of $y$, we ensure that both the observed $\hat{f}(y)$ and the number of observations in $D$ are retained in $D^*$. However, this choice of the distribution of resampled $Y$ is not a requirement for the back-door causal bootstrap to be valid. If $Y$ is continuous, the values $y_n$ are all distinct and cannot be grouped to simplify the computations. Instead, the observed distribution $\hat{f}(y)$ is reproduced exactly by simulating a single intervention for each sample $y_n$. However, as with the discrete case, we do not have to reproduce the observed, marginal distribution of $Y$ when generating deconfounded data; indeed we can simulate any interventional dataset we wish. For example, when $N$ is very large, it may be more practical to produce a smaller, deconfounded dataset across a uniformly sampled, representative range of values of $Y$ instead.

2.4 Front-door causal bootstrap

A somewhat more complex situation that arises in some observational settings is that of so-called front-door confounding. Here, multiple back-door paths composed of unobserved variables exist between
the prediction target $Y$ and the observed feature data $X$, interfering with the causal relationship $Y, X$ (Figure 2b). Since we cannot observe these back-door variables, we cannot block using back-door deconfounding. However, there is also a variable $Z$, known as a mediator, such that $Y \rightarrow Z \rightarrow X$. In this situation, we can use do-calculus to derive an expression for $f(x|do(y))$ such that we do not need to explicitly block any of the back-door paths.

The front-door criterion is in three parts: (i) the mediator must intercept all paths between $Y$ and $X$, (ii) all back-door paths from $Z$ to $X$ must be blocked by $Y$, and (iii) there should be no other paths between $Z$ and $X$. If these conditions hold, we get the following interventional distribution [Pearl, 2010]:

$$f(x|do(y)) = \int \left( \int f(x|y', z) f(y') dy' \right) f(z|y) dz$$

(13)

As with back-door deconfounding, using the interventional formula (6)-(8) leads to the following front-door adjusted KDE (see Appendix A: Proofs for derivation):

$$f(x|do(y)) \approx \frac{1}{N} \sum_{n \in \mathcal{N}} K[x_n - x] \frac{\hat{f}(z_n|y)}{\hat{f}(z_n|y_n)}$$

(14)

This gives us the front-door causal bootstrap, Algorithm (2), which we describe for supervised machine learning applications. As with the back-door algorithm, the computations may be simplified by looping over each $y \in \Omega_Y$ in the discrete interventional variable case.

**Algorithm 2** Front-door causal bootstrapping for supervised classification and regression problems.

**Input:** $N$ marginal samples $\mathcal{D} = (x_n, y_n, z_n), \ n \in \mathcal{N} = \{1, 2, \ldots, N\}$ from the front-door confounded causal graphical model. The variables are: arbitrary feature data (vector) $X$, prediction target $Y$ and mediator $Z$, with sample spaces $\Omega_X, \Omega_Y$ and $\Omega_Z$.

**Output:** $N$ deconfounded samples $\mathcal{D}^* = (x_m, y_m), m \in \mathcal{N}$ approximating samples from $f(x|do(y))$.

1. Find empirical EDF $\hat{f}(z, y)$ from $\mathcal{D}$ to compute $\hat{f}(z|y)$.

2. For each $n \in \mathcal{N}$:

3. Produce new sample $\mathcal{D}^* = (x_i, y_n)$, where index $i$ is selected from $\mathcal{N}$ with weights:

$$w_i = \frac{\hat{f}(z_i|y_n)}{N \hat{f}(z_i|y)}$$

2.5 Truncated factorization causal bootstrap

More generally, for a causal graphical model $G$ with vertices $\mathcal{V} = \{x, \mathcal{E}, y\}$ and $\mathcal{E} = \mathcal{P}(x) \setminus y$, the joint distribution is given by:

$$f(x, \mathcal{E}, y) = f(x|\mathcal{P}(x)) f(y|\mathcal{P}(y)) \prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))$$

(15)

If all the variables are observed, we can use the truncated factorization formula to compute the interventional distribution [Pearl, 2010]:

$$f(x, \mathcal{E}|do(y)) = f(x|\mathcal{P}(x)) \prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))$$

