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 supervised learning or regression method in machine learning and statistics to estimate the Conditional Average Treatment Effect (CATE) function. Meta-algorithms build on base algorithms—such as Random Forests (RF), Bayesian Additive 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 in another, and it can exploit structural properties of the CATE function. For example, if the CATE function is 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 extensive simulation studies, the X–learner performs favorably, although none of the meta-learners is uniformly the best. In two persuasion field experiments from political science, we demonstrate how our new X–learner can be used to target treatment regimes and to better understand causal mechanisms. We introduce a new estimator called the X–learner, and we characterize it and many CATE estimators into a unified meta-learner framework. Their performance is compared using extensive simulations, theory, and two data sets from randomized field experiments in political science.

In the first randomized experiment, we estimate the effect of a mailer on voter turnout (1), and in the second, we measure the effect of door-to-door conversations on prejudice against gender nonconforming individuals (2). In both experiments, the treatment effect is found to be non–constant, and we quantify this heterogeneity by estimating the CATE. We obtain insights into the underlying mechanisms, and the results allow researchers to better target the treatment.

To estimate the CATE, we build on regression or supervised learning methods in statistics and machine learning, which are widely used and successful in a wide range of applications. Specifically, we study meta-algorithms or meta-learners for estimating the CATE. They decomposed estimating the CATE into several sub-regression problems that can be solved with any regression or supervised learning method.

The most common meta-algorithm for estimating heterogeneous treatment effects takes two steps. First, it uses so-called base learners to estimate the conditional expectations of the outcomes given predictors under control and treatment separately. In randomized experiments and observational studies. Instead, they often seek to estimate Conditional Average Treatment Effects (CATE) to personalize treatment regimes and to better understand causal mechanisms. We introduce a new estimator called the Two-Tree estimator and we will, there-
The rest of the paper is organized as follows. We start with a formal introduction of the meta-learners and provide intuitions for why we can expect the X–learner to perform well when the CATE is smoother than the response outcome functions and when the sample sizes between treatment and control are unequal. We then present the results of an extensive simulation study and provide advice for practitioners before we present theoretical results on the convergence rate for different meta-learners. Finally, we examine two field experiments using several meta-algorithms and illustrate how the X–learner can find useful heterogeneity with fewer observations.

Framework and Definitions

We employ the Neyman-Rubin potential outcome framework (10 11), and assume a super population or distribution \( \mathcal{P} \) from which a realizations of \( N \) independent random variables are given as the training data. That is, \( (Y_i(0), Y_i(1), X_i, W_i) \sim \mathcal{P} \), 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 \( i \) is assigned to the control group, and \( Y_i(1) \) is the potential outcome when \( i \) is assigned to the treatment group. With this definition, the Average Treatment Effect is defined as

\[
\text{ATE} := E[Y(1) - Y(0)].
\]

It is also useful to define the response under control, \( \mu_0 \), and the response under treatment, \( \mu_1 \), as

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

Furthermore, we use the following representation of \( \mathcal{P} \):

\[
\begin{align*}
X &\sim \Lambda, \\
W &\sim \text{Bern}(\epsilon(X)), \\
Y(0) &\equiv \mu_0(X) + \epsilon(0), \\
Y(1) &\equiv \mu_1(X) + \epsilon(1),
\end{align*}
\]

where \( \Lambda \) is the marginal distribution of \( X \), \( \epsilon(0) \) and \( \epsilon(1) \) are noise random variables with mean zero conditioning on \( X \), and \( \epsilon(x) = \mathbb{P}(W = 1|X = x) \) 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. Hence we denote the observed data as

\[
\mathcal{D} = (Y_i, X_i, W_i)_{1 \leq i \leq N},
\]

with \( Y_i = Y_i(W_i) \). Note that the distribution of \( \mathcal{D} \) is specified by \( \mathcal{P} \). To avoid the problem that with a small
but non-zero probability all units are under control or under treatment, we will analyze the behavior of different estimators conditional on the number of treated units. That is, for a fixed $n$ with $0 < n < N$, we condition on the event that

$$\sum_{i=1}^{N} W_i = n.$$  

This will enable us to state the performance of an estimator in terms of the number of treated units $n$ and the number of control units $m = N - n$.

For a new unit $i$ with covariate vector $x_i$, in order to decide whether to give the unit the treatment, we wish 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 $D_i$ is not identifiable without strong additional assumptions because one can construct data generating processes with the same distribution of the observed data, but different $D_i$ (Example 2). Instead, we will estimate the CATE function which is defined as

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

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

$$E[(D_i - \hat{\tau})^2|X_i = x_i] = E[(D_i - \tau(x_i) + \tau(x_i) - \hat{\tau})^2|X_i = x_i]$$

and

$$E[(D_i - \tau(x_i))^2|X_i = x_i] + E[(\tau(x_i) - \hat{\tau})^2].$$

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 with a small Expected Mean Squared Error (EMSE) for estimating the CATE,

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

The expectation is here taken over $\hat{\tau}$ and $X \sim \Lambda$ which is independent of $\tau$ and has the same distribution of the features $X$.

To aid our ability to estimate $\tau$, we need to assume that there are no hidden confounders (12):

**Condition 1**

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

This assumption is, however, not sufficient to identify the CATE. One additional assumption that is often made to obtain identifiability of the CATE in the support of $X$ is to assume that the propensity score is bounded away from 0 and 1,

**Condition 2** There exists $e_{\min}$ and $e_{\max}$ such that for all $x$ in the support of $X$,

$$0 < e_{\min} < e(x) < e_{\max} < 1.$$  

**Meta-Algorithms**

In this section, we formally define a meta-algorithm (or meta-learner) for the CATE as the result of combining supervised learning or regression estimators (i.e., base learners) in a specific manner while allowing the base learners to take on any form. Meta-algorithms thus have the flexibility to appropriately leverage different sources of prior information in separate sub-problems of the CATE estimation problem: they can be chosen to fit a particular type of data, and they can directly take advantage of existing data analysis pipelines.

