

Meta-learners for Estimating Heterogeneous Treatment Effects using Machine Learning*

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Abstract

There is growing interest in estimating and analyzing heterogeneous treatment effects in experimental and observational studies. We describe a number of meta-algorithms that can take advantage of any machine learning or regression method to estimate the conditional average treatment effect (CATE) function. Meta-algorithms build on base algorithms—such as OLS, the Nadaraya-Watson estimator, Random Forests (RF), Bayesian Average Regression Trees (BART) or neural networks—to estimate the CATE, a function that the base algorithms are not designed to estimate directly. We introduce a new meta-algorithm, the X-learner, that is provably efficient when the number of units in one treatment group is much larger than another, and it can exploit structural properties of the CATE function. For example, if the CATE function is parametrically linear and the response functions in treatment and control are Lipschitz continuous, the X-learner can still achieve the parametric rate under regularity conditions. We then introduce versions of the X-learner that use RF and BART as base learners. In our extensive simulation studies, the X-learner performs favorably, although none of the meta-learners is uniformly the best. We also analyze two real data applications, and provide a software package that implements our methods.

Keywords— Causal Inference | Random Forests | Minimax Optimality

1 Introduction

Machine learning (ML), as a frontier field of both Statistics and Computer Science, has been making great strides in recent years, and statistical causal inference methods are having ever greater impact in many fields including the social sciences, medicine, and the IT industry. The power of ML methods is clear: prediction competitions are typically won by ML algorithms. Causal inference problems, however, are not simply prediction problems because treatment effects are never directly observed. We cannot simply tag observations with observed and validated treatment effects. Therefore, the use of ML methods for causal inference problems is not straightforward, and causal effects must always be estimated under some assumptions.

In this paper we focus on meta-algorithms for estimating Conditional Average Treatment Effects (CATE). Meta-algorithms build on base algorithms—such as OLS,

*Software that implements our methods is available at <https://github.com/soerenkuenzel/hte>.

Random Forests (RF), Bayesian Additive Regression Trees (BART) or neural networks—to estimate functions that the base algorithms are not designed to estimate directly. Researchers have long noted that under the assumption of strong ignorability, treatment effect estimation reduces to response surface estimation. This leads to a number of meta-learners.

The most common meta-algorithm for estimating heterogeneous treatment effects involves estimating the outcomes under control and treatment separately and then taking the difference of these estimates. This has been done using linear regression (e.g., Foster, 2013) and also tree-based approaches (e.g., Athey and Imbens, 2015). When used with trees, this has been called the *Two-Tree* estimator because it builds two separate trees: one tree to estimate the treated outcomes and a second tree to estimate the control outcomes. The CATE estimator is defined to be the difference between the two trees. We will refer to the general idea of estimating the response functions separately as *T-learner*. A similar algorithm is often used with OLS to perform covariate adjustment in randomized experiments to obtain variance gains. For example, Tsiatis et al. (2008) proposed a semi-parametric method where the researcher independently models the response curve for the treatment group and the control group and then adjusts the estimated average treatment effect with a function of these two curves.

Closely related to the T-learner is the idea of doing response modeling as usual in the regression problem but to include the treatment indicator as a covariate. The predicted CATE for an individual unit is the difference between the predicted values when the treatment assignment variable is changed from control to treatment, but all other features are held fixed. This meta-algorithm is used by Hill (2011) and Green and Kern (2012) with BART as the base learner, and it has been studied for regression trees by Athey and Imbens (2015), where it was called *Single Tree* because only one regression tree is constructed. We refer to this meta-algorithm as *S-learner*.¹

Recently, progress has been made using other machine learning algorithms for estimating heterogeneous treatment effects. For example, Athey and Imbens (2016, 2015) develop Classification and Regression Trees (CART) for CATE estimation, and Wager and Athey (2015) provide asymptotically valid inference methods for causal forests—a variant of Random Forests that is particularly amenable to theoretical analysis because it uses honesty (Biau, 2012; Biau and Scornet, 2015).

Our main contribution is the introduction of a new meta-algorithm, which we call *X-learner*, that builds on the T-learner. Suppose we could observe the individual treatment effects directly. This would make the estimation of the CATE simple: we could estimate the CATE function by regressing the vector of individual treatment effects on covariates. Moreover, if we knew that the CATE function had some properties such as linearity or sparsity, we would be able to use an estimator that could exploit or learn them. Of course, we do not observe individual treatment effects because we only observe the outcome under control or treatment, but never both. The X-learner approximates the individuals treatment effects by using a weighted average of two different estimators of outcomes (one for treated and one for control), and it then estimates the CATE function in a second step. We prove that the X-learner is efficient when the number of units in one treatment group is much larger than in the other, and that it can exploit structural properties of the CATE function. That is, if the CATE function is linear, but the response functions in treatment and control only satisfy that they are Lipschitz continuous, the X-learner can still achieve the parametric rate if one of the treatment groups is much larger than the other.

With the rise of big data, it is often the case that one has many more observations for one of the treatment groups, usually the control group. This occurs because (con-

¹Note that in the case of linear models like OLS, there is no clear distinction between the T and S learners. For example, one may estimate the linear model with a full set of interactions between the covariates and the treatment indicator in one step (Lin, 2013).

trol) outcomes and covariates are easy to obtain using data collected by administrative agencies, electronic medical record systems or on-line platforms in routine practice. This is the case with our first data application where election turnout decisions in the U.S. are recorded by local election administrators for all registered individuals. The X-learner can exploit the extra information that is available.

In order to study the finite sample properties of the X-learner, we produce an implementation that uses honest Random Forests as the base learner and another one that uses BART. In our simulations, although none of the meta-learners is uniformly the best, the X-learner performs favorably. We also show that the choice of base learner matters for performance.

In Section 2, we formally introduce the meta-learners we discuss. We also provide some intuition for why we can expect the X-learner to perform well when the CATE is smoother than the response functions and when the sample sizes between treatment and control are unequal. In Section 3, we provide convergence rate results for the X-learner. We conduct a simulation study in which we compare the meta-algorithms (Section 4), and we examine two data applications (Section 5).

1.1 A framework for estimating the CATE

We employ the Neyman-Rubin potential outcomes framework (Rubin, 1974; Splawa-Neyman et al., 1990), and assume a super population or distribution \mathcal{P} from which a realizations of N independent random variables are given as the training data: $(Y_i(0), Y_i(1), X_i, W_i) \sim \mathcal{P}$, where $X_i \in \mathbb{R}^d$ is a d dimensional covariate or feature vector, $W_i \in \{0, 1\}$ is the treatment assignment indicator (to be defined precisely later), $Y_i(0) \in \mathbb{R}$ is the potential outcome of unit i when i was assigned to the control group, and $Y_i(1)$ is the potential outcome when i was assigned to the treatment group. It is useful to define the response under control, μ_0 , and the response under treatment, μ_1 , as

$$\mu_0(x) := \mathbb{E}[Y(0)|X = x] \quad \text{and} \quad \mu_1(x) := \mathbb{E}[Y(1)|X = x].$$

With this notation, we can characterize \mathcal{P} as

$$\begin{aligned} X &\sim \lambda, \\ W &\sim \text{Bern}(e(X)), \\ Y(1) &= \mu_1(X) + \varepsilon(0), \\ Y(0) &= \mu_0(X) + \varepsilon(1), \end{aligned} \tag{1}$$

where λ is the marginal distribution of X , $\varepsilon(0)$ and $\varepsilon(1)$ are noise terms with mean zero conditioning on X , and $e(x) = \mathbb{P}(W = 1|X = x)$ is the propensity score.

The fundamental problem of causal inference is that for each unit in the training dataset we either observe the potential outcome under control ($W_i = 0$) or the potential outcome under treatment ($W_i = 1$) but never both and we, therefore, denote the observed data as:

$$\mathcal{D} = (Y_i^{obs}, X_i, W_i)_{1 \leq i \leq N},$$

with $Y_i^{obs} = Y_i(W_i)$. Note that the distribution of \mathcal{D} is implicitly specified by \mathcal{P} .

To decide for a new unit i with covariate vector given by x_i whether to give her the treatment, we want to estimate the Individual Treatment Effect (ITE) of unit i , D_i , which is defined as

$$D_i := Y_i(1) - Y_i(0).$$

However, we do not observe D_i for any unit, and even worse, D_i is not identifiable, in that one can construct two data generating processes (DGP) such that the observed data has the same distribution for both DGPs, but the D_i are different across the DGPs (cf. Example B.1). Instead, we will estimate the CATE function which is defined as

$$\tau(x) := \mathbb{E}[D|X = x] = \mathbb{E}[Y(1) - Y(0)|X = x],$$

and we note that the best estimator for the CATE is also the best estimator for the ITE. To see that, let $\hat{\tau}_i$ be an estimator for D_i and decompose the MSE at x_i as

$$\begin{aligned} & \mathbb{E}[(D_i - \hat{\tau}_i)^2 | X_i = x_i] \\ &= \mathbb{E}[(D_i - \tau(x_i) + \tau(x_i) - \hat{\tau}_i)^2 | X_i = x_i] \\ &= \mathbb{E}[(D_i - \tau(x_i))^2 | X_i = x_i] + \mathbb{E}[(\tau(x_i) - \hat{\tau}_i)^2]. \end{aligned} \quad (2)$$

Since we cannot influence the first term in the last expression, the estimator which minimizes the MSE for the ITE of i also minimizes the MSE for the CATE at x_i .

In this paper, we are interested in estimators which have a small expected mean squared error (EMSE),

$$\text{EMSE}(\mathcal{P}) = \mathbb{E}[(\tau(\mathcal{X}) - \hat{\tau}(\mathcal{X}))^2].$$

Here the expectation is taken over both the distribution of $\hat{\tau}$ and \mathcal{X} .

To aid our ability to estimate τ , we need to assume that there are no hidden confounders, and we therefore follow Rosenbaum and Rubin (1983) by assuming ignorability:

$$(\varepsilon(0), \varepsilon(1)) \perp W | X.$$

This assumption is necessary for the CATE to be identifiable, but it is not sufficient. For our theoretical results in Section 3, we will assume that the CATE function and the response functions are in some class of functions that can be estimated at a particular rate. Note that under those assumptions, we do not need the *strong* ignorability assumption.

2 Meta-Algorithms

In this section, we formally define a meta-algorithm for the CATE as the result of combining supervised learning or regression estimators in a specific way while allowing the supervised or regression estimators (or components of the meta-algorithm) to take on many forms. Meta-algorithms thus have the flexibility to appropriately leverage different sources of prior information in different decomposed parts of the CATE estimation problem.

We review both T and S learners. We then propose our new X-learner that can take advantage of the fact that often m (the size of the control group) is much larger than n (the size of the treatment group); it can also take advantage of a different (say, simpler) structure form of the CATE function $\tau(x)$ from those of $\mu_0(x)$ and $\mu_1(x)$. Obviously, flexibility is a gain only if the components in the meta-algorithm match well prior information for these components; otherwise, flexibility could lead to bias and/or large variance of the meta-algorithm.

Let us now review the two-step T-learner. In the first step, the control response function,

$$\mu_0(x) = \mathbb{E}[Y(0) | X = x],$$

is estimated by any supervised learning or regression estimator using the observations in the control group, $\{(X_i^0, Y_i^0)\}_{i=1}^{n_0}$, and we denote the estimated function $\hat{\mu}_0$. In the second step, we estimate the treatment response function,

$$\mu_1(x) = \mathbb{E}[Y(1) | X = x],$$

with potentially a different estimator using observed treated observations, and we denote the estimator as $\hat{\mu}_1$. Then a T-learner CATE estimator can be obtained as

$$\hat{\tau}^T(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x). \quad (3)$$

Pseudo code for this procedure can be found in the Appendix A as Algorithm 1 in Appendix A.

In the S-learner, the treatment indicator is included as a feature like all of the other features without the indicator being given any special role. We thus estimate the combined response function,

$$\mu(x, w) := \mathbb{E}[Y^{obs}|X = x, W = w],$$

using any ML algorithm on the entire data set, and we denote the estimator as $\hat{\mu}$. The CATE estimator is then given by

$$\hat{\tau}^S(x) = \hat{\mu}(x, 1) - \hat{\mu}(x, 0). \quad (4)$$

Pseudo code is provided as Algorithm 2 in the appendix.

Other meta-algorithms exist in the literature, which we do not discuss in detail. For example, one may transform the outcomes so any regression method can estimate CATE directly using Algorithm 4 reported in Appendix A. Athey and Imbens (2015) and Tian et al. (2014), among others, discuss this approach.² In our simulations, the algorithm performs poorly, and we do not discuss it further, but it may do well in other settings.

2.1 X-learner

In this section, we propose the X-learner and provide an illustrative example to highlight the motivations behind it. “X” appears in the name because it crosses the residuals like an “X” as seen below. The basic idea of the X-learner can be described in three steps:

1. Estimate the response functions

$$\mu_0(x) = \mathbb{E}[Y(0)|X = x], \text{ and} \quad (5)$$

$$\mu_1(x) = \mathbb{E}[Y(1)|X = x], \quad (6)$$

using any machine learning algorithm and denote the estimated functions $\hat{\mu}_0$ and $\hat{\mu}_1$. We call this the first stage, and the algorithms used are referred to as the base learners for the first stage. This stage is the same as the first stage in the T-learner.

2. Compute the residuals (or impute the treatment effects) for the individuals in the treated group based on the control outcome estimator, and the residuals (or imputed treatment effects) for individuals in the control group based on the treatment outcome estimator, that is:

$$\tilde{D}_i^1 := Y_i^1 - \hat{\mu}_0(X_i^1), \text{ and} \quad (7)$$

$$\tilde{D}_i^0 := \hat{\mu}_1(X_i^0) - Y_i^0, \quad (8)$$

and call these the pseudo residuals (or imputed treatment effects). Use any desired supervised or regression method(s) to estimate $\tau(x)$ in two ways: using the imputed \tilde{D} 's as the response variable in the treatment group to obtain $\hat{\tau}_1(x)$, and similarly to obtain $\hat{\tau}_0(x)$ for the control group.

Call $\hat{\tau}_1(x)$ and $\hat{\tau}_0(x)$ base learners of the second stage.

3. Define the CATE estimate by a weighted average of the two estimates in stage 2:

$$\hat{\tau}(x) = g(x)\hat{\tau}_0(x) + (1 - g(x))\hat{\tau}_1(x) \quad (9)$$

where $g \in [0, 1]$ is a weight function.

²This transform approach was first proposed in the Ph.D. thesis of James Sinovitch, Harvard University.

See Algorithm 3 in Appendix A for pseudo code.

Remark 1 $\hat{\tau}_0$ and $\hat{\tau}_1$ are both estimators for τ and g is chosen to combine those two estimators to one improved estimator $\hat{\tau}$. Some good choices of g involve choosing g to be an estimator of the propensity score, $g = \hat{e}$, but it can also make sense to choose $g = 1$ or 0 , if the number of treated units is very large or small compared to the number of control units. For some estimators it might even be possible to compute the variance of $\hat{\tau}_1$ and $\hat{\tau}_0$ and one could then choose g to minimize the variance of $\hat{\tau}$.

2.2 How do the meta-learners compare?

The X -learner can use information from the control group to derive better models for the treatment group and vice versa. We will illustrate this using a simple example. Suppose we wanted to study a treatment, and we are interesting in estimating the CATE as a function of one covariate, x . We observe, however, very few treated units and many units in the control group. This situation often arises with the growth of administrative and on-line data sources: data on control units is often far more plentiful than for treated units.