(16)
Marginalizing out other effect variables $E$ isolates the causal effect of $Y$ on $X$:

$$f(x|do(y)) = \int f(x|P(x)) \prod_{v \in E} f(v|P(v)) dE$$  \hspace{1cm} (17)$$

This is in the form of interventional distribution (6), and it follows that the causal bootstrap weights for $f(x|do(y))$ are those given by plugging in the KDEs $\hat{f}(P(x))$ and $\hat{f}(v|P(v))$ for all $v \in E$ and into (7). This leads to Algorithm 3 suitable for supervised learning applications. As above, the computations may be simplified by looping over each for $y \in \Omega_Y$ in the discrete interventional variable case.

Algorithm 3 Truncated factorization causal bootstrapping for supervised classification and regression.

**Input:** $N$ samples $D = (x_n, E_n, y_n), n \in \mathcal{N} = \{1, 2, \ldots, N\}$ from the joint distribution over the graphical causal model $\mathcal{G}$ with variables $\mathcal{V} = \{x, E, y\}$, where $X$ is an arbitrary multidimensional feature data (vector), $Y$ is the prediction target, and arbitrary additional variables $E$, with sample spaces $\Omega_X, \Omega_Y$ and $\Omega_E$.

**Output:** $N$ samples $D* = (x_m, y_m), m \in \mathcal{N}$ approximating the interventional distribution $f(x|do(y))$.

1. Using $D$, find empirical KDEs $\hat{f}(v|P(v))$, for all $v \in E$, and the joint KDE $\hat{f}(P(x))$.
2. For each $n \in \mathcal{N}$:
3. Produce new sample $D* = (x_i, y_n)$, where index $i$ is selected from $\mathcal{N}$ with weights $w_i$ given by:

$$w_i = \frac{1}{N} \times \begin{cases} K[y_i - y_n] \bar{w}_i & \text{if } y \in P(x) \\ \bar{w}_i & \text{otherwise} \end{cases}$$

$$\bar{w}_i = \left| \prod_{v \in E} \hat{f}(v|P(v)) \right|_{y \in U : u = u_i}$$

where $K[\cdot] = 1[\cdot]$ for discrete prediction target $Y$, or another suitable kernel otherwise.

3 Experiments and results

Next, we run several numerical experiments to demonstrate the application of the above algorithms in practice. For full details of these experiments, see Appendix B: Details of experiments.

3.1 Synthetic Gaussian mixtures

In this section, we demonstrate a simple, confounded model involving bivariate Gaussian features and discrete targets, confounder and mediator (Figure 3). We apply back-door (Algorithm 1) and (when there is a mediator) front-door causal bootstrapping in order deconfound the data. Trained on the deconfounded data, a simple linear discriminant (LDA) classifier achieves typical accuracies of 85-95% on both confounded and deconfounded data (Table 1). This easily outperforms LDA trained on the original, confounded data and tested on the deconfounded data where reaches at best 73% (back-door) and collapses to chance accuracy in the front-door case. Figure 3 gives us an intuitive explanation for how causal bootstrapping works in these cases: it changes the density of samples in feature space such that the confounded boundary is dominated by the desired target boundary instead.
Figure 3: Synthetic example illustrating causal bootstrapping for classification. Left: bivariate Gaussian feature data \( X \) depends upon both the discrete confounder \( U \), and the discrete classification target (red versus black points) \( Y \). The target \( Y \) also depends upon the confounder. In this situation, the ideal boundary to correctly classify on the basis of the target is vertical, whereas, the confounded boundary is horizontal. The black line is the boundary which would be determined using linear discriminant analysis (LDA).

Right: data after applying back-door or front-door causal bootstrapping. The resampling causes the LDA boundary to almost entirely coincide with the correct classification target \( Y \) boundary.