We first review both T and S learners, and we then propose the X–learner, which is a new meta-algorithm that can take advantage of unbalanced designs (i.e., the control or the treated group is much larger than the other group) and existing structures of the CATE (e.g., smoothness or sparsity). Obviously, flexibility is a gain only if the base learners in the meta-algorithm match the features of the data and the underlying model well.

The T–learner takes two steps. First, the control response function,

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

is estimated by a base learner, which could be any supervised learning or regression estimator using the observations in the control group, $\{(X_i, Y_i)\}_{W_i = 0}$. We denote the estimated function as $\hat{\mu}_0$. Second, we estimate the treatment response function,

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

with potentially a different base learner using the treated observations and we denote the estimator as $\hat{\mu}_1$. A T–learner is then obtained as

$$\hat{\tau}_T(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x).$$

Pseudo code for this T–learner can be found in Algorithm 1.

In the S–learner, the treatment indicator is included as a feature similar to all 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 base learner (supervised machine learning or regression algorithm) on the entire data set. We denote the estimator as \( \hat{\mu} \). The CATE estimator is then given by
\[ \hat{\tau}_S(x) = \hat{\mu}(x, 1) - \hat{\mu}(x, 0), \quad (4) \]
and pseudocode is provided in Algorithm 2.

There are other meta-algorithms in the literature, but we do not discuss them here in detail because of limited space. For example, one may transform the outcomes further, but it may do well in other settings.

**X–learner**

We propose the X–learner, and provide an illustrative example to highlight its motivations. The basic idea of the X–learner can be described in three stages:

1. Estimate the response functions
\[ \mu_0(x) = \mathbb{E}[Y(0)|X = x], \quad \text{and} \quad \mu_1(x) = \mathbb{E}[Y(1)|X = x], \quad (5, 6) \]
using any supervised learning or regression algorithm and denote the estimated functions \( \hat{\mu}_0 \) and \( \hat{\mu}_1 \). The algorithms used are referred to as the base learners for the first stage.

2. Impute the treatment effects for the individuals in the treated group based on the control outcome estimator, and the treatment effects for individuals in the control group based on the treatment outcome estimator, that is:
\[ \hat{D}^1_i := Y^1_i - \hat{\mu}_0(X^1_i), \quad \text{and} \quad \hat{D}^0_i := \hat{\mu}_1(X^0_i) - Y^0_i, \quad (7, 8) \]
and call these the imputed treatment effects.

We can employ any supervised learning or regression method(s) to estimate \( \tau(x) \) in two ways: using the imputed treatment effects 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 the supervised learning or regression algorithms 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.

**Figure 1:** Intuition behind the X–learner with an unbalanced design.

See Algorithm 3 for pseudo code.

**Remark 1** \( \hat{\tau}_0 \) and \( \hat{\tau}_1 \) are both estimators for \( \tau \). While \( g \) is chosen to combine these 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 estimate the covariance matrix of \( \hat{\tau}_1 \) and \( \hat{\tau}_0 \). One may then wish to choose \( g \) to minimize the variance of \( \hat{\tau} \).

**Intuition behind the meta–learners**

The X–learner can use information from the control group to derive better estimators for the treatment group and vice versa. We will illustrate this using a simple example. Suppose we want to study a treatment, and we are interested 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 units 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, let us only look at the treated outcome. When we 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 \( \mu_1 \). For the control group, we notice observations with \( x \in [0, 0.5] \) seem to be different, and we end up modeling \( \hat{\mu}_0(x) = \mathbb{E}[Y(0) | X = x] \) with a piecewise linear function with jumps at 0 and 0.5 (solid line). This is a relatively complex function, but we are not worried about overfitting since we observe many data points.

The \( T \)-learner would now use estimator \( \hat{\tau}_T(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x) \) (see Figure 1(c) solid line), which is a relatively complicated function with jumps at 0 and 0.5, while the true \( \tau(x) \) is a constant. This is, however, problematic because we are estimating a complex CATE function based on ten observations in the treated group.

When choosing an estimator for the treatment group, we correctly avoided overfitting, and we found a good estimator for the treatment response function, but as a result, we chose a relatively complex estimator for the CATE—the quantity of interest. We should have selected a piecewise linear function with jumps at 0 and 0.5, but this is, of course, unreasonable when just looking at the treated group. If we were to also take the control group into account, this function may be a natural choice. In other words, we should change our objective for \( \hat{\mu}_1 \) and \( \hat{\mu}_0 \). We want to estimate \( \hat{\mu}_1 \) and \( \hat{\mu}_0 \) in such a way that their difference is a good estimator for \( \tau \).

The \( X \)-learner enables us to do exactly that. It allows us to use structural information about the CATE and to make efficient use of an unbalanced design. The first stage of the \( X \)-learner is the same as the first stage of the \( T \)-learner, but in its second stage, the estimator for the controls is subtracted from the observed treated outcomes and similarly the observed control outcomes are subtracted from estimated treatment outcomes to obtain the imputed treatment effects,

\[
\begin{align*}
\hat{D}_1^1 &:= Y_1^1 - \hat{\mu}_0(X_1^1), \\
\hat{D}_0^1 &:= \hat{\mu}_1(X_0^1) - Y_0^1.
\end{align*}
\]

Here we use the notation that \( Y_i^0 \) and \( Y_i^1 \) are the \( i \)th observed outcome of the control and the treated group, respectively. \( X_1^1, X_0^1 \) are the corresponding feature vectors. Figure 1(b) shows the imputed treatment effects, \( \hat{D} \). By choosing a simple—here linear—function to estimate \( \tau_1(x) = \mathbb{E}[\hat{D}_1^1 | X_1 = x] \) we effectively estimate a model for \( \mu_1(x) = \mathbb{E}[Y^1 | X = x] \), which has a similar shape to \( \hat{\mu}_0 \).