Figure 1 (a) shows the outcome for the patients in the treatment group (circles) and the outcome of the untreated (crosses). In this example, the CATE is constant and equal to one. For the moment, only look at the treated outcome. When we try to find a good model to estimate $\mu_1(x) = \mathbb{E}[Y(1)|X = x]$, we must be careful not to overfit the data since we only observe 10 data points. We might decide to use a linear model, $\hat{\mu}_1(x)$ (dashed line), to estimate μ_1 . For the untreated group, we notice that patients with $x \in [0, 0.5]$ seem to behave very differently, and we end up modeling $\mu_0(x) = \mathbb{E}[Y(0)|X = x]$ with a piecewise linear function with jumps at 0 and 0.5 (solid line). This is a relatively complex function, but we don't fear that we are overfitting since we observe many data points.

The T -learner would now estimate $\hat{\tau}_T(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x)$, Figure 1 (c). This is a rather complicated function, which has jumps at 0 and 0.5 and that is a problem since we chose such a complex function based on only ten observations in the treated group. When choosing a model for the treatment group, we correctly avoided overfitting, and we found a good estimator for the treatment response function, but by doing so, we chose a complex model for the CATE—the quantity we are interested in. What we should have done is to select a piecewise linear function with jumps at 0 and 0.5. This is, of course, unreasonable when just looking at the treated group, but when looking at the outcomes of the controls, this seems to be a natural choice. In other words, we should change our objective for $\hat{\mu}_1$ and $\hat{\mu}_0$. We don't want to choose simple function, but we want to choose functions whose difference is simple.

The X -learner enables us to do exactly that. In the second stage, the model of the controls is subtracted from the observed treated outcomes:

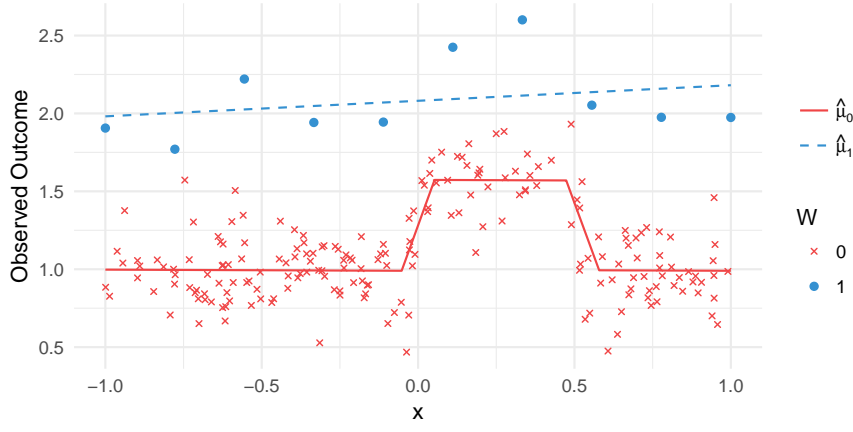
$$\tilde{D}_i^1 := Y_i^1 - \hat{\mu}_0(X_i^1) \quad (10)$$

$$\tilde{D}_i^0 := \hat{\mu}_1(X_i^0) - Y_i^0. \quad (11)$$

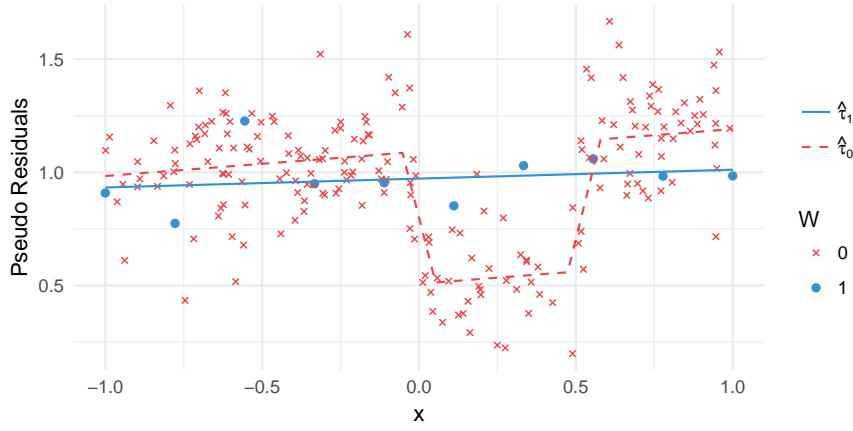
Figure 1 (b) shows the Pseudo Residuals, \tilde{D} . By choosing a simple function to estimate $\tau_1(x) = \mathbb{E}[\tilde{D}^1|X^1 = x]$ we effectively estimate a model for $\mu_1(x) = \mathbb{E}[Y^1|X^1 = x]$, which has a similar shape to $\hat{\mu}_0$. We can see that by choosing a relatively poor model for $\mu_1(x)$, \tilde{D}^0 is relatively far away from $\tau(x)$. The model for τ_0 will thus be relatively poor. However, our final estimator combines these two estimators according to

$$\hat{\tau}(x) = g(x)\hat{\tau}_0(x) + (1 - g(x))\hat{\tau}_1(x), \quad (12)$$

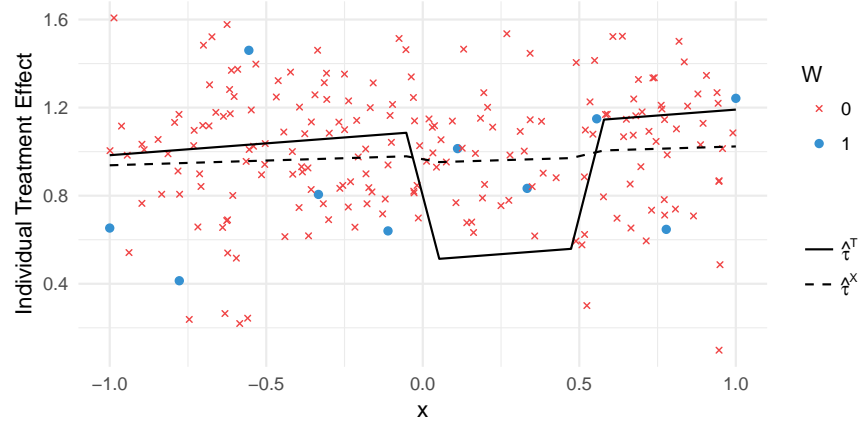
and we choose $g(x) = \hat{e}(x)$, an estimator for the propensity score. Note that since we have many more observations in the control group than in the treatment group,



(a) Observed outcomes and base learners of the first stage



(b) Pseudo residuals and the base learners of the second stage



(c) Comparison of *T*-learner and *X*-learner in a setting.

Figure 1: Intuition behind the X-learner with a constant treatment effect and unbalanced design.

$\hat{e}(x)$ is very small and thus $\hat{\tau}$ will be very similar to $\hat{\tau}_1(x)$. Figure 1 (c) compares the performance of the T-learner and the X-learner for our simple example.

It is difficult to compare the behavior of the S-learner to the X-learner in this example. Note, however, that if we choose random forest or regression trees for our ML algorithm, the feature which represents the treatment assignment is crucial for predicting Y^{obs} , and the first split will likely be on this feature. If that is the case, from there on the S-learner and the T-learner are the same, and we would expect them to perform similarly poorly in this scenario.

We end this section with some general remarks regarding the strengths and weaknesses of the S, T, and X learners, in order to provide some insights and qualitative guidance to practitioners when they choose among the three to fit their situation at hand.

- The S-learner is using the treatment assignment as a usual variable without giving it a special role. Depending on the base learner method, this variable can be completely ignored, and the S-learner is thus excellent in detecting no treatment effects, but— as we will see in section 4—it is often biased towards 0.
- The T-learner, on the other hand, does not combine the treated and control group. As we shall see in the simulations, this can be a disadvantage when the treatment effect is simple, because by not pooling the data, it is more difficult to learn a trend which appears in both the control and treatment response functions. Furthermore, if the outcome is continuous, it is often impossible for the T-learner to detect a true zero. This is because the likelihood of $\hat{\mu}_0(x) = \hat{\mu}_1(x)$ has for many base learners zero probability. If, however, the treatment effect is very complicated, and there are no common trends in μ_0 and μ_1 , then it will perform particularly well.
- The X-learner is not as specialized as the S or T learner, and it is not as readily clear from its structure when it performs particularly well or poorly. In the sections to come, we provide theoretical and simulation evidence on when it will perform well.

3 Comparison of Convergence Rates

In this section, we provide conditions under which the X-learner can be proven to outperform the T-learner in terms of pointwise estimation rate. These results can be viewed as attempts at rigorous formulations of intuitions regarding when X-learner is desirable. They corroborate our intuition that X-learner outperforms T-learner when one group is much larger than the other group or when the CATE function has a simpler form than those of the underlying response functions themselves.

Let us start by reviewing some of the basic results in the field of minimax non-parametric regression estimation: Bretagnolle and Huber (1979); Stone (1982); Birgé (1983); Bickel et al. (1998); Korostelev and Tsybakov (2012), also see textbooks Györfi et al. (2006) and Bickel and Doksum (2015). In the standard regression problem, one observes n independent and identically distributed tuples $(X_i, Y_i)_i \in \mathbb{R}^{d \times n} \times \mathbb{R}^n$ generated from some distribution \mathcal{P} and one is interested in estimating the conditional expectation of Y given some feature vector x , $\mu(x) = \mathbb{E}[Y|X = x]$. The error of an estimator $\hat{\mu}_n$ can be evaluated by the Expected Mean Squared Error (EMSE),

$$\text{EMSE}(\mathcal{P}, \hat{\mu}_n) = \mathbb{E}[(\hat{\mu}_n(\mathcal{X}) - \mu(\mathcal{X}))^2].$$

For a fixed \mathcal{P} , there are always estimators which have a very small EMSE. For example, choosing $\hat{\mu}_n \equiv \mu$ would have no error. However, \mathcal{P} and thus μ is unknown, and we do not know the EMSE for any estimator. Instead, one usually wants to find an estimator which achieves a small EMSE for a relevant set of distributions (such a

set is relevant if it captures domain knowledge or prior information of the problem). Ideally, we would like to find an estimator which has a small EMSE for all possible distributions. There is, however, no hope because there is no methods (including the most advanced machine learning techniques) which can achieve a small EMSE uniformly all the time. To make this problem feasible, one usually analyzes the worst performance of an estimator over a class or family, F , of distributions or one takes the minimax approach. The goal is to find an estimator which has a small EMSE for all distributions in this family. For example, if F_0 is the family of distributions \mathcal{P} such that $X \sim \text{Unif}[0, 1]$, $Y = \beta X + \varepsilon$, $\varepsilon \sim N(0, 1)$, and $\beta \in \mathbb{R}$, then it is well known that the OLS estimator achieves the parametric rate. That is, there exists a constant $C \in \mathbb{R}$ such that for all $\mathcal{P} \in F_0$,

$$\text{EMSE}(\mathcal{P}, \hat{\mu}_n^{\text{OLS}}) \leq Cn^{-1}.$$

If, however, F_1 is the family of all distributions \mathcal{P} such that $X \sim \text{Unif}[0, 1]$, $Y \sim \mu(X) + \varepsilon$ and μ is a Lipschitz continuous function with Lipschitz constant bounded by a constant, then there exists no estimator which achieves the parametric rate uniformly for all possible distributions in F_1 . To be precise, we can at most expect to find an estimator which achieves a rate of $n^{-2/3}$ and there exists a constant C' , such that

$$\liminf_{n \rightarrow \infty} \inf_{\hat{\mu}_n} \sup_{\mathcal{P} \in F_1} \frac{\text{EMSE}(\mathcal{P}, \hat{\mu}_n)}{n^{-2/3}} > C' > 0.$$

Estimators such as the Nadaraya-Watson and k -nearest neighbors can achieve this rate (Bickel and Doksum, 2015; Györfi et al., 2006).

Crucially, the fastest rate of convergence which holds uniformly for a family F is a property of the family to which the underlying data generating distribution belongs. It will be useful for us to define the sets of families for which a particular rate is achieved.

Definition 1 (*Family $S(a)$ of distributions with minmax rate n^{-a}*). For $a \in (0, 1]$, we define $S(a)$ to be the set of all families, F , of distributions of (X, Y) such that there exists an estimator $\hat{\mu}$ and a constant C such that for all $n \geq 1$,

$$\sup_{\mathcal{P} \in F} \text{EMSE}(\mathcal{P}, \hat{\mu}_n) \leq Cn^{-a}.$$

Furthermore, we define $S^*(a) \subset S(a)$ to be the set of all families which are in $S(a)$, but not in $S(b)$ for any $b < a$,

$$S^*(a) = S(a) \setminus (\cup_{b < a} S(b)).$$

Note that $S(a)$ is here not a family of distributions, but a set of families of distributions. From the examples from above, it is clear that $F_0 \in S(1)$ and $F_1 \in S(2/3)$.

Even though the minimax rate of EMSE is not very practical since one rarely knows that the true data generating process is in some reasonable family of distributions, it is nevertheless one of the very few useful theoretical tools to compare different nonparametric estimators. If for a big class of distributions, the worst EMSE of an estimator $\hat{\mu}^A$ is smaller than the worst EMSE of $\hat{\mu}^B$, then one might prefer estimator $\hat{\mu}^A$ over estimator $\hat{\mu}^B$. Furthermore, if the estimator of choice does not have a small error for a family which we think could be important, then we might expect $\hat{\mu}$ to have a large EMSE in real data.

Let us now employ the minimax approach to the problem of estimating the CATE. Recall that we assume a super population of random variables $(Y(0), Y(1), X, W)$ according to some distribution \mathcal{P} . We observe n treated and m control units from this super-population, and our goal is to find an estimator $\hat{\tau}_{mn}$ which has a small EMSE,

$$\text{EMSE}(\mathcal{P}, \hat{\tau}_{mn}) = \mathbb{E}[(\tau(\mathcal{X}) - \hat{\tau}_{mn}(\mathcal{X}))^2].$$

Similar to the regression case, we can again study the performance of estimators when \mathcal{P} lies in some family of distributions and in the following we will introduce families for which estimators based on the X-learner achieve provably a smaller EMSE than estimators based on the T-learner.

Similar to Definition 1, we define sets of families of super-populations.

Definition 2 (*Set of Superpopulations with given convergence rates*) For $a_\mu, a_\tau \in (0, 1]$, we define $S(a_\mu, a_\tau)$ to be the set of all distributions \mathcal{P} of $(Y(0), Y(1), X, W)$ such that

1. ignorability holds,
2. the distribution of $(X, Y(0))$ given $W = 0$ is in a class $F_0 \in S(a_\mu)$,
3. the distribution of $(X, Y(1))$ given $W = 1$ is in a class $F_1 \in S(a_\mu)$, and
4. the distribution of $(X, Y(1) - \mu_0(X))$ given $W = 1$ is in a class $F_{\tau 1} \in S(a_\tau)$.
5. the distribution of $(X, \mu_1(X) - Y(0))$ given $W = 0$ is in a class $F_{\tau 0} \in S(a_\tau)$.

A simple example of a family in $S(2/3, 1)$, would be the set of distributions \mathcal{P} for which $X \sim \text{Unif}[0, 1]$, $W \sim \text{Bern}(1/2)$, μ_0 is any Lipschitz continuous function, and τ is linear.

The difference between the T and X learner is that the T-learner estimates the response functions separately, and does not benefit from the possible smoothness of the CATE. Hence, if m is the number of control units and n is the number of treated units, one can expect that T with the right base learners estimates the CATE at a rate of $\mathcal{O}(m^{-a_\mu} + n^{-a_\mu})$, but, as we will see, we cannot expect it to be any faster.