Table 1: Accuracy of classifiers (linear discriminant analysis, LDA, and random forests, RF) applied to both confounded sample data, and sample data deconfounded using back-door and front-door causal bootstrapping (Algorithms 1-2). Classes are balanced so that chance predictions have 50% accuracy. Data samples 1 & 2 are confounded, whereas data sample 3 is non-confounded. When making predictions for non-confounded data, classifiers trained on deconfounded data clearly outperform classifiers trained on the original, confounded data (bold figures). By contrast, training on the original, confounded data produces classifiers which perform very poorly on non-confounded data, often no better than chance. However, training and testing on confounded data shows high test classification accuracy, giving a misleading indication of performance in practice where the data is not confounded.
3.2 Semi-synthetic “background-MNIST”

In these examples, we simulate measured (back-door) or unmeasured/unknown (front-door) confounding in an image recognition problem. Here, a set of MNIST digits are modified such that the brightness is altered depending upon the digit. The task is to recognize the digit. More specifically, the brightness is altered in a way which depends upon the digit label. This makes the brightness a strong confounder, and this clear signal is likely to be exploited by any predictor instead of actually detecting the configuration of pixels in the image (Figure 1). The setup is similar to the situation in medical imaging which sometimes occurs, where the settings of the imaging machine are inadvertently linked to the disease category which is to be classified [Zech et al., 2018]. A random forest (RF) classifier trained on the causal bootstrapped data performs well across both confounded and non-confounded data, whereas the same classifier trained on the original, confounded training data performs well on the confounded test data, but on the non-confounded data it collapses down to nearly chance performance (Table 1).

3.3 Real-world data: Parkinson’s voice

In this final example, we test back-door causal bootstrapping on real-world experimental data captured from individuals with Parkinson’s disease (PD). The experimental goal is to detect, from digital voice recordings, whether the individual has been diagnosed with PD or not. Nine voice features are extracted from the recordings, which are then input to a classifier. Three separate experiments have been conducted under varying conditions (different labs in different countries, speakers of different languages, slightly different age and sex grouping). In order to improve statistical estimation, the aim is to merge the data from the experiments together. However, the differences in experimental conditions mean that the distribution of the features differ. At the same time, there is an imbalance in the number of recordings collected from each experiment. Combined, these cause confounding meaning that a classifier may get a spurious advantage from detecting the experimental setup rather than PD/healthy status. This is a significant problem with voice-based disease characterization [Little et al., 2017].

Indeed, we find that an RF classifier trained on the confounded data, whilst performing well on an independent, confounded test set, performs significantly worse than an RF classifier trained on the same data deconfounded using back-door causal bootstrapping (Table 1). However, the performance of the classifier on the confounded data is much higher, strong evidence that the classifier relies heavily on the confounding signal in order to make classification decisions.

4 Related work

Causal modelling analysis is well established across certain disciplines, but the introduction of causal graphical models with probabilistic foundations led to defining causal phenomena such as interventions, confounding, collider and mediation variables in one unified framework [Pearl, 2009]. The awareness that (supervised) machine learning algorithms are prone to spurious confounding, and what to do about it, has a relatively long history, but it is only recently that rigorous solutions are being proposed, see Kaufman et al. [2012]. More recently, Zech et al. [2018], Voets et al. [2019] examine confounding in the context of deep learning for high-dimensional predictors. Little et al. [2017] discussed proposals for identification of confounding involving cross-validation stratified on the confounding variable. Similarly, to detect confounding, Neto [2018] suggested the use of stratified permutation testing and Ferrari et al. [2019] use train/test sets stratified on both prediction target and confounder. These studies do not detail a method for constructing deconfounded predictors and are restricted to the problem of classification under a single measured confounding variable (see Figure 2a).

The problem has only very recently started to be expressed in explicitly causal terms. Use of the back-door adjustment formula with explicit probabilistic prediction models has been proposed in Landeiro and Culotta [2016] and Landeiro and Culotta [2017]. These methods require an explicit
probabilistic model for the predictor and so do not apply to all supervised machine learning algorithms. Perhaps closest to this work, Chyzhyk et al. [2018] propose importance sampling to create deconfounded data from observational data. However, this does not guarantee that the marginal distributions of the confounder and target variables are retained which is problematic because a predictor can be sensitive to these marginals. Furthermore, it can only create test sets which are a subset of the training data. It is restricted to the situation with a single measured confounder as in Figure 2a.