We can see that by choosing a relatively poor model for \( \mu_1(x) \), \( \hat{D}_0^1 \) is relatively far away from \( \tau(x) \). The model for \( \tau_0(x) = \mathbb{E}[\hat{D}_0^0 | X = x] \) will thus be relatively poor. However, our final estimator combines these two estimators according to

\[
\hat{\tau}(x) = g(x)\hat{\tau}_0(x) + (1 - g(x))\hat{\tau}_1(x).
\]

If we choose \( g(x) = \hat{e}(x) \), an estimator for the propensity score, \( \hat{\tau} \) will be very similar to \( \hat{\tau}_1(x) \), since we have many more observations in the control group—i.e., \( \hat{e}(x) \) is small.

Figure 1(c) shows the \( T \)-learner and the \( X \)-learner. It is difficult to assess the general behavior of the \( S \)-learner in this examples because we must choose a base learner. For example, when we use RF as the base learner for this data set, the \( S \)-learner’s first split is on the treatment indicator in 97.5% of all trees in our simulations because the treatment assignment is very predictive of the observed outcome, \( Y \) (also see Figure 1). From there on, the \( S \)-learner and \( T \)-learner are the same, and we observe them to perform similarly poorly in this example.

**Simulation Results**

We conduct an extensive simulation study to compare the different meta-learners, and in this section, we summarize our findings and provide general remarks on the strengths and weaknesses of the \( S \), \( T \), and \( X \) learners while leaving details to the SI. The simulations are key to providing an understanding of the performance of the methods we consider for model classes that are not covered by our theoretical results.

Our simulation study is designed to consider a range of situations, making sure to include conditions where we think that the \( S \)-learner or the \( T \)-learner are likely to perform the best, and we include simulations setups proposed by previous researchers \( (12) \). We consider cases where the treatment effect is zero for all units and so pooling treatment and control groups is advantageous, and cases where the treatment and control response functions are completely different and so pooling would be harmful. We consider cases with and without confounding, and cases with equal and unequal sample sizes across treatment conditions. All simulations discussed in this section are based on synthetic data. For details, please see Section A. We provide additional simulations based on actual data when we discuss our applications.

We compare the \( S \), \( T \), and \( X \) learners with RF and BART as base learners. We implemented a version of RF for which the tree structure is independent of the leaf prediction given the observed features, so called honest RF in an R package called \texttt{hte} \((13)\). This version of RF is particularly accessible from a theoretical point of view, it performs well in noisy settings, and it is better suited for inference \((7, 16)\). For BART, our software uses the \texttt{dbarts} \((17)\) implementation for the base learner.

Comparing the use of different base learners enables us to demonstrate two things. On the one hand, it shows
that the conclusions we draw about the S, T and X learner are not specific to a particular base learner and on the other hand, it demonstrate that the choice of base learners can make a large difference in the prediction accuracy. The latter is an important advantage of meta-learners since subject knowledge can be used to choose base learners that perform well. For example, in Simulations 2 and 3, the response functions are globally linear, and we observe that estimators which act globally such as BART have a significant advantage in these situations or when the data set is small. If, however, there is no global structure or when the data set is large, then more local estimators such as RF seem to have an advantage (Simulations 3 and 5).

We observe that the choice of meta-learner can make a large difference, and for each meta-learner there exist cases where it is the best performing estimator.

The S-learner is treating the treatment indicator like any other predictor. For some base learners such as k-nearest neighbors it is not a sensible estimator, but for others, it can perform well. Since the treatment indicator is given no special role, algorithms such as the lasso and regression trees can completely ignore the treatment assignment by not choosing/splitting on it. This is excellent if the CATE is in many places 0 (Simulations 2 and 3), but—as we will see in our second data example—the S-learner can be biased towards 0.

The T-learner, on the other hand, does not combine the treated and control groups. This can be a disadvantage when the treatment effect is very complicated, and there are no common trends in the treatment groups is much larger than the other (Simulation 1 and 3). In the case where the CATE is 0, it is significantly better than the T-learner (Simulations 4 and 5). In the case where the CATE is 0, it usually does not perform as well as the S-learner, but it is significantly better than the T-learner (Simulations 1, 5 and 6). In the case of a very complex CATE, it often even outperforms the T-learner (Simulations 2 and 6). These simulation results have led us to the conclusion that unless one has a strong belief that the CATE is mostly 0, as a rule of thumb, one should use the X-learner with BART for small datasets and RF for bigger ones. In the sections to come, we will further support these claims with additional theoretical results and empirical evidence from real data and data-inspired simulations.

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 to rigorously formulate intuitions regarding when the X-learner is desirable. They corroborate our intuition that the X-learner outperforms the T-learner when one group is much larger than the other group and 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 nonparametric regression estimation (18, 19, 20). In the standard regression problem, one observes N independent and identically distributed tuples \((X_i, Y_i)\), \(i = 1, \ldots, N\) 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),

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

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 \(\mu\) is unknown. 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 about the problem). To make this problem feasible, a typical approach is the minimax approach where one analyzes the worst performance of an estimator over a family, \(\mathcal{F}\), of distributions (21). The goal is to find an estimator which has a small EMSE for all distributions in this family. For example, if \(\mathcal{F}_0\) is the family of distributions \(\mathcal{P}\) such that \(Y \sim \text{Unif}[0,1]\), \(Y = \beta X + \epsilon\), \(\epsilon \sim \text{N}(0,1)\), and \(\beta \in \mathbb{R}\), then it is well known that the OLS estimator achieves the optimal parametric rate. That is, there exists a constant \(C \in \mathbb{R}\) such that for all \(\mathcal{P} \in \mathcal{F}_0\),

\[
\text{EMSE}(\mathcal{P}, \hat{\mu}_{\text{OLS}}) \leq CN^{-1}.
\]

If, however, \(\mathcal{F}_1\) is the family of all distributions \(\mathcal{P}\) such that \(X \sim \text{Unif}[0,1]\), \(Y \sim \mu(X) + \epsilon\) and \(\mu\) is a Lipschitz continuous function with bounded Lipschitz constant, then there exists no estimator that achieves the parametric rate uniformly for all possible distributions in \(\mathcal{F}_1\). To be precise, we can at most expect to find an estimator that achieves a rate of \(N^{-2/3}\) and there exists a constant \(C'\), such that

\[
\liminf_{N \to \infty} \inf_{\hat{\mu}_N} \sup_{\mathcal{P} \in \mathcal{F}_1} \frac{\text{EMSE}(\mathcal{P}, \hat{\mu}_N)}{N^{-2/3}} > C'> 0.
\]

Estimators such as Nadaraya-Watson and k-nearest neighbors can achieve this optimal rate (20, 22).
Crucially, the fastest rate of convergence that 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 sets of families for which particular rates are achieved.