We can now analyze the difference between the T and X learner. The X-learner, on the other hand, can be seen as a weighted average of the two estimators, $\hat{\tau}_0$ and $\hat{\tau}_1$. Each of which consists of a base learner for one of the response functions which achieves a rate of at most a_μ , and a base learner which estimates the CATE and should intuitively achieve a rate of at most a_τ . We, therefore, expect $\hat{\tau}_1$ to achieve a rate of $\mathcal{O}(m^{-a_\mu} + n^{-a_\tau})$ and $\hat{\tau}_0$ to achieve a rate of $\mathcal{O}(m^{-a_\tau} + n^{-a_\mu})$. It turns out to be mathematically very challenging to show that these rates hold in general. We will show this result in two cases: In the first example (Section 3.1), we assume the CATE to be linear. This implies that $a_\tau = 1$, and we achieve the parametric rate in n , which is in particular impressive when the number of control units is large. In the second example (Section 3.2), we consider the other extreme where we don't have any assumptions on the CATE. In this case, there is nothing which can be inferred from the control units about the treated units and vice versa. Consequently, the T-learner is here in some sense the best strategy, and achieves the minimax optimal rate of $\mathcal{O}(m^{-a_\mu} + n^{-a_\mu})$. However, we believe that a_μ is in most cases a lower bound for a_τ , and therefore the X-learner achieves the same rate. We will show this phenomena in the case of Lipschitz continuous functions.

3.1 Unbalanced class sizes and simple CATE

Even though it is theoretically possible that a_τ is of the same order of a_μ , our experience with real data suggests that it is often bigger (or the treatment effect IS simpler than the potential outcomes). Let us intuitively understand the difference between the T- and X-learner for a class $F \in S(a_\mu, a_\tau)$ with $a_\tau > a_\mu$. The T-Learner splits the problem of estimating the CATE into the two subproblems of estimating μ_0 and μ_1 separately. By choosing the right estimators, we can expect to achieve the rates of a_μ ,

$$\sup_{\mathcal{P}_0 \in F_0} \text{EMSE}(\mathcal{P}_0, \hat{\mu}_0^m) \leq C m^{-a_\mu}, \quad \text{and} \quad \sup_{\mathcal{P}_1 \in F_1} \text{EMSE}(\mathcal{P}_1, \hat{\mu}_1^n) \leq C n^{-a_\mu}, \quad (13)$$

where C is some constant. Those rates translate immediately to rates for estimating τ , since

$$\begin{aligned} \sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_{nm}^T) &\leq 2 \sup_{\mathcal{P}_0 \in \mathcal{F}_0} \text{EMSE}(\mathcal{P}_0, \hat{\mu}_0^m) + 2 \sup_{\mathcal{P}_1 \in \mathcal{F}_1} \text{EMSE}(\mathcal{P}_1, \hat{\mu}_1^n) \\ &= 2C (m^{-a_\mu} + n^{-a_\mu}). \end{aligned} \quad (14)$$

In general, we cannot expect to do better than this, when using an estimation strategy which falls in the class of T-Learners, because the subproblems in (13) are treated completely independent and neither $\hat{\mu}_0$ nor $\hat{\mu}_1$ is learning from the other class.

In some cases we observe that the number of control units is much larger than the number of treated units, $m \gg n$. This happens for example if we test a new treatment and we have a large number of previous (untreated) observations which can be used as the control group. In that case we get a stronger bound than (14), because essentially the error of the regression problem for the treated group dominates,

$$\sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_{nm}^T) = \sup_{\mathcal{P}_1 \in \mathcal{F}_1} \text{EMSE}(\mathcal{P}_1, \hat{\mu}_1^n) \leq Cn^{-a_\mu}. \quad (15)$$

This is an improvement over (14), but it still does not lead to the fast rate, a_τ .

The X-learner, on the other hand, can achieve the fast rate a_τ (or n^{-a_τ} to be precise). An expansion of the EMSE into two squared error terms and also a cross term involving biases can be used to show that the T-learner can not achieve this fast rate in the unbalanced case. To see the faster rate for the X-learner, recall that the number of control units is assumed so large that μ_0 can be predicted almost perfectly and choose the weighing function g equal to 0 in (9). It follows that the error of the first stage of the X-learner is negligible and the treated pseudo residuals satisfy $D_i^1 = \tau(X_i(1)) + \varepsilon_i$. Per assumption 5, $\mathbb{E}[D^1|X = x]$ can now be estimated using an estimator achieving the desired rate of a_τ ,

$$\sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_{nm}^X) \leq Cn^{-a_\tau}.$$

This is a substantial improvement over (15) and intuitively demonstrates that, in contrast to the T-learner, the X-learner can exploit structural assumptions on the treatment effect. However, even for large m , we cannot expect to perfectly estimate μ_0 . The following theorem deals carefully with this estimation error in the case where τ is linear, but the response functions can be estimated at any nonparametric rate.

Theorem 1 *Assume we observe m control units and n treated units from some super population of independent and identically distributed observations $(Y(0), Y(1), X, W)$ coming from a distribution \mathcal{P} given in (1) and satisfies the following assumptions:*

A1 *The error terms ε_i are independent given X , with $\mathbb{E}[\varepsilon_i|X = x] = 0$ and $\text{Var}[\varepsilon_i|X = x] \leq \sigma^2$.*

A2 *\mathcal{X} has finite second moments,*

$$\mathbb{E}[\|\mathcal{X}\|_2^2] \leq C_{\mathcal{X}}.$$

A3 *Ignorability holds.*

A4 *There exists an estimator $\hat{\mu}_0^m$ with*

$$\text{EMSE}(\mathcal{P}, \hat{\mu}_0^m) = \mathbb{E}[(\mu_0(\mathcal{X}) - \hat{\mu}_0^m(\mathcal{X}))^2] \leq C_0 m^{-a}.$$

A5 *The treatment effect is parametrically linear, $\tau(x) = x^T \beta$, with $\beta \in \mathbb{R}^d$.*

A6 *The eigenvalues of the sample covariance matrix of X^1 are well conditioned, in the sense that there exists an n_0 , such that*

$$\sup_{n > n_0} \gamma_{\min}(\hat{\Sigma}_n) \geq C_{\Sigma}. \quad (16)$$

Then the X-learner with $\hat{\mu}_0^m$ in the first stage, OLS in the second stage and weighing function $g \equiv 0$ has the following upper bound on its EMSE: for all $n > n_0$,

$$EMSE(\mathcal{P}, \hat{\tau}^{mn}) = \mathbb{E} \left[\|\tau(\mathcal{X}) - \hat{\tau}^{mn}(\mathcal{X})\|^2 \right] \leq C(m^{-a} + n^{-1})$$

with $C = \max(C_0, \sigma^2 d) C_{\mathcal{X}} C_{\Sigma}$. In particular, if there are a lot of control units, such that $m/n^{1/a} \leq c_3$, then the X-learner achieves the parametric rate in n , or

$$EMSE(\mathcal{P}, \hat{\tau}^{mn}) \leq (1 + c_3) C n^{-1}.$$

It is mathematically symmetric that similar results hold if n (size of the treatment group) is much larger than m (size of the control group). Furthermore, we note that an equivalent statement also holds for the pointwise MSE, and we show this result in Theorem 3.

3.2 Balanced class sizes and complex CATE

In the previous section, we considered the case when the distribution of $(Y(0), Y(1), W, X)$ was assumed to be in some family $F \in S(a_\mu, a_\tau)$ with $a_\tau > a_\mu$, and we showed that one can expect the X-learner to outperform the T-learner in this case. Now we want to explore the case when $a_\tau \leq a_\mu$.

As discussed above, we expect the T-learner with the right base learners to achieve a rate of at least $\mathcal{O}(m^{-a_\mu} + n^{-a_\mu})$ (c.f. (14)). To understand the convergence rate of the X-learner, let us recall that the X-learner is an average of the two base learners of the second stage. As motivated above, we would expect $\hat{\tau}_1$ to achieve a rate of $\mathcal{O}(m^{-a_\mu} + n^{-a_\tau})$, and $\hat{\tau}_0$ to achieve a rate of $\mathcal{O}(m^{-a_\tau} + n^{-a_\mu})$.

Let us consider the case, when $a_\tau < a_\mu$. This is a somewhat artificially case, since having response functions in $S(a_\mu)$ (Assumption 2 and 3 in Definition 2) imply that the CATE cannot be too complicated (Assumption 4 and 5). For example, if μ_0 and μ_1 is Lipschitz continuous, then the CATE is Lipschitz continuous as well, and we would expect $a_\tau = a_\mu$. Even though it is hard to construct a case, with $a_\tau < a_\mu$, we cannot exclude such a situation, and we would expect in such a case the T-learner to be the better meta learner.

We believe that the case when $a_\tau \approx a_\mu$ is not very common, but still much more reasonable than the case when $a_\tau < a_\mu$. In this case, we would expect the T and X learner to perform similarly when compared by their convergence rate. Let us try to backup this intuition with a specific example. Note that Theorem 1 already confirms that $\hat{\tau}_1$ achieves the expected rate,

$$\mathcal{O}(m^{-a_\mu} + n^{-a_\tau}),$$

for the case when the CATE is linear. In the following we will consider another example, where the CATE is of the same order as the response functions.

Let us first introduce a class of distributions with Lipschitz continuous regression functions:

Definition 3 (Lipschitz continuous regression functions) Let F^L be the class of distributions on $(X, Y) \in [0, 1]^d \times \mathbb{R}$ such that:

1. the features, X_i , are iid uniformly distributed in $[0, 1]^d$,
2. the observed outcomes are given by

$$Y = \mu(X) + \varepsilon,$$

where ε is independent and normally distributed with mean 0 and variance σ^2 ,

3. X and ε are independent, and

4. μ are Lipschitz continuous with parameter L .

Remark 2 The optimal rate of convergence for the regression problem of estimating $x \mapsto \mathbb{E}[Y|X = x]$ defined in Definition 3 is given by $n^{-2/(2+d)}$. Furthermore, the KNN algorithm with the right choice of neighbors achieves this rate, and it is thus minimax optimal for this regression problem. We can conclude that $F^L \in S(\frac{2}{2+d})$.

Now, let's define a very related distribution on $(Y(0), Y(1), W, X)$.

Definition 4 Let \mathcal{D}_{mn}^L be the class of distributions of $(Y(0), Y(1), W, X) \in \mathbb{R}^N \times \mathbb{R}^N \times \{0, 1\}^N \times [0, 1]^{d \times N}$ such that:

1. $N = m + n$,
2. the features, X_i , are iid uniformly distributed in $[0, 1]^d$,
3. there are exactly n treated units,

$$\sum_i W_i = n,$$

4. the observed outcomes are given by

$$Y_i(w) = \mu_w(X_i) + \varepsilon_{wi},$$

where ε_{wi} is independent normally distributed with mean 0 and variance σ^2 .³

5. X, W and $\varepsilon = (\varepsilon_{wi})$ are independent, and
6. μ_0, μ_1 are Lipschitz continuous with parameter L .

Note that if $(Y(0), Y(1), W, X)$ is distributed according to a distribution in \mathcal{D}_{mn}^L , then $(Y(0), X)$ given $W = 0$ and $(Y(1), X)$ given $W = 1$ have marginal distributions in F^L , and $(X, Y(0) - \mu_0(X))$ given $W = 0$ and $(X, Y(1) - \mu_1(X))$ given $W = 1$ have a distributions in F^{2L} , and thus we can conclude that $\mathcal{D}_{mn}^L \in S\left(\frac{2}{2+d}, \frac{2}{2+d}\right)$. In Theorem 5, we prove that the best possible rate for this problem is given by $\mathcal{O}(n^{2/(2+d)} + m^{2/(2+d)})$. This is precisely the rate the T-learner with the right base learners achieves. In Section C.1, we show that the X-learner with the KNN estimator for both stages achieves this optimal rate as well, and we can thus conclude that both the T- and X-learner achieve the minimax optimal rate for this problem.

Theorem 2 Assume $(X, W, Y(0), Y(1)) \sim \mathcal{P} \in \mathcal{D}_{mn}^L$. In particular, μ_0 and μ_1 are Lipschitz continuous with constant L ,

$$|\mu_w(x) - \mu_w(z)| \leq L\|x - z\| \quad \text{for } w \in \{0, 1\},$$

and $X \sim \text{Unif}([0, 1]^d)$. Then the X-learner with the KNN algorithms for both stages is minimax optimal,

$$\mathbb{E}\|\tau - \hat{\tau}^{mn}\|^2 \leq c\sigma^{\frac{4}{d+2}} L^{\frac{2d}{2+d}} \left(m^{-2/(2+d)} + n^{-2/(2+d)}\right). \quad (17)$$

with c a constant which does not depend on \mathcal{P} , L , and σ .

Note that \mathcal{D}_{mn}^L is a very special family, but we expect that this result holds in much greater generality.

³We do not assume that $\varepsilon_{0i} \perp \varepsilon_{1i}$.

4 Simulation Studies

In this section, we compare the S, T, and X learner in several simulation studies. We examine prototypical situations where one learner is preferred over the others. In practice, we recommend choosing powerful machine learning algorithms such as RFs (Breiman, 2001) or BART (Hill, 2011) for the base learners, since such methods perform well for a large variety of data sets. We, therefore, choose all base learners to be either the BART or honest RF algorithms, and we refer to those meta learners as S-RF, T-RF, X-RF, S-BART, T-BART, and X-BART respectively. Using two machine learning algorithms helps us demonstrate that the effects we see are not specific to a particular machine learning algorithm and that choice of base learner affects prediction accuracy. That is, some machine learning algorithms (i.e. potential base learners) perform especially well for a particular type of data. For example, if the data set is very large and the features are pixels of images, then convolutional neural networks performs very well, and one should prefer it over other methods which are not performing well on image data.

Remark 3 (BART and RF) *BART and RF are regression tree based algorithms, they both use all observations for each prediction, and they are in that sense global methods. However, BART seems to use global information more seriously than RF, and it performs in particular well when the data generating process exhibits some global structures (e.g. globally sparsity or global linearity). RF, on the other hand, are relatively better when the data has locally some structure which does not necessarily generalize to the entire space.*

4.1 Tuning meta-learners

Tuning algorithms for causal inference problems is not straightforward because of the lack of obvious goodness-of-fit metrics. Unlike in the usual prediction problem, the target quantity, the CATE or the individual treatment effects are unobserved and goodness-of-fit methods such as Cross-Validation (CV) cannot be used directly.

One feature of the meta-learners is that they can be decomposed into sub-prediction tasks which can be tuned separately. For each of these prediction tasks the target is observed (or available through estimation by the first stage as in the X-learner), and goodness-of-fit measures such as CV or base learner specific goodness-of-fit metrics such as the Out-Of-Bag (OOB) error for RF can be used to tune the learners.