Related methods for constructing interventional predictors are now being explored in the machine learning community. For example, Kallus et al. [2018] investigate the special situation where a small, interventional sample is available which overlaps with a larger observational study, where the overlap contains sufficient information to construct an interventional predictor. The approach is not fully nonparametric, relying on a parametric correction of an predictor constructed from the observational data. A broader approach invokes causal stability [Pearl, 2009], that is, constructing predictors which only exploit information that does not, or is not expected to, change across different observational settings. For example, invariant causal prediction methods combine data from multiple interventional samples; using this they select, or more generally find a representation of, the variables that are parents of the prediction target [Peters et al., 2016, Arjovsky et al., 2019] to construct a predictor which is invariant across differing experimental or observational settings. These methods rely upon the existence of multiple datasets collected under different settings. By contrast, if information about which parts of the causal graph may change is available, Subbaswamy et al. [2019] present an algorithm for identifying a stable interventional distribution (if one can be found).

5 Discussion and conclusions

In this paper we have shown how, given a structural causal model and observational data from that model, it is possible to derive simple algorithms to draw bootstrap samples from that data which are consistent with a desired interventional distribution. We have developed several algorithms for supervised machine learning, which may be of general usefulness, including those based on closing back-door confounding paths, unmeasured and unknown confoundings satisfying the front-door criterion, and more generally, an algorithm for any given interventional distribution. Through empirical experiments, we have demonstrated that effective interventional predictors can be trained using this technique that do not merely make associational predictions. At the same time, these results highlight the striking negative impact of failure to take confounding properly into account in supervised machine learning.

There are certain limitations to this approach. In particular, we need to know the causal graphical model for the observational data. This can be difficult for situations where there is significant ambiguity. However, in many situations we do not need to know all the causal relationships, and large parts of the graph may be unknown. Consider for instance front-door deconfounding: provided the criteria hold, we do not need to know about, or measure, all the variables on the back-door causal paths which are intercepted by the target \(Y\). This makes front-door causal bootstrapping fairly generic as a deconfounding tool. It may also be possible to use structural discovery algorithms and hence recover an estimate of the causal model for the observational data [Chickering, 2002].

Another problem with this approach is where the distribution of a variable needs to be estimated yet it is high-dimensional, for example the distribution \( \hat{f}(y|S) \) in Algorithm 1. Although we have suggested using KDEs, these estimates can be unreliable when there is a paucity of data available. However, we note that the causal bootstrap algorithms proposed here do not stipulate the form of these distribution estimates, and parametric estimates may be more reliable, particularly if additional information about these variables is available.

Bootstrapping necessarily involves producing repeated observations of the effect variable \(X\). In some applications this is problematic. For example, given an observational sample, we may want to test the performance of a causal predictor by bootstrapping multiple interventional samples from that original data. However, these multiple samples will share individual observations with the original data, this will introduce an optimistic bias into the performance estimates, which is particularly problematic for
modern complex predictors such as deep learning that can memorize individual observations [Belkin et al., 2018]. One solution to this is to use bootstrap bias correction methods [Hastie et al., 2009, Section 7.11]. An alternative is to use split-sample approaches for example, mimicking cross-validation, whereby the original observational sample is bootstrapped once and the bootstrap is split into multiple subsamples. The predictor is trained and tested on non-overlapping subsamples of the bootstrap such that no observations are shared between train and test.

Although we have generally emphasised the use of the Dirac delta function for the effect variable $X$ in the causal bootstrap algorithms, a different direction is to use a kernel other than the delta function. This naturally leads to the causal analogue of *smoothed bootstrapping* [Silverman and Young, 1987]. One advantage of such smoothed bootstraps is that all causal bootstraps consist of genuinely unique observations (assuming $X$ is continuous) not shared with the original observational sample. This will mitigate the above problem of observation memorization for out-of-sample performance testing. However, it is often the case that $X$ will be high-dimensional so that the smoothed bootstraps may deviate quite substantially from the underlying (and unknown) distribution of $X$, if the observational sample is not sufficiently large.