**Definition 1 (Families with bounded minimax rate)**

For \( a \in (0, 1] \), we define \( S(a) \) to be the set of all families, \( F \), with a minimax rate of at most \( N^{-a} \).

Note that for any family \( F \in S(a) \) there exists an estimator \( \hat{\mu} \) and a constant \( C \) such that for all \( N \geq 1 \),

\[
\sup_{\mathcal{P} \in F} \text{EMSE}(\mathcal{P}, \hat{\mu}_N) \leq CN^{-a}.
\]

From the examples above, it is clear that \( F_0 \in S(1) \) and \( F_1 \in S(2/3) \).

Even though the minimax rate of the 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 that we believe based on domain information could be relevant in practice, then we might expect \( \hat{\mu} \) to have a large EMSE in real data.

**Implication for CATE estimation**

Let us now employ the minimax approach to the problem of estimating the CATE. Recall that we assume a superpopulation, \( \mathcal{P} \), of random variables \((Y(0), Y(1), X, W)\) according to \( \mathcal{F} \), and we observe \( N \) outcomes, \((X_i, W_i, Y_{i\text{obs}})_{i=1}^N \). To avoid the problem that with a small but non-zero probability all units are treated or untreated, we analyze the expected mean squared error of an estimator given that there are \( 0 < n < N \) treated units.

\[
\text{EMSE}(\mathcal{P}, \hat{\tau}^{mn}) = \mathbb{E} \left[ (\tau(X) - \hat{\tau}^{mn}(X))^2 \right] \sum_{i=1}^N W_i = n.
\]

The expectation is taken over the observed data, \((X_i, W_i, Y_i)_{i=1}^N \), given that we observe \( n \) treated units, and \( X \) which is distributed according to \( \mathcal{F} \).

Similar to Definition 1, we characterize families of superpopulations by the rates at which the response functions and the CATE function can be estimated.

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1 Refer to Section E for a careful treatment of the distributions involved.

**Definition 2 (Superpopulations with given rates)**

For \( a_\mu, a_\tau \in (0, 1] \), we define \( S(a_\mu, a_\tau) \) to be the set of all families of distributions \( \mathcal{P} \) of \((Y(0), Y(1), X, W)\) such that ignorability holds (Condition 1), the overlap condition (Condition 2) is satisfied, and the following conditions hold.

1. The distribution of \((X, Y(0))\) given \( W = 0 \) is in a family \( F_0 \in S(a_\mu) \).
2. The distribution of \((X, Y(1))\) given \( W = 1 \) is in a family \( F_1 \in S(a_\mu) \).
3. The distribution of \((X, \mu_1(X) - Y(0))\) given \( W = 0 \) is in a family \( F_{\tau_0} \in S(a_\tau) \), and
4. The distribution of \((X, Y(1) - \mu_0(X))\) given \( W = 1 \) is in a family \( F_{\tau_1} \in S(a_\tau) \).

A simple example of a family in \( S(2/3, 1) \) is the set of distributions \( \mathcal{P} \) for which \( X \sim \text{Unif}[0, 1] \), \( W \sim \text{Bern}(1/2) \), \( \mu_0 \) is any Lipschitz continuous function, \( \tau \) is linear, and \( \varepsilon(0), \varepsilon(1) \) are independent standard normal distributed.

We can also build on existing results from the literature to characterize many families in terms of smoothness conditions on the CATE and on the response functions.

**Example 1** Let \( C > 0 \) be an arbitrary constant and consider the family, \( F_2 \), of distributions for which \( X \) has compact support in \( \mathbb{R}^d \), the propensity score \( e \) is bounded away from 0 and 1 (Condition 2), \( \mu_0, \mu_1 \) are \( C \) Lipschitz continuous, and the variance of \( \varepsilon \) is bounded. Then it follows (20) that

\[
F_2 \in S \left( \frac{2d}{2 + d}, \frac{2d}{2 + d} \right).
\]

Note that we don’t have any assumptions on \( X \) apart from its support being bounded. If we are willing to make assumptions on the density (e.g., \( X \) is uniformly distributed), then we can characterize many distributions by the smoothness conditions of \( \mu_0, \mu_1, \) and \( \tau \).

**Definition 3** Let \( p = k + \beta \) for some \( k \in \mathbb{N} \) and \( 0 < \beta \leq 1 \), and let \( C > 0 \). A function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) is called \((p, C)\)-smooth if for every \( \alpha = (\alpha_1, \ldots, \alpha_d) \), \( \alpha_i \in \mathbb{N} \), \( \sum_{j=1}^d \alpha_j = k \) the partial derivative \( \frac{\partial^k f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \) exists and satisfies

\[
\left| \frac{\partial^k f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}(x) - \frac{\partial^k f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}(z) \right| \leq C \|x - z\|^\beta.
\]

**Example 2** Let \( C_1, C_2 \) be arbitrary constants and consider the family, \( F_3 \), of distributions for which \( X \sim \text{Unif}[0, 1]^d \), \( e \equiv c \in (0, 1) \), \( \varepsilon \) is two-dimensional normally distributed, \( \mu_0 \) and \( \mu_1 \) are \((p_\mu, C_1)\)-smooth, and \( \tau \)
is $(p_r, C_2)$-smooth. Then it follows \[ F_3 \in S \left( \frac{2d}{2p_\mu + d}, \frac{2d}{2p_r + d} \right). \]