Take, for example, the T-learner. It consists of two well separated estimators: one which estimates the treated response function, $\mu_1 = \mathbb{E}[Y(1)|X = x]$, and one which estimates the control response function, μ_0 . For both estimators the response variable and the features or predictors are observed, and we can tune them separately.⁴ This procedure does not necessarily lead to the best parameter selection for the T-learner, not only because every goodness-of-fit metric is to some extent an approximation, but also because the parameters that minimize the expected MSE or EMSE of the individual learners do not necessarily minimize the EMSE for the CATE. To investigate this approximation in detail, let us decompose the EMSE of the T-learner as follows,

$$\text{EMSE}(\tau^T) := \mathbb{E} \left(\tau(\mathcal{X}) - \hat{\tau}^T(\mathcal{X}) \right)^2 = \text{EMSE}_1 + \text{EMSE}_0 - 2\mathbb{E}[\text{BIAS}_1(\mathcal{X})\text{BIAS}_0(\mathcal{X})]$$

with the notation, that $\text{EMSE}_w = \mathbb{E}(\mu_w(\mathcal{X}) - \hat{\mu}_w^T(\mathcal{X}))^2$ and $\text{BIAS}_w(x) = \mathbb{E}\hat{\mu}_w^T(x) - \mu_w(x)$. When tuning the parameters separately for each base learner, we essentially pick parameters such that EMSE_0 and EMSE_1 are minimized, and we ignore the bias terms. In general, we cannot expect to find the base learner parameter setting which minimizes the $\text{EMSE}(\tau^T)$. However, in many situations the bias term is small or the

⁴An example implementation can be found in Algorithm 7 in Appendix A.

discrepancy due to this approximation is negligible, then the approximation works well. For the S-learner, one can essentially make the same argument to motivate tuning the base model with a standard goodness-of-fit or model error metric.

Parameter tuning for the the X-learner is more complicated than for the S and T learners, since the predictor variables in the second stage depend on the base learners of the first stage and there is one extra step of combining the two estimators for the CATE. We recommend tuning $\hat{\tau}_1$, and $\hat{\tau}_0$ separately, and then choose a g to combine $\hat{\tau}_1$ and $\hat{\tau}_0$ in an extra step.

Let us first discuss how one could choose g . While the choice of g can have a large impact on CATE estimation if the two estimated response models differ, we often observe in simulations that choosing g to be the propensity leads to good performance. For example, in the unbalanced case studied in Simulation 1, the choice of g is very important. Based on simulation evidence, we generally recommend to either estimate the covariance matrix of $\hat{\tau}_1$ and $\hat{\tau}_0$ using a bootstrap procedure and then choose the best g that minimizes the variance of the combined estimator, $\hat{\tau}$, or to use an estimate for the propensity score for g .

Tuning $\hat{\tau}_1$ and $\hat{\tau}_0$ is usually more challenging. Let us restrict our analysis and only consider $\hat{\tau}_1$, since $\hat{\tau}_0$ can be similarly treated. Denote by γ the vector of tuning parameters for the control response estimator of the first stage, $\hat{\mu}_0$, and θ the tuning parameters of $\hat{\tau}_1$. We want to choose γ and θ such that the EMSE of $\hat{\tau}_1$ as an estimator for τ ,

$$\text{EMSE}(\hat{\tau}_1) := \mathbb{E}(\tau(\mathcal{X}) - \hat{\tau}_1(\mathcal{X}))^2, \quad (18)$$

is small. Note, however, that in the second stage (when $\hat{\tau}_1$ is estimated), $\hat{\mu}_0$ was already estimated, and it is fixed. $\hat{\tau}_1$ is then estimated with $\tilde{D}_i^1 = Y_i^1 - \hat{\mu}_0(X_i^1)$ as the dependent variable. It is therefore trying to estimate the function,

$$x \mapsto \mathbb{E}[\tilde{D}^1 | X = x] = \mu_1(x) - \hat{\mu}_0(x),$$

and not τ directly. It will be useful to also define the EMSE for this regression function,

$$\text{EMSE}(\hat{\tau}_1 | \hat{\mu}_0) := \mathbb{E}[(\mu_1(\mathcal{X}) - \hat{\mu}_0(\mathcal{X}) - \hat{\tau}_1(\mathcal{X}))^2 | \hat{\mu}_0]. \quad (19)$$

It is then straightforward to decompose the EMSE($\hat{\tau}_1$) as follows:

$$\begin{aligned} \text{EMSE}(\hat{\tau}_1) &= \text{EMSE}_0 + \mathbb{E}[\text{EMSE}(\hat{\tau}_1 | \hat{\mu}_0)] \\ &\quad - 2\mathbb{E}[\text{Cov}(\hat{\mu}_0(\mathcal{X}), \hat{\mu}_0(\mathcal{X}) + \hat{\tau}_1^\theta(\mathcal{X}) | X)] - 2\mathbb{E}[\text{BIAS}_0(\mathcal{X}) \text{BIAS}_1^\top(\mathcal{X})]. \end{aligned} \quad (20)$$

where $\text{BIAS}_1^\top(x) = \mathbb{E}\hat{\tau}_1(x) - \tau(x)$, and EMSE_0 and $\text{BIAS}_0(x)$ is defined above in the analysis for the S and T learner.

However, since we neither observe the ITEs nor the CATE, we approximate the EMSE by ignoring the bias terms as for the T and S learners and also the covariance term that did not exist for the other two learners,

$$\text{EMSE}(\hat{\tau}_1) \approx \text{EMSE}_0 + \text{EMSE}(\hat{\tau}_1 | \hat{\mu}_0).^5 \quad (21)$$

The advantage of this approximation is that EMSE_0 is the EMSE which occurs when estimating $x \mapsto \mathbb{E}[Y(0) | X = x]$ in the first stage, and $\text{EMSE}(\hat{\tau}_1 | \hat{\mu}_0)$ is the EMSE for the regression problem of estimating $x \mapsto \mathbb{E}[\tilde{D}^1 | X = x]$ in the second stage of the X-learner. In the same way, as for S and T learner, both quantities can now be estimated using either generic methods such as CV, or learner specific methods such as OOB errors.

We can now tune γ and θ separately by first tuning γ for the base learner in the first stage, and then ($\hat{\mu}_0$ is now fix) tuning θ for the second stage. However, due to

⁵Using a bootstrap algorithm, it is possible to approximate MSE($\hat{\tau}_1$) in a better way. This, however, is computationally expensive and therefore not suited for parameter tuning.

$\text{EMSE}(\hat{\tau}_1|\hat{\mu}_0)$ depending on both γ and θ , we recommend to tune them jointly. That is, if we wanted to find the best values for (γ, θ) out of a list of k candidates, $\{(\gamma_i, \theta_i)\}_{i=1}^k$, we would use approximation (21) together with some procedure for estimating EMSE_0 and $\text{EMSE}(\hat{\tau}_1|\hat{\mu}_0)$ to estimate $\text{EMSE}(\hat{\tau}_1)$ for each (γ_i, θ_i) , and we would select the pair with the smallest estimated EMSE.

We note that similar to our approximation for the EMSE of the S and T learners, we omit the bias terms in our approximation and we approximate the expected MSE of the base learner in the second stage, $\mathbb{E}[\text{EMSE}(\hat{\tau}_1|\hat{\mu}_0)]$ by the EMSE given the realization of $\hat{\mu}_0$, $\text{EMSE}(\hat{\tau}_1|\hat{\mu}_0)$. Those approximations seem reasonable, but to omit the covariance term, $\mathbb{E}[\text{Cov}(\hat{\mu}_0(\mathcal{X}), \hat{\mu}_0(\mathcal{X}) + \hat{\tau}_1^\theta(\mathcal{X})|X)]$ seems striking at first. However, note that $\hat{\tau}_1^\theta(x) = \hat{\mathbb{E}}[Y(1) - \hat{\mu}_0(X)|X = x]$ is very close to $\mu_1(x) - \hat{\mu}_0(x)$, and thus

$$\text{Cov}(\hat{\mu}_0(\mathcal{X}), \hat{\mu}_0(\mathcal{X}) + \hat{\tau}_1^\theta(\mathcal{X})|X = x) \approx \text{Cov}(\hat{\mu}_0(\mathcal{X}), \mu_1(\mathcal{X})|X = x) = 0$$

is close to 0.

Those approximations seem crude, but we want to note that even if this approximation for the EMSE does not work well, we might still be able to find good tuning parameters, that lead to a good performance of the X-learner. That is, as long as the minimizers of EMSE and its approximations are close, we are fine even though the EMSE and its approximation can be far apart (for example, there is roughly a constant off-set).

4.2 Simulation setup

For each simulation, we specify the propensity score, e , the response functions μ_0 and μ_1 , the dimension, $d \in \mathbb{N}$, of the feature space and a parameter, α , which specifies the amount of confounding between features. To simulate an observation, i , in the training set, we simulate its feature vector, X_i , its treatment assignment, W_i , and its observed outcome, Y_i^{obs} , independently in the following way:

1. First, we simulate a d -dimensional feature vector,

$$X_i \stackrel{iid}{\sim} \mathcal{N}(0, \Sigma). \quad (22)$$

with Σ being a correlation matrix which is created using the `vine` method as it is discussed by Lewandowski et al. (2009).

2. Next, we create the potential outcomes according to

$$\begin{aligned} Y_i(1) &= \mu_1(X_i) + \varepsilon_i(1) \\ Y_i(0) &= \mu_0(X_i) + \varepsilon_i(0) \end{aligned}$$

where $\varepsilon_i(1), \varepsilon_i(0) \stackrel{iid}{\sim} \mathcal{N}(0, 1)$.

3. And finally, we simulate the treatment assignment according to

$$W_i \sim \text{Bern}(e(X_i)),$$

we set $Y_i^{\text{obs}} = Y(W_i)$ and we return $(X_i, W_i, Y_i^{\text{obs}})$.⁶

We train each CATE estimator on a training set of N units, and we evaluate its performance against a test set of 10^4 units for which we know the true CATE. We repeat each experiment 30 times, and we report the averages.

⁶This is slightly different from the DGP we were considering for our theoretical results, because here m , the number of control units and n , the number of treated units are both random. The difference is, however, very small, since in our setups $N = m + n$ is very large.

4.3 The unbalanced case with a simple CATE

We have already seen in Theorem 1, and in the Section 2.2 that the X-learner performs particularly well when the treatment group sizes are very unbalanced. We will verify this effect in the following. We choose the propensity score to be constant and very small, $e(x) = 0.01$, such that on average only one percent of the units receive treatment. Furthermore, we choose the response functions in such a way that the CATE function is comparatively simple to estimate. To be precise, we choose

Simulation 1 (unbalanced treatment assignment)

$$\begin{aligned} e(x) &= 0.01, \quad d = 20, \\ \mu_0(x) &= x^T \beta + 5 \mathbb{I}(x_1 > 0.5), \quad \text{with } \beta \sim \text{Unif}([-5, 5]^d), \\ \mu_1(x) &= \mu_0(x) + 8 \mathbb{I}(x_2 > 0.1). \end{aligned}$$

The CATE function $\tau(x) = \mathbb{I}(x_2 > 0.1)$ is a one-dim indicator function, and thus simpler than the 20-dim linear function for the response functions $\mu_0(\cdot)$ and $\mu_1(\cdot)$. We can see in Figure 2 that the X-learner indeed performs much better in this unbalanced setting with both the BART and the RF as the base-learners.

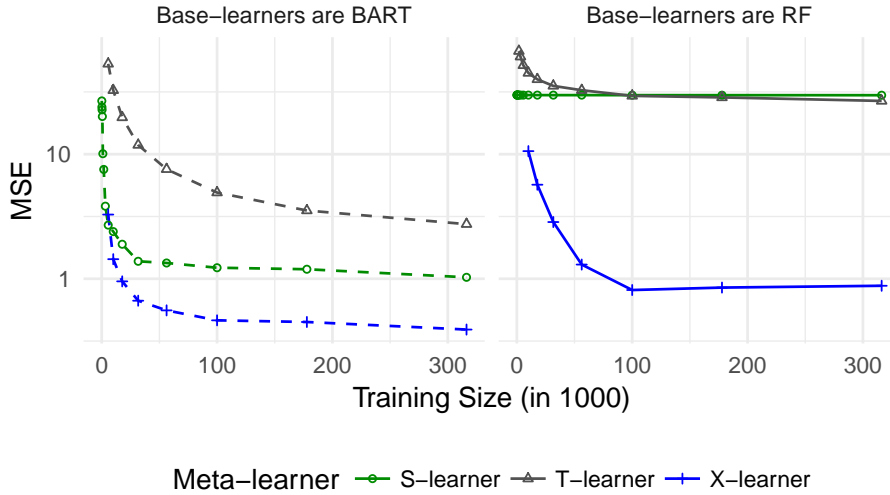


Figure 2: Comparison of S, T, and X with BART (left) and RF (right) as base learners in Simulation 1

4.4 Balanced cases without confounding

Next let us analyze the two extreme cases of a very complex CATE and no treatment effect. We will show that for the case of no treatment effect, the S-learner performs very well, since it is good at predicting a zero treatment effect by not splitting on the treatment indicator. On the other hand, for the complex CATE case, there is nothing to be learned from the treated group about the control group and vice versa. Here the T-learner performs very well, while the S-learner is often biased towards zero. Unlike the T-learner, the X-learner is pooling the data, and it is therefore performing well for the simple CATE case. And unlike the S-learner, the X-learner is not biased towards zero. It, therefore, performs well in the both cases.

4.4.1 Complicated CATE

Let us first consider the case where the treatment effect is as complicated as the response functions in the sense that it does not satisfy regularity conditions such as sparsity or linearity which the response functions do not satisfy. To be precise, we study two Simulations here, and we choose for both the dimension to be $d = 20$, and the propensity score to be $e(x) = 0.5$. In the first setup (complex linear) the response functions are different linear functions of the entire feature space:

Simulation 2 (complex linear)

$$\begin{aligned} e(x) &= 0.5, \quad d = 20, \\ \mu_1(x) &= x^T \beta_1, \quad \text{with } \beta_1 \sim \text{Unif}([-5, 5]^d), \\ \mu_0(x) &= x^T \beta_0, \quad \text{with } \beta_0 \sim \text{Unif}([-5, 5]^d). \end{aligned}$$

The second setup (complex non-linear) is motivated by Wager and Athey (2015). Here the response function are non-linear functions:

Simulation 3 (complex non-linear)

$$\begin{aligned} e(x) &= 0.5, \quad d = 20, \\ \mu_1(x) &= \frac{1}{2} \varsigma(x_1) \varsigma(x_2), \\ \mu_0(x) &= -\frac{1}{2} \varsigma(x_1) \varsigma(x_2) \end{aligned}$$

with

$$\varsigma(x) = \frac{2}{1 + e^{-12(x-1/2)}}.$$

Figure 3 shows the MSE performance of the different learners. In this case, it is best to separate the CATE estimation problem into the two problems of estimating μ_0 and μ_1 since there is nothing one can learn from the other assignment group. The T-learner follows exactly this strategy and should perform very well. The S-learner, on the other hand, pools the data and it needs to learn that the response function for the treated and the response function for the control group are very different. However, in the simulations we studied here, the difference seems to matter only very little.

Another interesting insight is that choosing BART or RF as the base learner can matter a lot. BART performs very well, when the response surfaces satisfy global properties such as being globally linear as in Simulation 2. This is, however, not satisfied in Simulation 3. Here the optimal splitting policy differs throughout the space and this non-global property is harming BART. Choosing RF as base learners performs here better. Researchers should use their subject knowledge when choosing the right base learner.

4.4.2 No treatment effect

Let us now consider the other extreme where we chose the response functions to be equal. This leads to a zero treatment effect, which is very favorable for the S-learner. We will again consider two simulations where the feature dimension is 20, and the propensity score is constant and 0.5.

We start with a global linear model (Simulation 4) for both response function. In Simulation 5, we simulate some interaction by slicing the space into three parts ($\{x : x_{20} < -0.4\}$, $\{x : -0.4 < x_{20} < 0.4\}$, $\{x : -0.4 < x_{20}\}$). For each of the three parts of the space a different linear model holds. We do this because we believe that in many data sets there is local structure which only appears in some parts of the space.