Finally, we note that the RKHS-based KDE for the joint distribution of $X$ and its parents, utilizing the reproducing property to derive the bootstrap weights, is not the only RKHS-based estimator. For example, we can also use semi-parametric RKHS *finite or infinite mixture models* [Little, 2019] which may be preferable in certain situations, for example when the data is naturally clustered and the size of observational data is too small to guarantee reliable bootstrap samples. We leave the derivation of the corresponding causal bootstrap algorithms for future work.

References

M. Arjovsky, L. Bottou, I. Gulrajani, and D. Lopez-Paz. Invariant Risk Minimization. *arXiv:1907.02893 [cs, stat]*, July 2019. URL http://arxiv.org/abs/1907.02893.

M. Belkin, D. Hsu, S. Ma, and S. Mandal. Reconciling modern machine learning practice and the bias-variance trade-off. *arXiv:1812.11118 [cs, stat]*, December 2018. URL http://arxiv.org/abs/1812.11118.

A. Berlinet and C. Thomas-Agnan. *Reproducing Kernel Hilbert Spaces in Probability and Statistics*. Springer Science & Business Media, June 2011.

D.M. Chickering. Optimal Structure Identification With Greedy Search. *Journal of Machine Learning Research*, 3(Nov):507–554, 2002.

D. Chyzhyk, G. Varoquaux, B. Thirion, and M. Milham. Controlling a confound in predictive models with a test set minimizing its effect. In *2018 International Workshop on Pattern Recognition in Neuroimaging (PRNI)*, Singapore, 2018. IEEE.

B. Efron and R. J. Tibshirani. *An Introduction to the Bootstrap*. CRC Press, May 1994.

E. Ferrari, A. Retico, and D. Bacciu. Measuring the effects of confounders in medical supervised classification problems: the Confounding Index (CI). *arXiv:1905.08871 [cs, stat]*, May 2019. URL http://arxiv.org/abs/1905.08871.

T. Hastie, R. J. Tibshirani, and J. Friedman. *The Elements of Statistical Learning*. Springer, New York, NY, 2nd ed. 2009 edition, October 2009.

N. Kallus, A.M. Puli, and U. Shalit. Removing hidden confounding by experimental grounding. In *NIPS’18 Proceedings of the 32nd International Conference on Neural Information Processing Systems*, Montreal, Canada, 2018.
Appendix A: Proofs

Bootstrap weights for interventional distributions

Here we prove that the causal bootstrapping weights in (4) from an interventional distribution where the set of unwanted (secondary) effect variables \( \mathcal{E} = \mathcal{P}(x) \setminus y \), are given by (7)-(8). Starting with the interventional distribution and expanding out the conditional \( f(x|\mathcal{P}(x)) \):

\[
f(x|\text{do}(y)) = \int f(x, \mathcal{P}(x)) \frac{\prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))}{f(\mathcal{P}(x))} d\mathcal{E}
\]

(18)

We now replace \( f(x, \mathcal{P}(x)) \) with the RKHS KDE:

\[
f(x, \mathcal{P}(x)) \approx \frac{1}{N} \sum_{n \in N} K[x - x_n] \prod_{u \in \mathcal{P}(x)} K[u - u_n]
\]

(19)

Inserting this into (18), and since \( x \notin \mathcal{E} \), we can factorize the multiple integral:

\[
f(x|\text{do}(y)) \approx \frac{1}{N} \sum_{n \in N} K[x - x_n] \int \prod_{u \in \mathcal{P}(x)} K[u - u_n] \frac{\prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))}{f(\mathcal{P}(x))} d\mathcal{E}
\]

(20)

such that the weights (7) are given by:

\[
w_n = \frac{1}{N} \int \prod_{u \in \mathcal{P}(x)} K[u - u_n] \frac{\prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))}{f(\mathcal{P}(x))} d\mathcal{E}
\]

(21)