Let us intuitively understand the difference between the T and X learners. The T-Learner splits the problem of estimating the CATE into the two subproblems of estimating $\hat{\mu}_0$ and $\hat{\mu}_1$ separately. By appropriately choosing the base learners, we can expect to achieve the minimax optimal rates of $m^{-a_r}$ and $n^{-a_r}$ respectively,

$$\sup_{\mathcal{P}_0 \in \mathcal{F}_0} \text{EMSE}(\mathcal{P}_0, \hat{\mu}_0^{m}) \leq C \, m^{-a_r},$$

$$\sup_{\mathcal{P}_1 \in \mathcal{F}_1} \text{EMSE}(\mathcal{P}_1, \hat{\mu}_1^{n}) \leq C \, n^{-a_r},$$

where $C$ is some constant. Those rates translate immediately to rates for estimating $\tau$,

$$\sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_T^{m}) \leq C \, (m^{-a_r} + n^{-a_r}).$$

In general, we cannot expect to do better than this, when using an estimation strategy that falls in the class of T-Learners, because the subproblems in Equation 10 are treated completely independently and there is nothing to be learned from the treatment group about the control group and vice versa.

In Section \[ \ref{sec:application} \] we present a careful analysis of this result and we prove the following theorem.

**Theorem 1 (Minimax rates of the T–learner)** For a family of superpopulations, $F \in S(a_\mu, a_r)$, there exist base learners to be used in the T–learner so that the corresponding T–learner estimates the CATE at a rate of

$$O(m^{-a_\mu} + n^{-a_r}).$$

The X–learner, on the other hand, can be seen as a locally weighted average of the two estimators, $\hat{\tau}_0$ and $\hat{\tau}_1$ (Eq. 9). Take for the moment, $\hat{\tau}_1$. It consists of an estimator for the outcome under control which achieves a rate of $m^{-a_r}$, and an estimator for the imputed treatment effects which should intuitively achieve a rate of $n^{-a_r}$. We, therefore, expect that under some conditions on $F \in S(a_\mu, a_r)$, there exist base learners such that $\hat{\tau}_0$ and $\hat{\tau}_1$ in the X–learner achieve the rates,

$$O(m^{-a_r} + n^{-a_r}) \quad \text{and} \quad O(m^{-a_\mu} + n^{-a_r}),$$

respectively.

Even though it is theoretically possible that $a_r$ is similar to $a_\mu$, our experience with real data suggests that it is often larger (i.e., the treatment effect is simpler to estimate than the potential outcomes), because the CATE function is often smoother or sparsely related to the feature vector. In this case, the X–learner converges at a faster rate than the T–learner.

**Remark 2 (Unbalanced groups)** In many real-world applications, 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 that can be used as the control group. In that case, the bound on the EMSE of the T–learner will be dominated by the regression problem for the treated response function,

$$\sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_T^{m}) \leq C_1 n^{-a_r}. \tag{13}$$

The EMSE of the X–learner, however, will be dominated by the regression problem for the imputed treatment effects and it will achieve a faster rate of $n^{-a_r}$,

$$\sup_{\mathcal{P} \in \mathcal{F}} \text{EMSE}(\mathcal{P}, \hat{\tau}_X^{m}) \leq C_2 n^{-a_r}. \tag{14}$$

This is a substantial improvement over 13 when $a_r > a_\mu$, and it demonstrates that in contrast to the T–learner, the X–learner can exploit structural conditions on the treatment effect. We, therefore, expect the X–learner to perform particularly well, when one of the treatment groups is larger than the other. This can also be seen in our extensive simulation study presented in Section \[ \ref{sec:results} \] and in the field experiment of social pressure on voter turnout presented in the appendix part of this paper.

**Example when the CATE is linear**

It turns out to be mathematically very challenging to give a satisfying statement for the extra conditions needed on $F$ in 12. However, they are satisfied under weak conditions when the CATE is Lipschitz continuous (c.f. Section \[ \ref{sec:theory} \] and, as we discuss in the following when the CATE is linear. We emphasize that we believe that this result holds in much greater generality.

Let us discuss in the following families of distributions with a linear CATE, but without assumptions on the response functions other than that they can be estimated at some rate $a$.

**Condition 3** The treatment effect is linear, $\tau(x) = x^T \beta$, with $\beta \in \mathbb{R}^d$.

**Condition 4** There exists an estimator $\hat{\mu}_0^{m}$ and constants $C_0, a > 0$ with

$$\text{EMSE}(\mathcal{P}, \hat{\mu}_0^{m}) = \mathbb{E}[|\hat{\mu}_0(X) - \hat{\mu}_0(X)|^2 | W = 0] \leq C_0 m^{-a}. \tag{15}$$
To help our analysis, we also assume that the noise terms are independent given $X$ and that the feature values are well behaved.

**Condition 5** The error terms $\varepsilon_t$ are independent given $X$, with $\mathbb{E}[\varepsilon_t | X = x] = 0$ and $\text{Var}[\varepsilon_t | X = x] \leq \sigma^2$.

**Condition 6** $X$ has finite second moments,

$$\mathbb{E}([X]_2) \leq C_X,$$

and the eigenvalues of the sample covariance matrix of $X^1$ are well conditioned, in the sense that there exists an $n_0 \in \mathbb{N}$ and a constant $C_{\Sigma} \in \mathbb{R}$ such that for all $n > n_0$,

$$\Pr \left( \gamma_{\min}^{-1}(\bar{\Sigma}_n) \leq C_{\Sigma} \right) = 1.$$  

Under these conditions, we can prove that the $X$–learner achieves a rate of $O(m^{-a} + n^{-1})$.

**Theorem 2** Assume we observe $m$ control units and $n$ treated units from a superpopulation that satisfies Conditions 4 and 5, then $\tilde{\tau}_1$ of the $X$–learner with $\mu_{0m}^T$ in the first stage and OLS in the second stage achieves a rate of $O(m^{-a} + n^{-1})$. Specifically, for all $n > n_0, m > 1$,

$$\text{EMSE}(\mathcal{P}, \hat{\tau}_1mn) \leq C(m^{-a} + n^{-1}),$$

with $C = \max \left( \frac{\max - \min}{\min - \min} \cdot C_0, \sigma^2d \right) C_X C_{\Sigma}$.