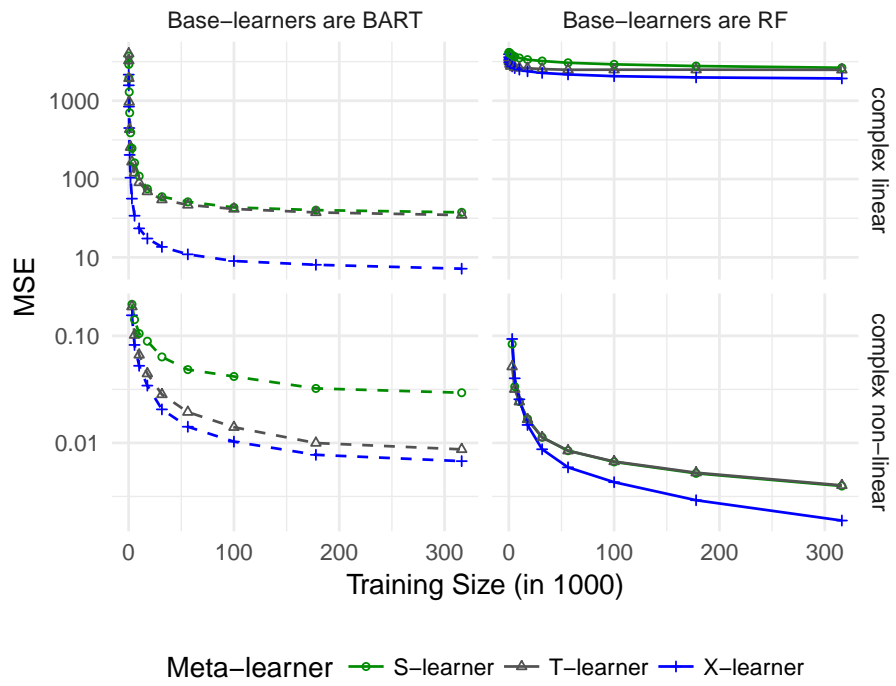


Figure 3: Comparison of S, T, and X with BART (left) and RF (right) as base learners for Simulation 2 (top) and Simulation 3 (bottom)

Simulation 4 (global linear)

$$\begin{aligned}
e(x) &= 0.5, \quad d = 20, \\
\mu_0(x) &= x^T \beta, \quad \text{with } \beta \sim \text{Unif}([-15, 15]^d) \\
\mu_1(x) &= \mu_0(x)
\end{aligned}$$

Simulation 5 (piecewise linear)

$$\begin{aligned}
e(x) &= 0.5, \quad d = 20, \\
\mu_0(x) &= \begin{cases} x^T \beta_l & \text{if } x_{20} < -0.4 \\ x^T \beta_m & \text{if } -0.4 \leq x_{20} \leq 0.4 \\ x^T \beta_u & \text{if } 0.4 < x_{20} \end{cases} \\
\mu_1(x) &= \mu_0(x)
\end{aligned}$$

with

$$\beta_l(i) = \begin{cases} \beta(i) & \text{if } i \leq 5 \\ 0 & \text{otherwise} \end{cases} \quad \beta_m(i) = \begin{cases} \beta(i) & \text{if } 6 \leq i \leq 10 \\ 0 & \text{otherwise} \end{cases} \quad \beta_u(i) = \begin{cases} \beta(i) & \text{if } 11 \leq i \leq 15 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\beta \sim \text{Unif}([-15, 15]^d).$$

Figure 4 shows the outcome of these simulation. For both simulations, the CATE is globally 0. As expected, the S-learner performs very well, since the treatment assignment has no predictive power for the combined response surface. It is thus often ignoring in the S-learner, and the S-learner correctly predicts a zero treatment effect.

We can again see that the global property of the BART harms its performance in the piecewise linear case since here the importance of features is different in different parts of the space.

4.5 Confounding

In preceding examples, the propensity score was globally equal to some constant. This is a special case, and in many experiments and observational studies, we cannot assume this to be true. All of the meta-learners we discuss can handle confounding, as long as the ignorability assumption holds. We test this in a setting which has also been studied by Wager and Athey (2015).

Simulation 6 (beta confounded)

$$\begin{aligned}
e(x) &= \frac{1}{4}(1 + \beta(x_1, 2, 4)) \\
\mu_0(x) &= 2x_1 - 1, \\
\mu_1(x) &= \mu_0(x),
\end{aligned}$$

5 Applications

In this section we consider two data examples, and we create simulations that are based on the real examples. In the first example, we consider a large Get-Out-The-Vote (GOTV) experiment that explored if social pressure can be used to increase voter turnout in elections in the United States (Green and Larimer, 2008). In the second example, we consider an experiment that explored if door-to-door canvassing can be used to durably reduce transphobia in Miami (Broockman and Kalla, 2016). In both

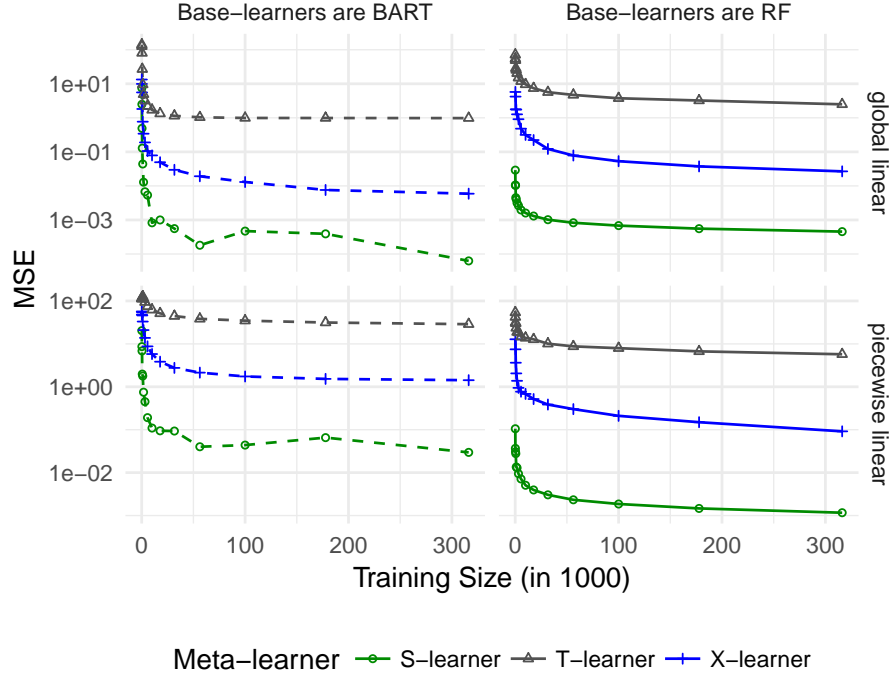


Figure 4: Comparison the of S, T, and X learner with BART (left) and RF (right) as base learners for Simulation 4 (top) and Simulation 5 (bottom)

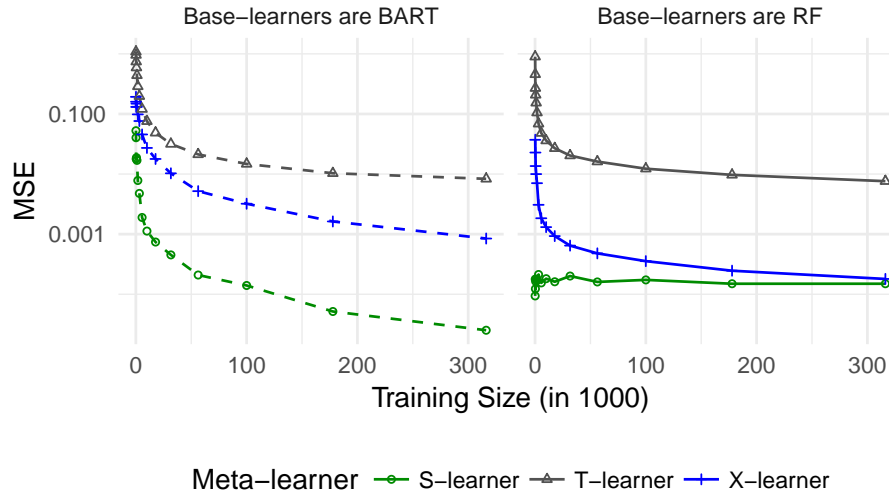


Figure 5: Comparison of S, T, and X with BART (left) and RF (right) as base learners for Simulation 6

examples, the original authors failed to find evidence of heterogeneous treatment effects using simple linear models, and subsequent researchers and policy makers are acutely interested in treatment effect heterogeneity that could be used to better target the interventions. We use our honest random forest implementation to conduct analysis because of the importance of obtaining valid confidence intervals in these applications. Confidence intervals are obtained using a bootstrap procedure (Algorithm 6).

5.1 Social pressure and voter turnout

In a large field experiment, Green and Larimer (2008) show that substantially higher turnout was observed among registered voters who received mailing promising to publicize their turnout to their neighbors. In the United States, whether someone is registered to vote and their history of voting is a matter of public record. Of course, *how* individuals voted is private. The Green and Larimer (2008) experiment has been highly influential both in the scholarly literature and in political practice. In our re-analysis we focus on two treatment conditions: the control group which was assigned to 191,243 individuals and the neighbors treatment, which was assigned to 38,218 individuals. Note the unequal sample sizes. The experiment was conducted in Michigan prior to the August 2006 primary election, which was a statewide election with a wide range of offices and proposals on the ballot. The authors randomly assigned households with registered voters to receive mailers. The outcome, whether someone voted, was observed in the primary election. The “neighbors” mailing opens with a message that states “DO YOUR CIVIC DUTY-VOTE!” It then continues by not only listing the household’s voting records but also the voting records of those living nearby. The mailer informed individuals that “we intent to mail an updated chart” after the primary.

The study consists of seven key individual-level covariates, most of which are discrete: gender, age, and whether the registered individual voted in the primary elections in 2000, 2002 and 2004 or the general election in 2000 and 2002. The sample was restricted to voters who had voted in the 2004 general election. The outcome of interest is turnout in the 2006 primary election, which is an indicator variable. Because compliance is not observed, all estimates are of the Intention-to-Treat (ITT) effect, which is identified by the randomization. The average treatment effect estimated by the authors is .081 with a standard error of (.003). Increasing voter turnout by 8.1% using a simple mailer is a large substantive effect, especially considering that many individuals may never have seen the mailer.

Figure 6 presents the histogram of estimated treatment effects using X-RF. The bins are colored by what proportion of observations in the given bin have confidence intervals that do not cover zero. The positive treatment effect appears to be isolate to a portion of the observations, and there is evidence of a negative backlash among a small number of people. Applied researchers have observed a backlash from these mailers—e.g., some recipients call their Secretary of States office or local election registrar to complain (Mann, 2010; Michelson, 2016). Having estimates of the heterogeneity would enable campaigns to better target the mailers in the future.

X-RF, S-RF and T-RF all provide similar estimates of the CATEs. This is unsurprising given the very large sample size, the small number of covariates, and their distributions. For example, the correlation between the CATE estimates of S-RF and T-RF is 0.99. (Results for S-RF and T-RF available upon request.)

We conduct a simulation study to see how these estimators would behave in smaller samples. We take the CATE estimates produced by T-RF, and we assume that they are the truth. We can then impute the potential outcomes, under both treatment and control for every observation. We then sample training data from the complete data and predict CATEs for the test data using S, T, and X RF. We keep the unequal treatment proportion observed in the full data fixed—i.e., $\mathbb{P}(T = 1) = 0.167$. Figure

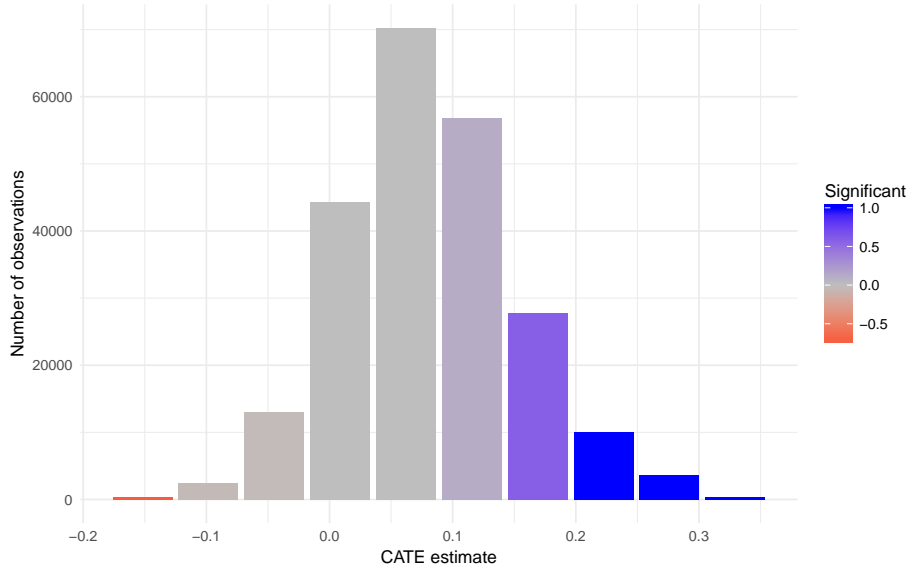


Figure 6: Social pressure and Voter Turnout. The absolute value of the scale is the proportion of observations in each bin which is significantly different from 0. Negative values corresponds to bins which are smaller than 0, and positive values corresponds to those which are bigger than 0.

7 presents the results for this simulation. The simulation shows that in small samples both X-RF and S-RF outperform T-RF, with X-RF performing the best, as one may conjecture given the unequal sample sizes.

5.2 Reducing transphobia: A field experiment on door-to-door canvassing

In an experiment that received wide-spread media attention, Broockman and Kalla (2016) show that brief (10 minute) but high quality door-to-door conversations can markedly reduce prejudice against non-gender conforming individuals for at least 3 months. This experiment was published in *Science* after the journal retracted an earlier article claiming to show the same in an experiment about gay rights (Bohannon, 2016). Broockman et al. (2015) showed that the earlier published study was fraudulent, and they conducted the new one to determine if the pioneering behavioral intervention of encouraging people to actively take the perspective of others was effective in decreasing prejudice.

There are important methodological differences between this example and our previous one. The experiment is a placebo-controlled experiment with a parallel survey that measures attitudes, which are the outcomes of interest. The authors follow the design of (Broockman et al., 2017). The authors first recruited registered voters ($n = 68,378$) via mail for an unrelated online survey to measure baseline outcomes. The authors then randomly assigned respondents of the baseline survey to either the treatment group ($n = 913$) or the placebo group that was targeted with a conversation about recycling ($n = 912$). Randomization was conducted at the household level ($n = 1295$), and because the design employs a placebo-control, the estimand of interest is the complier-average-treatment effect. Outcomes were measured by the online survey three days, three weeks, six weeks, and three months after the door-to-door

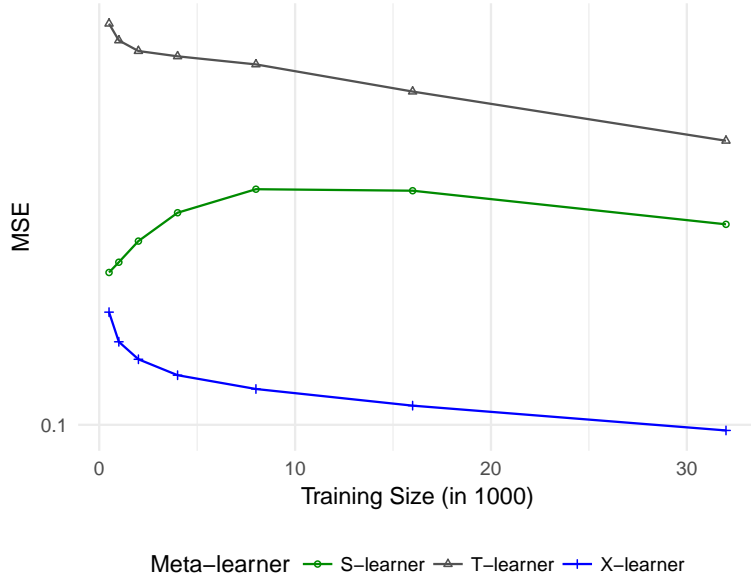


Figure 7: Simulation, Social pressure and Voter Turnout

conversations. We analyze results for the first follow-up.