Now, picking one \( u' \in \mathcal{E} \), the integral above can be further factorized:

\[
\int \prod_{u \in \mathcal{P}(x) \setminus u} K[u - u_n] \int K[u' - u'_n] \frac{\prod_{v \in \mathcal{E}} f(v|\mathcal{P}(v))}{f(\mathcal{P}(x))} du'd(\mathcal{E} \setminus u')
\]

(22)

and evaluating the inner integral using the reproducing property we get:
Here we derive the back-door weighted KDE (12) using (7)-(8). Here $\mathcal{E} = \{S\}$, the interventional parents are $\mathcal{P}(\mathbf{x}) = \{y, S\}$ (so $y \in \mathcal{P}(\mathbf{x})$), and $\mathcal{P}(\mathcal{S}) = \emptyset$, giving $w_n = N^{-1}K[y - y_n] \bar{w}_n$ with:

$$\bar{w}_n = \frac{\hat{f}(S_n)}{\hat{f}(y, S_n)} = \frac{1}{\hat{f}(y|S_n)}$$

and substituting these $w_n$ into (4) gives (12).

Similarly, for the front-door formula (14), we have $\mathcal{E} = \{y', z\}$, interventional distribution parents $\mathcal{P}(\mathbf{x}) = \{y', z\}$ (so $y \notin \mathcal{P}(\mathbf{x})$), $\mathcal{P}(y') = \emptyset$, $\mathcal{P}(z) = \{y\}$, leading to:

$$w_n = \frac{\hat{f}(y_n) \hat{f}(z_n|y_n)}{N \hat{f}(y_n, z_n)} = \frac{\hat{f}(z_n|y_n)}{N \hat{f}(z_n|y_n)}$$

and substituting these $w_n$ into (4) gives (14).

Finally, we prove the form of the weights (10) for the interventional distribution given in Tikka and Karvanen [2017]. Here, $\mathcal{E} = \{y', z, w\}$, with interventional parents $\mathcal{P}(\mathbf{x}) = \{w, y', z\}$ (implying that $y \notin \mathcal{P}(\mathbf{x})$), $\mathcal{P}(y') = \{w\}$, $\mathcal{P}(z) = \{w, y\}$ and $\mathcal{P}(w) = \emptyset$ giving:

$$w_n = \frac{\hat{f}(y_n|w_n) \hat{f}(z_n|w_n, y_n) \hat{f}(w_n)}{N \hat{f}(w_n, y_n, z_n)} = \frac{\hat{f}(z_n|w_n, y_n)}{N \hat{f}(z_n|w_n, y_n)}$$

### Appendix B: Details of experiments

Each sample is indexed by the environment or sample variable $e \in \{1, 2, 3\}$. All prediction estimates are replicated over 10 runs, obtained by either synthesising entirely new data, or randomly permuting the observations before splitting into distinct samples. MATLAB code which implements these experiments is available on request from the authors.

### Synthetic Gaussian mixtures

The target and mediator variables take on values $\Omega_Y, \Omega_Z, \Omega_U = \{1, 2\}$. The model is:

\[
\begin{align*}
U & \sim \text{Bernoulli} (p) \\
Y|U & \sim \text{Bernoulli} (q_e (u)) \\
Z|Y & \sim \text{Bernoulli} (r (y)) \\
X_1|Z, U & \sim \mathcal{N} (\mu_1 (z), \sigma = 1) \\
X_2|Z, U & \sim \mathcal{N} (\mu_2 (u), \sigma = 1)
\end{align*}
\]
The parameters depend upon the sample and whether the model is back-door or front-door. For back-door, we set $p = 0.85$. The parameter $q_e(1) = 0.95$ and $q_e(2) = 0.05$ for $e = 1, 2$, and we set $q_3(u) = 0.5$ (thus making the target independent of the confounder for sample 3). The mediator plays no role in this model and so $r(1) = 1$ and $r(2) = 0$. The feature parameters are $\mu_1(1) = 1.5$ and $\mu_1(2) = -1.5$, and $\mu_2(1) = 2.4$ and $\mu_2(2) = -2.4$.