We note that an equivalent statement also holds for the pointwise MSE (Theorem 4) and for $\tilde{\tau}_0$.

This example also supports Remark 2, because if there are many control units,

$$m \geq n^{1/a},$$

then the $X$–learner achieves the parametric rate in $n$,

$$\text{EMSE}(\mathcal{P}, \hat{\tau}_1mn) \leq Cn^{-1}.$$

In fact as Theorem 4 shows, even if the number of control units are of the same order, we can often achieve the parametric rate.

**Applications**

In this section, we consider two data 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 [1]. In the second example, we consider an experiment that explored if door-to-door canvassing can be used to durably reduce transphobia in Miami [2]. In both examples, the original authors failed to find evidence of heterogeneous treatment effects using simple linear models without basis expansion, 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 [13] because of the importance of obtaining valid confidence intervals in these applications. Confidence intervals are obtained using a bootstrap procedure (Algorithm 6).

**Social pressure and voter turnout**

In a large field experiment, Gerber et al. show that substantially higher turnout was observed among registered voters who received mailing promising to publicize their turnout to their neighbors [1]. In the United States, whether someone is registered to vote and their past voting turnout is a matter of public record. Of course, how individuals voted is private. The experiment has been highly influential both in the scholarly literature and in political practice. In our reanalysis, we focus on two treatment conditions: the control group which was assigned to 191,243 individuals and the “neighbor’s” treatment, which was assigned to 38,218 individuals. Note the unequal sample sizes. The experiment was conducted in Michigan before 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 0.081 with a standard error of (0.003). Increasing voter turnout by 8.1% using a simple mailer is a substantive effect, especially considering that many individuals may never have seen the mailer.

Figure 2 presents the estimated treatment effects using X–RF where the potential voters are grouped by their voting history. The upper panel of the figure shows the proportion of voters with a significant positive (blue) and a significant negative (red) CATE estimate. We can see
that there is evidence of a negative backlash among a small number of people who only voted once in the past five elections prior to the general election 2004. 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 (25, 26). The lower panel shows the distribution of CATE estimates for each of the subgroups. Having estimates of the heterogeneity enables campaigns to better target the mailers in the future. For example, if the number of mailers is limited, one should target potential voters who voted three times during the last five elections, since this group has the highest average treatment effect and it is a very big group of potential voters.

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 can be found in Figure 10). We conducted a data-inspired 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., \( P(W = 1) = 0.167 \). Figure 3 presents the results for this simulation. They show 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.

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

In an experiment that received wide-spread media attention, Broockman et al. show that brief (10 minutes) but high-quality door-to-door conversations can markedly reduce prejudice against gender nonconforming individuals for at least three months (2). This experiment was published in Science after the journal retracted an earlier article claiming to show the same in an experiment about gay rights (27). Broockman et al. 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 (28).

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 (29). The authors

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3In praxis, it is not necessary to identify a particular subgroup. Instead, one can simply target units for which the predicted CATE is large.
first recruited registered voters (n = 68,378) via mail for an unrelated online survey to measure baseline outcomes. They 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 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 that 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 find an average treatment effect of 0.22 (SE: 0.072, t-stat: 3.1) on their transgender tolerance scale. 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. Figure 4(a) 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 within half a standard deviation of the ATE that the authors report.

Unlike our previous data example, there are marked differences in the treatment effects estimated by our three learners. Figure 4(b) presents the estimates from T–RF. These estimates are similar to those of X–RF, but with a larger spread. Figure 4(c) 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-stat=3.1).

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. Unlike the previous data example, the covariates are strongly predictive of the outcomes, and the splits in the S-RF are mostly on the features rather than the treatment indicator, because they are more predictive of the observed outcomes than the treatment assignment (c.f., Figure 11).

**Conclusion**

This paper reviewed meta-algorithms for CATE estimation including the T and S learners. It then introduced a new meta-algorithm, the X–learner, that can translate any supervised learning or regression algorithm or a combination of such algorithms into a CATE estimator. The X–learner is adaptive to various settings. For example,
both theory and data examples show that it performs 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. Specifically, if the CATE function is linear, but the response functions in treatment and control only satisfy Lipschitz continuous conditions, the X–learner can still achieve the parametric rate if one of the treatment groups is much larger than the other (Theorem 2). If there are no regularity conditions on the CATE function and the response functions are Lipschitz continuous, then both the X–learner and the T–learner obtain the same minimax optimal rate (Theorem 7). We conjecture that these results hold for more general model classes than those in our theorems.

We have presented an extensive set of simulations to understand the finite sample behaviors of different implementations of these learners, especially for model classes that are not covered by our theoretical results. We have also examined two data applications. Although none of the meta-algorithms is always the best, the X–learner performs well overall, 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 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 response 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). Other situations are possible and lead to different preferred estimators. For example, one could slightly change the S–learner so that it shrinks to the estimated ATE instead of zero, and it would then be preferred when the treatment effect is constant and non-zero. One hopes that the X–learner can adapt to these different settings. The simulations and real data studies presented have demonstrated the X–learner’s adaptivity. However, further studies and experience with more real datasets are necessary.

In ongoing research, we are investing using other supervised learning algorithms, and we are creating a deep learning architecture for estimating CATE. We are also exploring an alternative to the X–learner, the U–learner (Algorithm 6), that takes advantage of situations where the propensity score is easy to estimate and when there is much confounding—e.g., Simulation 6 (30). The U–learner is in some sense similar to the ATE estimator of Chernozhukov et al. (31) and an estimator for partially linear models by Robinson (32), but for nonparametric CATE estimation. A very recent paper proposes a modified version of the U–learner which is not a meta-learner because it requires the adaptation of the base learner in the second stage (33). We do not believe that under our assumptions, this modification of the U–learner or the U–learner generally performs better than the S–learner or the T–learner, but we want to explore the properties of the U–learner in future research.