The final experimental sample consists of only 501 observations. The experiment was well powered despite its small sample size because it includes a baseline survey of respondents as well as post-treatment surveys. The survey questions were designed to have high over-time stability. The R^2 of regressing the outcomes of the placebo-control group on baseline covariates using OLS is 0.77. Therefore, covariate adjustment greatly reduces sampling variation. There are 26 baseline covariates which include basic demographics (gender, age, ethnicity) and baseline measures of political and social attitudes and opinions about prejudice and views towards Miami’s nondiscrimination law.

The authors report an average treatment effect of 0.257 (SE: 0.075, t-stat: 3.4) on their transgender tolerance scale.⁷ The scale is coded so that a larger number implies greater tolerance. The variance of the scale is 1.14, with a minimum observed value of -2.3 and maximum observed value of 2. This is a large effect given the scale. For example, the estimated decrease in transgender prejudice is greater than Americans’ average decrease in homophobia from 1998 to 2012, when both are measured as changes in standard deviations of their respective scales.

The authors report finding no evidence of heterogeneity in the treatment effect that can be explained by the observed covariates. Their analysis is based on linear models (OLS, lasso and elastic net) (without basis expansions).⁸

Figure 8 presents our results for estimating the CATE using X-RF. We find that there is strong evidence that the positive effect that the authors find is only found among a subset of respondents, that can be targeted based on observed covariates. The average of our CATE estimates is indistinguishable from the ATE that the authors report.

Unlike our previous data example, there are marked differences in the treatment

⁷The authors’ transgender tolerance scale is the first principle component of combining five -3 to +3 Likert scales. See Brookman and Kalla (2016) for details.

⁸Brookman and Kalla (2016) estimate the CATE using Algorithm 4 in Appendix A.

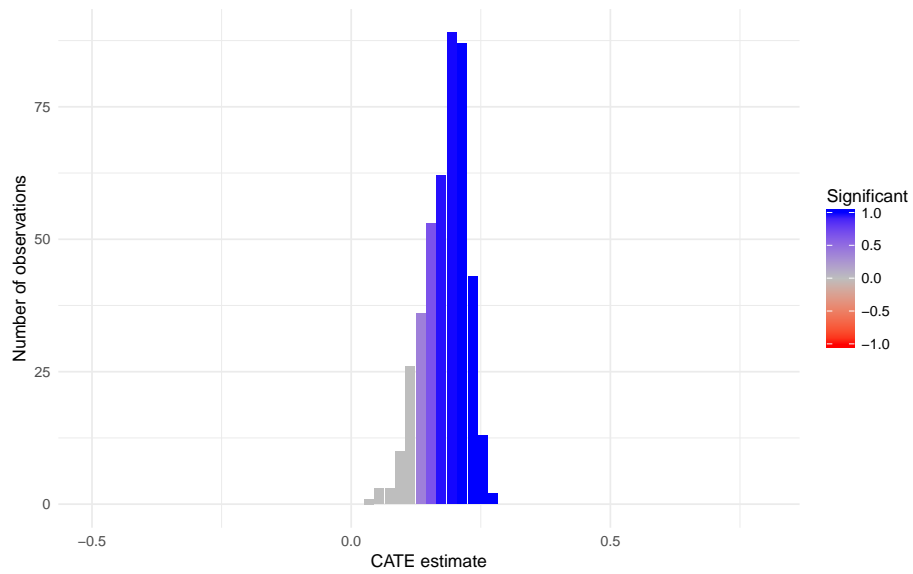


Figure 8: Reducing Transphobia: X-RF

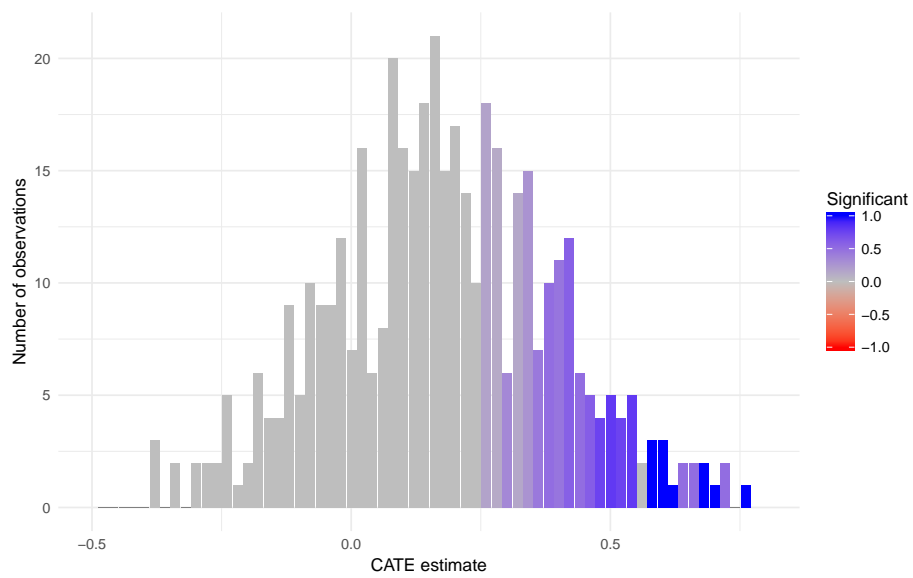


Figure 9: Reducing Transphobia: T-RF

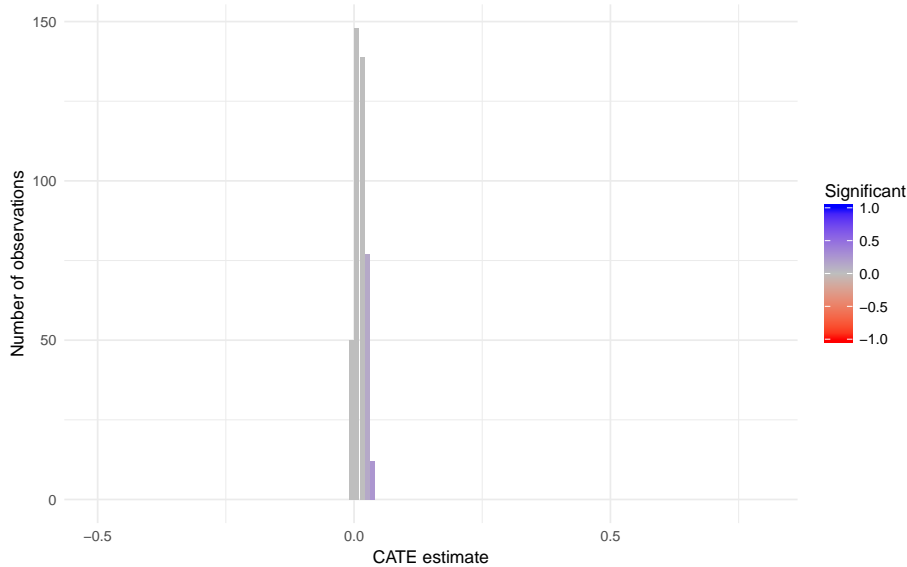


Figure 10: Reducing Transphobia: S-RF

Algorithm	RMSE	Bias
X-RF	1.102	0.0122
T-RF	1.090	0.0110
S-RF	1.207	-0.1073

Table 1: Reducing Transphobia: Simulation

effects estimated by our three learners. Figure 9 presents the estimates from T-RF. These estimates are similar to those of X-RF, but with a larger spread. Figure 10 presents the estimates from S-RF. Note that the average CATE estimate of S-RF is much lower than the ATE reported by the original authors and the average CATE estimates of the other two learners. And almost none of the CATE estimates are significantly different from zero. Recall that the ATE in the experiment was estimated with precision, and was large both substantively and statistically ($t\text{-stat}=3.4$).

In this data, S-RF appears to be shrinking the treatments estimates towards zero. The ordering of the estimates we see in this data application is often what we have observed in simulations: The S-learner has the least spread around zero, the T-learner has the largest spread, and the X-learner is somewhere in between.

Of course, with actual data we do not know what ground truth is. In order to better understand the performance of our learners in this data, we create a simulation study based on the application. However, we cannot use our previous real-data simulation design because the sample size is too small. Instead, we follow an approach used by previous authors and use matching to create ground truth. We take the experimental data, and conduct 1-to-1 matching based on the baseline measure of the respondents attitude towards Miami’s nondiscrimination law. We then split the sample in half, and use that for training and the balance for test. The simulation results are consistent with what we find when analyzing the actual data: X-RF and T-RF perform similarly, but S-RF shows markedly different behavior. Results are reported in Table 1. S-RF has a RMSE that is approximately 1.1 times higher than that of the other two algorithms

and a bias that is 10 times larger. S-RF is biased downward in this simulation, as we suspect it is in the actual data application. Unlike the previous data example, the covariates are strongly predictive of outcomes, and we suspect that pooling the data across treatment and control groups is not helpful because of the heterogeneity.

6 Conclusion

This paper reviews general meta-algorithms for CATE estimation including the T-learner and the S-learner. It then introduces a new meta-algorithm, the X-learner, that can translate any supervised learning algorithm or a combination of such algorithms into a CATE estimator in a number of stages. The hope is that the X-learner is adaptive to various settings. It is expected to perform particularly well when one of the treatment groups is much larger than the other or when the separate parts of the X-learner are able to exploit the structural properties of the response and treatment effect functions. This intuition is supported by theoretical results under specific regularity conditions on the response and CATE functions. Specifically, if the CATE function is linear, but the response functions in treatment and control only satisfy that they are Lipschitz continuous, the X-learner can still achieve the parametric rate, if one of the treatment groups is much larger than the other (Theorem 1). We have also shown that if there are no regularity conditions on the CATE function, but the response functions are Lipschitz continuous, then both the X-learner and the T-learner obtain the same minimax optimal rate for a particular feature distribution and treatment assignment (Theorem 2) and we expect this result to hold for more general data generating processes.

We have presented an extensive set of simulations to understand the finite sample behavior of different implementations of these learners. We have also examined two applications, each with accompanying simulations exercises. Although none of the meta-algorithms is always the best, the X-learner performs well, especially in the real data examples. In practice, in finite samples, there will always be gains to be had if one accurately judges the underlying data generating process. For example, if one thinks that the treatment effect is simple, or even zero, then pooling the data across treatment and control conditions will be beneficial when estimating the response model (i.e., the S-learner will perform well). However, if the treatment effect is strongly heterogeneous and the responses surfaces of the outcomes under treatment and control are very different, pooling the data will lead to worse finite sample performance (i.e., the T-learner will perform well). One hopes that the X-learner can adapt to these different settings. In the simulation and real data studies presented earlier, X-learner seems to adapt, but we would like to see more studies and more experience with real data on X-learner and other meta-algorithms from ourselves and others.

We are currently working on an alternative to X-learner, the U-learner, that takes advantage of situations where the propensity score is easy to estimate and when there is much confounding (Appendix A). The U-learner is in some sense similar to the ATE estimator of Chernozhukov et al. (2016), but for CATE estimation. We are also investigating using other supervised learning algorithms such as deep learning with the X-learner, and we recognize that work needs to be done on architecture design for deep learning algorithms to estimate CATE.

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A Pseudo Code

In this section, we use the following notation: Y^0 and Y^1 are the observed outcomes for the control and the treated group. For example, Y_i^1 is the observed outcome of the i th unit in the treated group. X^0 and X^1 are the features of the control and treated units, and hence, X_i^1 corresponds to the feature vector of the i th unit in the treated group. $M_k(Y \sim X)$ is here the notation for a regression estimator, which estimates $x \mapsto \mathbb{E}[Y|X = x]$.

Algorithm 1 T-learner

- 1: **procedure** T-LEARNER(X, Y^{obs}, W)
 - 2: $\hat{\mu}_0 = M_0(Y^0 \sim X^0)$ ▷ Estimate μ_1 and μ_0
 - 3: $\hat{\mu}_1 = M_1(Y^1 \sim X^1)$
 - 4: $\hat{\tau}(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x)$ ▷ Difference is the CATE estimator:
-

Algorithm 2 S-learner

- 1: **procedure** S-LEARNER(X, Y^{obs}, W)
 - 2: $\hat{\mu} = M(Y^{obs} \sim (X, W))$
 - 3: $\hat{\tau}(x) = \hat{\mu}(x, 1) - \hat{\mu}(x, 0)$
-

Algorithm 3 X-learner

- 1: **procedure** X-LEARNER(X, Y^{obs}, W, g)
 - 2: $\hat{\mu}_0 = M_1(Y^0 \sim X^0)$ ▷ Estimate response function
 - 3: $\hat{\mu}_1 = M_2(Y^1 \sim X^1)$
 - 4: $\tilde{D}_i^1 = Y_i^1 - \hat{\mu}_0(X_i^1)$ ▷ Compute pseudo residuals
 - 5: $\tilde{D}_i^0 = \hat{\mu}_1(X_i^0) - Y_i^0$
 - 6: $\hat{\tau}_1 = M_3(\tilde{D}^1 \sim X^1)$ ▷ Estimate CATE for treated and control
 - 7: $\hat{\tau}_0 = M_4(\tilde{D}^0 \sim X^0)$
 - 8: $\hat{\tau}(x) = g(x)\hat{\tau}_0(x) + (1 - g(x))\hat{\tau}_1(x)$ ▷ Average the estimates
-

$g(x) \in [0, 1]$ is a weighing function which is chosen to minimize the variance of $\hat{\tau}(x)$. It is sometimes possible to estimate $\text{Cov}(\tau_0(x), \tau_1(x))$, and compute the best g based on this estimate. However, we have made good experiences by choosing g to be an estimate of the propensity score.