For front-door confounding, we have $p = 0.5$, for $e = 1, 2$ we set $q_e(1) = 0.98$ and $q_e(2) = 0.02$, and $q_3(u) = 0.5$ (non-confounded sample). The mediator has conditional parameter $r(1) = 0.90$ and $r(2) = 0.10$. The feature parameters are the same as for the back-door case.

**Background-MNIST data**

In this example, we embed and modify the 28 by 28 pixel digit image data from the MNIST dataset [LeCun, 2019] inside a back-door or front-door causal graph. We use the 2,000 test images for digits ‘2’ and ‘6’. For convenience, the back-door samples are generated using the following model (note that we can always find the equivalent conditional $Y|U$ using Bayes’):

\[
\begin{align*}
U|Y & \sim \text{Bernoulli}(q_e(y)) \\
Y & \sim \text{Bernoulli}(p) \\
X|Y,U & \sim \text{MNIST}(y,u)
\end{align*}
\]

(28)

where $p = 0.5$, and $q_e(1) = 0.95$, $q_e(2) = 0.05$ and $q_3(y) = 0.5$ (non-confounded sample 3). Here, $\text{MNIST}(y,u)$ is a random function which retrieves a unique MNIST image $x$ representing digit ‘2’ for $y = 1$ and digit ‘6’ for $y = 2$. The brightness of the image data is then modified by converting $x \mapsto \min(x + b(u), 255)$ where $b(u)$ is a 28 by 28 image of pixels all with the same value 100 if $u = 1$, and value 0 otherwise.

For the front-door case, the model is:

\[
\begin{align*}
U & \sim \mathcal{N}(0, 5) \\
Y|U & \sim \text{Bernoulli}(q_e(u)) \\
Z|Y & \sim \text{Bernoulli}(r(y)) \\
X|Z,U & \sim \text{MNIST}(z,u)
\end{align*}
\]

(29)

Here, the Bernoulli parameter for $Y$ depends upon the confounder in the following way:

\[
q_e(u) = \frac{q^u}{q^u + (1 - q)^u}
\]

where $q = 0.8$ for $e = 1, 2$ and $q = 0.5$ for $e = 3$ (making the target independent of the confounder for sample 3). The mediator parameter is $r(1) = 0.95$ and $r(2) = 0.05$. As above, $\text{MNIST}(z,u)$ is a random function which retrieves a unique MNIST image $x$ representing digit ‘2’ for $z = 1$ and digit ‘6’ for $z = 2$. Then, the brightness of the image data is modified by converting $x \mapsto \min(x + b(u), 255)$ where $b(u)$ is a 28 by 28 image of pixels all with values:

\[
v(u) = 100 \times \left(\frac{1}{2} \arctan\left(\frac{1}{5} u\right) + \frac{1}{2}\right)
\]

which maps the continuous confounder values onto the scaled background brightness values in the range $[0, 100]$.

**Parkinson’s voice data**

This dataset is based on features extracted from the sustained phonations of three sets of patients with Parkinson’s disease and healthy controls, recorded in separate labs based in the US [Little, 2008],
Turkey [Sakar, 2018] and Spain [Naranjo et al., 2019]. For further details of how these samples were recorded, see references therein. Features which are common across all three datasets are extracted, to give a feature dataset \( \mathbf{X} \) of \( 9 \times 1191 \), along with a target class from \( \Omega_Y = \{1, 2\} \) for each, representing healthy control versus Parkinson’s. The goal is to predict whether any single observation is from an individual with or without Parkinson’s.

The confounder \( U \) takes values in \( \Omega_U = \{1, 2, 3\} \) denoting the dataset. For illustrative purposes, for the confounded environment samples 1 & 2, the effect of different labs, patient populations and experimental protocols is enhanced by resampling with replacement from the combined dataset to ensure that the confounding across datasets, conditioned on the target variable, is in the proportion 5%, 5%, 90% for \( Y = 1 \) and 90%, 5%, 5% for \( Y = 2 \), whilst simultaneously ensuring that the target variable is balanced across classes. For sample 3, the proportion of data from each dataset is 47.5%, 5%, 47.5% independent of \( Y \) (so that sample 3 is non-confounded).