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A. 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 BART [5], Neural Networks or RFs [34] for the base learners, since such methods perform well for a large variety of datasets. In the following, we choose all base learners to be either BART or honest RF algorithms—as implemented in the hte R package [15]—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 to demonstrate that the effects we see are not specific to a particular machine learning algorithm and that the choice of base learner affects prediction accuracy. That is, some machine learning algorithms (i.e., potential base learners) perform exceptionally well for some data structures. For example, if the dataset is very large and the features are pixels of images, then convolutional neural networks perform very well, and one should prefer it over other methods which are not working 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., global sparsity or 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.

Causal Forests

A very related estimator to the T–RF and S–RF is Causal Forests (CF) [7] because all these three estimators can be defined as

\[ \hat{\tau}(x) = \hat{\mu}(x, w = 1) - \hat{\mu}(x, w = 0), \]

where \( \hat{\mu}(x, w) \) is a form of random forests with different constraints on the split on the treatment assignment, \( W \). To be precise, in the S-learner the standard squared error loss function will decide where to split on \( W \), and it can, therefore, happen anywhere within the tree. In the T-learner the split on \( W \) must occur in the very beginning. For CF the split on \( W \) is always the split before the leaves. To obtain the right splits, the splitting criterion has to be changed, and we refer to the original paper for a precise explanation of the algorithm. Figure 5 shows the differences between these learners for full trees with 16 leaves.

CF is not a meta-learner since the algorithm has to be changed. However, its similarity to T-RF and S-RF make it interesting to evaluate its performance as well. Furthermore, one could think about generalizations of CF to other tree-based learners such as BART. To our knowledge, this is not implemented yet, and we will, therefore, compare it in the following simulations to S, T, and X–RF.

![Figure 5: Illustration of the structural form of the trees in T–RF, S–RF, and CF.](image)

Simulation setup

Let us here introduce the general framework of the following simulations. For each simulation, we specify the propensity score, \( c \), the response functions \( \mu_0 \) and \( \mu_1 \), the dimension, \( d \in \mathbb{N} \), of the feature space and a parameter, \( \alpha \), 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, \( Y_i \), independently in the following way:

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In the original statement of the algorithm we train separate RF estimators for each of the treatment groups, but that is exactly equivalent.
1. First, we simulate a $d$–dimensional feature vector,

$$X_i \overset{iid}{\sim} \mathcal{N}(0, \Sigma).$$

(16)

with $\Sigma$ being a correlation matrix which is created using the vine method \cite{36}.

2. Next, we create the potential outcomes according to

$$Y_i(1) = \mu_1(X_i) + \varepsilon_i(1)$$
$$Y_i(0) = \mu_0(X_i) + \varepsilon_i(0)$$

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

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

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

we set $Y_i = Y(W_i)$ and we return $(X_i, W_i, Y_i)$\footnote{This 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.}

We train each CATE estimator on a training set of $N$ units, and we evaluate its performance against a test set of $10^5$ units for which we know the true CATE. We repeat each experiment 30 times, and we report the averages.

A.1. The unbalanced case with a simple CATE

We have already seen in Theorem 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.

**Simulation 1 (unbalanced treatment assignment)**

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

The CATE function $\tau(x) = \mathbb{I}(x_2 > 0.1)$ is a one-dimensional indicator function, and thus simpler than the 20-dim function for the response functions $\mu_0(\cdot)$ and $\mu_1(\cdot)$. We can see in Figure 6 that the X–learner indeed performs much better in this unbalanced setting with both the BART and the RF as the base–learners.

A.2. 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 sometimes does not split on the treatment indicator at all and it tends to be biased towards zero. On the other hand, for the complex CATE case simulation we have chosen, 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 both cases.
Figure 6: Comparison of S–, T–, and X–BART (left) and S–, T–, and X–BART and CF (right).

A.2.1. Complex CATE

Let us first consider the case where the treatment effect is as complex 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. We study two Simulations here, and we choose for both the dimension to be $d = 20$, and the propensity score to be $e(x) = 0.5$.

Simulation 2 (complex linear)

$$e(x) = 0.5, \quad d = 20,$$
$$\mu_1(x) = x^T \beta_1, \text{ with } \beta_1 \sim \text{Unif}[1, 30]^{20},$$
$$\mu_0(x) = x^T \beta_0, \text{ with } \beta_0 \sim \text{Unif}[1, 30]^{20}.$$  

The second setup (complex non–linear) is motivated by (7). Here the response function are non–linear functions.

Simulation 3 (complex non-linear)

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

with

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

Figure 7 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 $\mu_0$ and $\mu_1$ 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 great deal. 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 perform here better. Researchers should use their subject knowledge when choosing the right base learner.
A.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 \( \{x : x_{20} < -0.4\}, \{x : -0.4 < x_{20} < 0.4\}, \) and \( \{x : -0.4 < x_{20}\}\). For each of the three parts of the space a different linear response function 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.

Simulation 4 (global linear)

\[
e(x) = 0.5, \quad d = 5, \\
\mu_0(x) = x^T \beta, \quad \text{with } \beta \sim \text{Unif}[1,30]^5 \\
\mu_1(x) = \mu_0(x)
\]

Simulation 5 (piecewise linear)

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

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

Figure 8 shows the outcome of these simulations. 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 ignored 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.

A.3. Confounding

In preceding examples, the propensity score was globally equal to some constant. This is a special case, and in many 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 (7). For this setting we choose $x \sim \text{Unif}([0, 1]^{20})$ and we use the notation that $\beta(x_1, 2, 4)$ is the $\beta$ distribution with parameters 2 and 4.

Simulation 6 (beta confounded)

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

Figure 9 shows that none of the algorithms is significantly suffering under confounding. We do not show the performance of causal forests, because—as noted by the authors—it is not designed for observational studies with only conditional unconfoundedness and it is not fair to compare it here (7).