Algorithm 4 F-learner

```
1: procedure F-LEARNER( $X, Y^{obs}, W$ )
2:    $\hat{e} = M_p[W \sim X]$ 
3:    $Y_i^* = Y_i^{obs} * (W_i - \hat{e}(X_i)) / \hat{e}(X_i)(W_i - \hat{e}(X_i))$ 
4:    $\hat{\tau} = M_\tau(Y^* \sim X)$ 
```

Algorithm 5 U-learner

```
1: procedure U-LEARNER( $X, Y^{obs}, W$ )
2:    $\hat{\mu}_{obs} = M_{obs}(Y^{obs} \sim X)$  ▷ Estimate  $\mu_m = E[Y^{obs}|X]$ 
3:    $\hat{e} = M_p[W \sim X]$  ▷ Estimate the p-score
4:    $R_i = (Y_i^{obs} - \hat{\mu}_{obs}(X_i)) / (W_i - \hat{e}(X_i))$ 
5:    $\hat{\tau} = M_\tau(R \sim X)$  ▷ Compute the main model
```

Algorithm 6 bootstrap Confidence intervals

```
1: procedure COMPUTECI(
   $x$ : feature vector of the training data,
   $w$ : treatment assignment of the training data,
   $y$ : observed outcome )
2:   for  $b$  in  $\{1, \dots, B\}$  do ▷ Sample  $n/2$  of the data
3:      $s = \text{sample}(1 : n, \text{replace} = \text{T}, \text{size} = \lceil n/2 \rceil)$ 
4:      $x_b^* = x_s$ 
5:      $w_b^* = w_s$ 
6:      $y_b^* = y_s$ 
7:      $\hat{\tau}_b^*(p) = \text{learner}(x_b^*, w_b^*, y_b^*)[p]$  ▷ Bootstrap CATE estimate for  $p$ :
8:    $\hat{\tau}(p) = \text{learner}(x, w, y)[p]$ 
9:    $\sigma = sd(\{\hat{\tau}_b^*(p)\}_{b=1}^B)$  ▷ Bootstrap standard deviation
10: return  $(\hat{\tau}(p) - q_{\alpha/2}\sigma, \hat{\tau}(p) + q_{1-\alpha/2}\sigma)$ 
```

Algorithm 7 T-learner — hyper parameter tuning

- 1: **procedure** T-LEARNER_TUNED(X, Y^{obs}, W)
 - 2: Tune θ_0 to minimize the EMSE($\mu_0, \hat{\mu}_0$) with $\hat{\mu}_0 = M_0(Y^0 \sim X^0, \theta_0)$ and call the best setting θ_0^* ,
 - 3: Tune θ_1 to minimize the EMSE($\mu_1, \hat{\mu}_1$) with $\hat{\mu}_1 = M_1(Y^1 \sim X^1, \theta_1)$ and call the best setting θ_1^* ,
 - 4: $\hat{\mu}_0 = M_0(Y^0 \sim X^0, \theta_0^*)$,
 - 5: $\hat{\mu}_1 = M_1(Y^1 \sim X^1, \theta_1^*)$,
 - 6: $\hat{\tau}(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x)$ ▷ Difference is the CATE estimator:
-

$M_w(Y^w \sim X^w, \theta_w)$ is here the notation for a machine learning method with tuning parameters θ_w . We do not identify the method for finding the best tuning parameters, because there are usually many methods of tuning a regression method, such as cross-validation with random search and out-of-bag-errors with gaussian process priors.

B Notes on the ITE

Example B.1 (D_i is not identifiable) Assume we observe a one-dimensional and uniformly distributed feature between 0 and 1, $X \sim \text{Unif}([0, 1])$, the treatment assignment was independent of the feature and Bernoulli distributed, $W \sim \text{Bern}(0.5)$, and the outcome under control was independent of the features and the treatment assignment, and it was Rademacher distributed,

$$P(Y(1) = 1) = P(Y(0) = -1) = 0.5.$$

Now consider two Data Generating Processes (DGP) identified by the distribution of the outcomes under treatment:

1. In the first DGP, the outcome under treatment is equal to the outcome under control:

$$Y(1) = Y(0),$$

2. In the second DGP, the outcome under treatment is the negative of the outcome under control:

$$Y(1) = -Y(0).$$

Note that the observed data, $\mathcal{D} = (Y_j^{obs}, X_j, W_j)_{1 \leq j \leq N}$, has the same distribution for both DGPs, but $D_i = 0$ for all i in the DGP 1, and $D_i \in \{-2, 2\}$ for all i in DGP 2. Thus no estimator based on \mathcal{D} for both DGPs can be consistent for D_i . The CATE, $\tau(X_i)$, is, however, equal to 0 in both DGP, and $\hat{\tau} \equiv 0$ is, for example, a consistent estimators for the CATE, $\tau(X_i)$.

C Convergence Rates Results

C.1 Theorem 1

C.1.1 Pointwise version of Theorem 1

First of all, we present here a pointwise version of Theorem 1.

Theorem 3 Assume we observe m control units and n treated units from some super population of independent and identically distributed observations $(Y(0), Y(1), X, W)$ coming from a distribution \mathcal{P} given in (1) that satisfies the following assumptions:

A1 The error terms ε_i are independent given X , with $\mathbb{E}[\varepsilon_i|X = x] = 0$ and $\text{Var}[\varepsilon_i|X = x] \leq \sigma^2$.

A2 Ignorability holds.

A3 There exists an estimator $\hat{\mu}_0$ with

$$\mathbb{E}[(\mu_0(x) - \hat{\mu}_0(x))^2] \leq C_x^0 m^{-a}.$$

A4 The treatment effect is parametrically linear, $\tau(x) = x^T \beta$, with $\beta \in \mathbb{R}^d$.

A5 The eigenvalues of the sample covariance matrix of the features of the treated units are well conditioned, in the sense that there exists an n_0 , such that

$$\sup_{n > n_0} \mathbb{E}[\gamma_{\min}^{-1}(\hat{\Sigma}_n)] < c_1 \quad \text{and} \quad \sup_{n > n_0} \mathbb{E}[\gamma_{\max}(\hat{\Sigma}_n)/\gamma_{\min}^2(\hat{\Sigma}_n)] < c_2. \quad (23)$$

Then the X -learner with $\hat{\mu}_0$ in the first stage, OLS in the second stage and weighing function $g \equiv 0$ has the following upper bound: for all $x \in \mathbb{R}^d$ and all $n > n_0$,

$$\mathbb{E}[\|\tau(x) - \hat{\tau}_X(x)\|^2] \leq C_x^1 m^{-a} + C_x^2 n^{-1}$$

with $C_x^1 = c_2 \|x\|^2 C_x^0$ and $C_x^2 = \sigma^2 d c_1 \|x\|^2$. In particular, if there are a lot of control units, such that $m/n^{1/a} \leq c_3$, then the X -learner achieves the parametric rate in n , or

$$\mathbb{E}[\|\tau(x) - \hat{\tau}_X(x)\|^2] \leq 2C_x^1 n^{-1}.$$

Proof. [Theorem 3]

In the following, we will write X instead of X^1 to simplify the notation. When using $g \equiv 0$ in (9), the X -learner will be equal to $\hat{\tau}_1$.

The pseudo residuals for the treated group can be written as

$$D_i^1 = Y_i - \hat{\mu}_0(X_i) = X_i \beta + \delta_i + \epsilon_i$$

with $\delta_i = \mu_0(X_i) - \hat{\mu}_0(X_i)$. In the second stage we estimate β using a simple OLS estimator,

$$\hat{\beta} = (X'X)^{-1} X' D^1.$$

We decompose the MSE of $\hat{\tau}(x)$ into two orthogonal error terms,

$$\begin{aligned} \mathbb{E}[(\tau(x) - \hat{\tau}_X(x))^2] &= \mathbb{E}[(x' \beta - x' \hat{\beta})^2] = \mathbb{E}[(x'(\beta - \hat{\beta}))^2] \leq \|x\|^2 \mathbb{E}[\|\beta - \hat{\beta}\|^2] \\ &= \|x\|^2 \mathbb{E}[\|(X'X)^{-1} X' \delta\|^2 + \|(X'X)^{-1} X' \epsilon\|^2]. \end{aligned} \quad (24)$$

Throughout the proof, we assume that $n > n_0$ such assumption A6 can be used. We will show that the second term decreases according to the parametric rate, n^{-1} , while the first term decreases with a rate of m^{-a} .

$$\begin{aligned} \mathbb{E}[(X'X)^{-1} X' \epsilon]^2 &= \mathbb{E}[\epsilon X (X'X)^{-1} (X'X)^{-1} X' \epsilon] \\ &= \mathbb{E}[\text{tr}(X (X'X)^{-1} (X'X)^{-1} X' \mathbb{E}[\epsilon \epsilon' | X])] \\ &\leq \sigma^2 \mathbb{E}[\text{tr}((X'X)^{-1})] \\ &= \sigma^2 \mathbb{E}[\text{tr}(\hat{\Sigma}_n^{-1})] n^{-1} \\ &\leq \sigma^2 d \mathbb{E}[\gamma_{\max}(\hat{\Sigma}_n^{-1})] n^{-1} \\ &\leq \sigma^2 d \mathbb{E}[\gamma_{\min}^{-1}(\hat{\Sigma}_n)] n^{-1} \\ &\leq \sigma^2 d c_1 n^{-1}. \end{aligned} \quad (25)$$

For the last inequality we used assumption A6.

Next, we are concerned with bounding the error coming from not perfectly predicting μ_0 :

$$\begin{aligned}
\mathbb{E}[\|(X'X)^{-1}X'\delta\|_2^2] &= \mathbb{E}[\|\hat{\Sigma}_n^{-1}X'\delta\|_2^2]n^{-2} \\
&\leq \mathbb{E}[\gamma_{\min}^{-2}(\hat{\Sigma}_n)\|X'\delta\|_2^2]n^{-2} \\
&\leq \mathbb{E}[\gamma_{\min}^{-2}(\hat{\Sigma}_n)\gamma_{\max}(XX')\|\delta\|_2^2]n^{-2} \\
&= \mathbb{E}[\gamma_{\min}^{-2}(\hat{\Sigma}_n)\gamma_{\max}(\hat{\Sigma}_n)\|\delta\|_2^2]n^{-1} \\
&= \mathbb{E}\left[\gamma_{\min}^{-2}(\hat{\Sigma}_n)\gamma_{\max}(\hat{\Sigma}_n)\mathbb{E}\left[\|\delta\|_2^2\middle|X\right]\right]n^{-1} \\
&\leq \mathbb{E}\left[\gamma_{\max}(\hat{\Sigma}_n)/\gamma_{\min}^2(\hat{\Sigma}_n)\right]C_x^0m^{-a} \\
&\leq c_2C_x^0m^{-a}.
\end{aligned} \tag{26}$$

here we used that $\gamma_{\max}(\hat{\Sigma}_n^{-2}) = \gamma_{\min}^{-2}(\hat{\Sigma}_n)$, and $\mathbb{E}\left[\|\delta\|_2^2\middle|X\right] = \mathbb{E}\left[\sum_{i=1}^n \delta^2(X_i)\middle|X\right] \leq n \sup_x \mathbb{E}\left[\delta^2(x)\middle|X\right] \leq nC_x^0m^{-a}$. Furthermore for the last statement, we used assumption A5.

C.1.2 Proof of Theorem 1

Proof. [Theorem 1]

This proof is very similar to the proof of Theorem 3. The difference is that here we evaluate the EMSE of the \mathcal{X} is random, and we have somewhat weaker assumptions, because $\hat{\mu}_0$ only satisfies that its EMSE converges at a rate of $-a$, but not necessary its MSE for every x .

We start with a similar decomposition as (24),

$$\begin{aligned}
\mathbb{E}[(\tau(\mathcal{X}) - \hat{\tau}_X(\mathcal{X}))^2] &= \mathbb{E}[(\mathcal{X}'\beta - \mathcal{X}'\hat{\beta})^2] = \mathbb{E}[(\mathcal{X}'(\beta - \hat{\beta}))^2] \leq \mathbb{E}[\|\mathcal{X}\|^2]\mathbb{E}[\|\beta - \hat{\beta}\|^2] \\
&= \mathbb{E}[\|\mathcal{X}\|^2]\mathbb{E}[\|(X'X)^{-1}X'\delta\|^2 + \|(X'X)^{-1}X'\varepsilon\|^2].
\end{aligned}$$

Following exactly the same steps as in (25), we receive

$$\mathbb{E}[\|(X'X)^{-1}X'\varepsilon\|^2] \leq \sigma^2 dC_\Sigma n^{-1}.$$

Bounding $\mathbb{E}[\|(X'X)^{-1}X'\delta\|^2]$ is now slightly different from (26),

$$\begin{aligned}
\mathbb{E}[\|(X'X)^{-1}X'\delta\|_2^2] &\leq \mathbb{E}[\gamma_{\min}^{-1}(X'X)\|X(X'X)^{-1}X'\delta\|_2^2] \\
&\leq \mathbb{E}[\gamma_{\min}^{-1}(X'X)\|\delta\|_2^2] \\
&\leq \mathbb{E}\left[\gamma_{\min}^{-1}(\Sigma_n)\frac{1}{n}\|\delta\|_2^2\right] \\
&\leq C_\Sigma \frac{1}{n} \sum_i \mathbb{E}[\|\delta_i\|_2^2] \\
&\leq C_\Sigma C_0 m^{-a}.
\end{aligned} \tag{27}$$

Lastly, we use the assumption that $\mathbb{E}[\|\mathcal{X}\|^2] \leq C_\mathcal{X}$ to conclude that

$$\mathbb{E}[(\tau(\mathcal{X}) - \hat{\tau}_X(\mathcal{X}))^2] \leq C_\mathcal{X}(C_\Sigma C_0 m^{-a} + \sigma^2 dC_\Sigma n^{-1}).$$

C.2 Proof of Theorem 2

The following is a more complete version of Theorem 2 in that it is more specific about the base learners used in this theorem. We will set $g \equiv 0$ which is equivalent to only analyzing $\hat{\tau}_1$. The analysis for $\hat{\tau}_0$ is equivalent.

Theorem 4 Assume $(X, W, Y(0), Y(1)) \sim \mathcal{P} \in \mathcal{D}_{mn}^L$. In particular, μ_0 and μ_1 are Lipschitz continuous with constant L ,

$$|\mu_w(x) - \mu_w(z)| \leq L\|x - z\| \quad \text{for } w \in \{0, 1\},$$

and $X \sim \text{Unif}([0, 1]^d)$ and let $\hat{\tau}^{mn}$ be the T -learner with

- $g \equiv 0$,
- the base learner of the first stage for the control, $\hat{\mu}_0$ is a KNN estimator with constant k_0 ,
- the base learner of the second stage for the treated group, $\hat{\mu}_1$, is a KNN estimator with constant k_1 .

Then $\hat{\tau}^{mn}$ is a consistent estimator for τ and there exists a constant C such that

$$\mathbb{E}\|\tau - \hat{\tau}^{mn}\|^2 \leq C \left(\frac{\sigma^2}{k_0} + L^2 \left(\frac{k_0}{m} \right)^{2/d} + \frac{\sigma^2}{k_1} + L^2 \left(\frac{k_1}{n} \right)^{2/d} \right). \quad (28)$$

Thus choosing

$$k_0 = (\sigma^2/L^2)^{\frac{d}{2+d}} m^{\frac{2}{d+2}} \quad (29)$$

$$k_1 = (\sigma^2/L^2)^{\frac{d}{2+d}} n^{\frac{2}{d+2}} \quad (30)$$

leads to the optimal rate as given in Theorem 5,

$$\mathbb{E}\|\tau - \hat{\tau}^{mn}\|^2 \leq c\sigma^{\frac{4}{d+2}} L^{\frac{2d}{2+d}} \left(m^{-2/(2+d)} + n^{-2/(2+d)} \right). \quad (31)$$

Lemma 1 Under the assumption of Theorem 2, $\hat{\mu}_0^m$ and $\hat{\mu}_1^n$ are consistent estimators for μ_0 and μ_1 and

$$\begin{aligned} \mathbb{E}[\|\hat{\mu}_0^m - \mu_0\|^2] &\leq \frac{\sigma^2}{k_m} + cL^2 \left(\frac{k_m}{m} \right)^{2/d}, \\ \mathbb{E}[\|\hat{\mu}_1^n - \mu_1\|^2] &\leq \frac{\sigma^2}{k_n} + cL^2 \left(\frac{k_n}{n} \right)^{2/d}. \end{aligned}$$

Proof. [Lemma 1] This is a direct implication of Theorem 6.2 in Györfi et al. (2006):

Lemma 2 Let $x \in [0, 1]^d$, $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Unif}([0, 1]^d)$ and $d > 2$. Define $\tilde{X}(x)$ to be the nearest neighbor of x , then there exists a constant c such that for all n ,

$$\mathbb{E}\|\tilde{X}(x) - x\|^2 \leq \frac{c}{n^{2/d}}.$$

Proof. [Lemma 2] First of all we consider

$$\mathbb{P}(\|\tilde{X}(x) - x\| \geq \delta) = (1 - \mathbb{P}(\|X_1 - x\| \leq \delta))^n \leq (1 - \tilde{c}\delta^d)^n \leq e^{-\tilde{c}\delta^d n} \quad (32)$$

Now we can compute the expectation:

$$\mathbb{E}\|\tilde{X}(x) - x\|^2 = \int_0^\infty \mathbb{P}(\|\tilde{X}(x) - x\| \geq \sqrt{\delta}) d\delta \quad (33)$$

$$\leq \int_0^d e^{-\tilde{c}\delta^{d/2} n} d\delta \quad (34)$$

$$\leq \int_0^d \min\left(1, \frac{1}{\tilde{c}\delta^{d/2} n}\right) d\delta \quad (35)$$

$$\leq \int_0^{(1/\tilde{c}n)^{2/d}} 1d\delta + \int_{(1/\tilde{c}n)^{2/d}}^d \frac{1}{\tilde{c}\delta^{d/2}n} d\delta \quad (36)$$

$$= \left(\frac{1}{\tilde{c}n}\right)^{2/d} + \frac{1}{\tilde{c}n} \left[\frac{d^{-d/2+1}}{-d/2+1} - \frac{(1/\tilde{c}n)^{-1+2/d}}{-d/2+1} \right] \quad (37)$$

$$\leq \frac{1 - \frac{1}{-d/2+1}}{(\tilde{c}n)^{2/d}} \quad (38)$$

Proof. [Theorem 2⁹] First of all we notice that in the third step, Equation (9), the two estimators from the second step are averaged:

$$\hat{\tau}^{mn}(x) = g(x)\hat{\tau}_0^{m,n}(x) + (1 - g(x))\hat{\tau}_1^{m,n}(x)$$

It is thus enough to show that these estimators from the second step achieve the optimal convergence rate. Furthermore, because of symmetry it is enough to restrict our analysis on $\hat{\tau}_1^{m,n}$.

We decompose this estimator as

$$\hat{\tau}_{m,n}^1(x) = \frac{1}{k_1} \sum_{i=1}^{k_1} [Y_{(i,n)}^1(x) - \hat{\mu}_0^m(X_{(i,n)}^1(x))] \quad (39)$$

$$= \hat{\mu}_1^n(x) - \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m(X_{(i,n)}^1(x)) \quad (40)$$

with the notation that $((X_{(1,n_w)}^w(x), Y_{(1,n_w)}^w(x)), \dots, (X_{(n_w,n_w)}^w(x), Y_{(n_w,n_w)}^w(x)))$ is a reordering of the tuples $(X_j^w(x), Y_j^w(x))$ such that $\|X_{(i,n_w)}^w(x) - x\|$ is increasing in i . With this notation we can write the estimators of the first stage as

$$\hat{\mu}_0^m(x) = \frac{1}{k_0} \sum_{i=1}^{k_0} Y_{(i,m)}^0(x), \quad (41)$$

$$\hat{\mu}_1^n(x) = \frac{1}{k_1} \sum_{i=1}^{k_1} Y_{(i,n)}^1(x), \quad (42)$$

$$(43)$$

and we can upper bound the problem with two terms:

$$\mathbb{E}[|\tau(\mathcal{X}) - \hat{\tau}_1^{m,n}(\mathcal{X})|^2] \quad (44)$$

$$= \mathbb{E}\left[\left|\mu_1(\mathcal{X}) - \mu_0(\mathcal{X}) - \hat{\mu}_1^n(\mathcal{X}) + \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m(X_{(i,n)}^1(\mathcal{X}))\right|^2\right] \quad (45)$$

$$\leq 2\mathbb{E}\left[|\mu_1(\mathcal{X}) - \hat{\mu}_1^n(\mathcal{X})|^2\right] + 2\mathbb{E}\left[\left|\mu_0(\mathcal{X}) - \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m(X_{(i,n)}^1(\mathcal{X}))\right|^2\right] \quad (46)$$

The first term is the regression problem for the first step of the X-learner and we can control this term with lemma 1,

$$\mathbb{E}[\|\mu_1 - \hat{\mu}_1^n\|^2] \leq \frac{\sigma^2}{k_1} + c_1 L^2 \left(\frac{k_1}{n}\right)^{2/d}. \quad (47)$$

⁹Many ideas of this proof are motivated by Györfi et al. (2006) and Bickel and Doksum (2015)

The second term is more challenging. To control it, we condition on the data $\mathcal{D} = (X_1^0, \dots, X_m^0, X_1^1, \dots, X_n^1)$ and the evaluation point, \mathcal{X} .

$$\frac{1}{2} \mathbb{E} \left[\left\| \mu_0(\mathcal{X}) - \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m(X_{(i,n)}^1(\mathcal{X})) \right\|^2 \right] \quad (48)$$

$$\leq \mathbb{E} \left\| \mu_0(\mathcal{X}) - \frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) \right\|^2 \quad (49)$$

$$+ \mathbb{E} \left\| \frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) - \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m(X_{(i,n)}^1(\mathcal{X})) \right\|^2 \quad (50)$$

This has the advantage that the second term, (50), can be bound as follows:

$$\begin{aligned} (50) &= \mathbb{E} \left(\frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) - Y_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right)^2 \\ &\leq \max_i \frac{1}{k_m^2} \sum_{j=1}^{k_0} \mathbb{E} \left(\mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) - Y_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right)^2 \\ &= \max_i \frac{1}{k_m^2} \sum_{j=1}^{k_0} \mathbb{E} \left[\mathbb{E} \left[\left(\mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) - Y_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right)^2 \middle| \mathcal{D}, \mathcal{X} \right] \right] \\ &\leq \frac{\sigma^2}{k_0} \end{aligned}$$

The last inequality follows from the assumption that conditional on \mathcal{D} ,

$$Y_{(j,m)}^0(x) \sim \mathcal{N}(\mu_0(X_{(j,m)}^0(x)), \sigma^2).$$

Next we upper bound (49):

$$(49) \leq \mathbb{E} \left(\frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \left\| \mu_0(\mathcal{X}) - \mu_0(X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X}))) \right\| \right)^2 \quad (51)$$

$$\leq \mathbb{E} \left(\frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} L \left\| \mathcal{X} - X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right\| \right)^2 \quad (52)$$

$$\leq L^2 \frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \mathbb{E} \left\| \mathcal{X} - X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right\|^2 \quad (53)$$

$$\leq L^2 \frac{1}{k_1} \sum_{i=1}^{k_1} \mathbb{E} \left\| \mathcal{X} - X_{(i,n)}^1(\mathcal{X}) \right\|^2 \quad (54)$$

$$+ L^2 \frac{1}{k_1 k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \mathbb{E} \left\| X_{(i,n)}^1(\mathcal{X}) - X_{(j,m)}^0(X_{(i,n)}^1(\mathcal{X})) \right\|^2 \quad (55)$$

where (53) follows with Jensen's inequality.

Let's consider (54): We partition the data into A_1, \dots, A_{k_1} sets, where the first $k_1 - 1$ sets have $\lfloor \frac{n}{k_1} \rfloor$ elements and we define $\tilde{X}_{i,1}(x)$ to be the nearest neighbor of x in A_i .

$$\frac{1}{k_1} \sum_{i=1}^{k_1} \mathbb{E} \left\| \mathcal{X} - X_{(i,n)}^1(\mathcal{X}) \right\|^2 \leq \frac{1}{k_1} \sum_{i=1}^{k_1} \mathbb{E} \left\| \mathcal{X} - \tilde{X}_{i,1}(\mathcal{X}) \right\|^2$$

$$\begin{aligned}
&= \frac{1}{k_1} \sum_{i=1}^{k_1} \mathbb{E} \left[\mathbb{E} \left[\left\| \mathcal{X} - \tilde{X}_{i,1}(\mathcal{X}) \right\|^2 \middle| \mathcal{X} \right] \right] \\
&\leq \frac{\tilde{c}}{\lfloor \frac{n}{k_1} \rfloor^{2/d}}
\end{aligned}$$

Where the last inequality follows from lemma 2. With exactly the same argument, we can bound (55) and we thus have:

$$(49) \leq L^2 \tilde{c} * \left(\frac{1}{\lfloor \frac{n}{k_1} \rfloor^{2/d}} + \frac{1}{\lfloor \frac{n_2}{k_2} \rfloor^{2/d}} \right) \leq 2\tilde{c}L^2 * \left(\left(\frac{k_1}{n} \right)^{2/d} + \left(\frac{k_0}{m} \right)^{2/d} \right)$$

Plugging everything in, we have

$$\mathbb{E}[|\tau(\mathcal{X}) - \hat{\tau}_1^{m,n}(\mathcal{X})|^2] \leq 2\frac{\sigma^2}{k_1} + 2(c_2 + 2\tilde{c})L^2 \left(\frac{k_1}{n} \right)^{2/d} + 2\frac{\sigma^2}{k_0} + 4\tilde{c}L^2 \left(\frac{k_0}{m} \right)^{2/d} \quad (56)$$

$$\leq C \left(\frac{\sigma^2}{k_1} + L^2 \left(\frac{k_1}{n} \right)^{2/d} + \frac{\sigma^2}{k_0} + \left(\frac{k_0}{m} \right)^{2/d} \right) \quad (57)$$

with $C = 2 \max(1, c_2 + 2\tilde{c}, 2\tilde{c})$.

C.3 Optimal Rate for the Balanced Case

Before, we derive the minimax optimal rate for \mathcal{D}_{mn}^L , we consider families of distributions which don't have any "extra" regularity conditions on the CATE, and all the smoothness for the CATE follows from the smoothness of the response functions. We define this set of families in Definition 5. First, recall the definition of S^* in Definition 1. For families in this class, there exists, an estimator $\hat{\mu}$ and constants c such that for all $n \geq 1$,

$$\sup_{\mathcal{P} \in F} \text{EMSE}(\hat{\mu}) \leq cn^{-a},$$

but for any $\tilde{a} > a$, there does not exist an estimator $\tilde{\mu}$, and a constant \tilde{c} , such that for all $n > 1$,

$$\sup_{\mathcal{P} \in F} \text{EMSE}(\hat{\mu}) \leq \tilde{c}n^{-\tilde{a}}.$$

Definition 5 • Let $H(F_0, F_1)$ be the class of distributions of $(Y(0), Y(1), W, X) \in \mathbb{R}^N \times \mathbb{R}^N \times \{0, 1\}^N \times [0, 1]^{d \times N}$ such that:

1. $N = m + n$,
2. the features, X_i , are iid uniformly distributed in $[0, 1]^d$,
3. there are exactly n treated units,

$$\sum_i W_i = n,$$

4. X and W are independent, and
- 5.

$$[(X, Y(0)) | W = 0] \in F_0,$$

$$[(X, Y(1)) | W = 1] \in F_1,$$

- For $a \in (0, 1]$, we define $G^*(a)$ to be the set of all families $H(F_0, F_1)$ with $F_0, F_1 \in S^*(a)$.

Theorem 5 (Minimax Lower Bound) Let $\hat{\tau}$ be an arbitrary estimator, $F \in G^*(a)$, and let $0 < a_1, a_2$, and c such that for all $n, m \geq 1$,

$$\sup_{\mathcal{P} \in F} \text{EMSE}(\mathcal{P}, \hat{\tau}) \leq c(m^{-a_0} + n^{-a_1}), \quad (58)$$

then a_1 and a_2 are at most a ,

$$a_0, a_1 \leq a.$$

Proof. [Theorem 5]

We will show that $a_1 \leq a$. The proof for a_0 is mathematically symmetric. Assume a_1 was bigger than a , then we will show that there exists a sequence of estimators $\hat{\mu}_{1n}$, such that

$$\sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{D_1^n \sim \mathcal{P}_1^n} \left[(\mu_1(\mathcal{X}) - \hat{\mu}_{1n}(\mathcal{X}; \mathcal{D}_1^n))^2 \right] \leq 2cn^{-a_1}$$

which is a contradiction, since $[(X, Y(1)) | W = 1] \sim \mathcal{P}_1 \in F_1 \in S^*(a)$.

Let \tilde{P}_0 be an arbitrary distribution in F_0 , and compute,

$$c(m^{-a_0} + n^{-a_1}) \geq \sup_{\mathcal{P} \in F} \mathbb{E}_{(\mathcal{D}_0^m \times \mathcal{D}_1^n) \sim \mathcal{P}} [(\tau(\mathcal{X}) - \hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n))^2] \quad (59)$$

$$= \sup_{\mathcal{P}_1 \in F_1} \sup_{\mathcal{P}_0 \in F_0} \mathbb{E}_{(\mathcal{D}_0^m \times \mathcal{D}_1^n) \sim \mathcal{P}_0^m \times \mathcal{P}_1^n} [(\tau(\mathcal{X}) - \hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n))^2] \quad (60)$$

$$\geq \sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{(\mathcal{D}_0^m \times \mathcal{D}_1^n) \sim \tilde{\mathcal{P}}_0^m \times \mathcal{P}_1^n} [(\tau(\mathcal{X}) - \hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n))^2] \quad (61)$$

$$= \sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{D_1^n \sim \mathcal{P}_1^n} \left[\mathbb{E}_{\mathcal{D}_0^m \sim \tilde{\mathcal{P}}_0^m} [(\tau(\mathcal{X}) - \hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n))^2] \right] \quad (62)$$

$$\geq \sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{D_1^n \sim \mathcal{P}_1^n} [(\tau(\mathcal{X}) - \mathbb{E}_{\mathcal{D}_0^m \sim \tilde{\mathcal{P}}_0^m} [\hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n)])^2] \quad (63)$$

$$= \sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{D_1^n \sim \mathcal{P}_1^n} [(\mu_1(\mathcal{X}) - \mu_0(\mathcal{X}) - \mathbb{E}_{\mathcal{D}_0^m \sim \tilde{\mathcal{P}}_0^m} [\hat{\tau}(\mathcal{X}; \mathcal{D}_0^m, \mathcal{D}_1^n)])^2] \quad (64)$$

Choose a sequence m_n in such a way that $c(m_n^{-a_1} + n^{-a_2}) \leq 2cn^{-a_1}$, and finally define

$$\hat{\mu}_{1n}(x; \mathcal{D}_1^n) = \mu_0(x) - \mathbb{E}_{\mathcal{D}_0^{m_n} \sim \tilde{\mathcal{P}}_0^{m_n}} [\hat{\tau}(x; \mathcal{D}_0^{m_n}, \mathcal{D}_1^n)].$$

Now (64) implies that

$$\sup_{\mathcal{P}_1 \in F_1} \mathbb{E}_{D_1^n \sim \mathcal{P}_1^n} [(\mu_1(\mathcal{X}) - \hat{\mu}_{1n}(\mathcal{X}; \mathcal{D}_1^n))^2] \leq c(m_n^{-a_0} + n^{-a_1}) \leq 2cn^{-a_1},$$

which is a contradiction to $F_1 \in S(a)$.

Theorem 6 $D_{mn}^L \in G^*(2/(2+d))$, and therefore the best possible rate of any estimator is given by

$$\mathcal{O}(n^{2/(2+d)} + m^{2/(2+d)}).$$

Proof. [Theorem 6] Note that $D_{mn}^L = H(F^L, F^L)$.