B. Notes on the ITE

We provide an example which demonstrates that the ITE is not identifiable without further assumptions. Similar arguments and examples have been given before, e.g., (35) and we only list it here for completeness.
Example 3 \((D_i \text{ is not identifiable})\) Assume we observe a one-dimensional and uniformly distributed feature between 0 and 1, \(X \sim \text{Unif}(0,1)\), a treatment assignment which is independent of the feature and Bernoulli distributed, \(W \sim \text{Bern}(0.5)\), and a Rademacher distributed outcome under control which is independent of the features and the treatment assignment,
\[
P(Y(0) = 1) = P(Y(0) = -1) = 0.5.
\]

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, \(D = (Y_j, X_j, W_j)_{1 \leq j \leq N}\), 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 the observed data \(D\) can be consistent for ITEs, \((D_i)_{1 \leq i \leq n}\). The CATE, \(\tau(X_i)\), is, however, equal to 0 in both DGPs. \(\hat{\tau} \equiv 0\) is, for example, a consistent estimator for the CATE.

C. Stability of the social pressure analysis across meta-learners

In Figure 2 we present how the CATE varies with the observed covariates. We find a very interesting behavior which is that the biggest treatment effect can be observed for potential voters which voted three or four times before the 2004 general election. The treatment effect for potential voters, who vote in none or all five observed elections, had a much smaller treatment effect. We concluded this based on the output of the X-learner. To show that a similar conclusion can be drawn using different meta-learners, we repeated our analysis with the S and T learner (c.f. Figure 10). We find that the output is almost identical to the output of the X-learner. This is not surprising since the data set is very large and most of the covariates are discrete.

D. The bias of the S-learner in the reducing transphobia study

For many base learner, the S-learner can completely ignore the treatment assignment and thus predict a 0 treatment effect. This often leads to a bias towards 0 as we can see in Figure 4. To further analyze this behavior, we trained a
random forests estimator on the transphobia dataset with 100,000 trees, and we explored how often the individual trees predict a 0 treatment effect by not splitting on the treatment assignment. Figure 11 shows that the trees very rarely split on the treatment assignment. This is not surprising for this data set since the covariates are very predictive of the control response function and the treatment assignment is a relatively weak predictor.

**Figure 10:** Results for the S–learner (left) and T–learner (right) for the get out the vote experiment.

**Figure 11:** This figure is created from an S–RF learner to show that the S–learner often ignores the treatment effect entirely. It is based on 100,000 trees and it shows the histogram of trees by what percentage of the support of \( X \) is not split on \( W \).

### E. Conditioning on the number of treated units

In our theoretical analysis, we assume a super-population and we conditioning on the number of treated units to avoid the problem that with a small but non-zero probability all units are in the treated or in the control group and to be able to state the performance of different estimators in terms of \( n \), the number of treated units, and \( m \), the number of control units. This conditioning, however, leads to nonindependent samples. The crucial step to deal with this dependent structure is to condition on the treatment assignment, \( W \).
Specifically, there are three models to be considered.

1. The first one is defined by 1. It specifies a distribution, \( P \), of \( (X, W, Y) \), and we assume to observe \( N \) independent samples from this distribution,

\[
(X_i, W_i, Y_i)_{i=1}^N \overset{iid}{\sim} P.
\]

We denote the joint distribution of \( (X_i, W_i, Y_i)_{i=1}^N \) by \( P^N \).

2. We state our technical results in terms of a conditional distribution. For a fixed \( n \) with \( 0 < n < N \), we consider the distribution of \( (X_i, W_i, Y_i)_{i=1}^N \) given that we observe \( n \) treated units and \( m = N - n \) control units. We denote this distribution as \( P_{nm} \).

\[
\left[ (X_i, W_i, Y_i)_{i=1}^N \mid \sum_{i=1}^N W_i = n \right] \sim P_{nm}.
\]

Note that under \( P_{nm} \) the \( (X_i, W_i, Y_i) \) are identical in distribution, but not independent.

3. For technical reasons, we also introduce a third distribution which we will only use in some of the proofs. Here, we condition on the vector of treatment assignments, \( W \).

\[
(X_i, W_i, Y_i)_{i=1}^N \mid W = w \sim P^w.
\]

Under this distribution \( W \) is non-random and \( (X_i, Y_i) \) are not identical in distribution. However, within each treatment group the \( (X_i, Y_i) \) tuples are independent and identical in distribution. To make this more precise, define \( P_1 \) to be the conditional distribution of \( (X, Y) \) given \( W = 1 \), then under \( P^w \), we have

\[
(X_i, Y_i)_{W_i = 1} \overset{iid}{\sim} P_1.
\]

We prove these facts in the following.

**Theorem 3** Let \( n \) and \( N \) be such that \( 0 < n < N \) and let \( w \in \{0, 1\}^N \) with \( \sum_{i=1}^N w_i = n \). Then under the distribution \( P^w \),

\[
(X_k, Y_k)_{W_k = 1} \overset{iid}{\sim} P_1.
\]

We prove this in two steps. In Lemma 1 we prove the independence and in Lemma 2 we prove that the identical distributions.

**Lemma 1 (independence)** Let \( n \), \( N \), and \( w \) be as in Theorem 3 and define \( S = \{j \in \mathbb{N} : w_j = 1\} \). Then for all \( \emptyset \neq I \subseteq S \), and all \( (B_i)_{i \in \mathcal{I}} \) with \( B_i \subseteq \mathbb{R}^p \times \mathbb{R} \),

\[
\mathbb{P} \left( \bigcap_{i \in \mathcal{I}} \{(X_i, Y_i) \in B_i \} \mid W = w \right) = \prod_{i \in \mathcal{I}} \mathbb{P} (X_i, Y_i) \in B_i \mid W = w),
\]

(17)

Note that another way of writing (17) is

\[
\mathbb{P}^w \left( \bigcap_{i \in \mathcal{I}} \{(X_i, Y_i) \in B_i \} \right) = \prod_{i \in \mathcal{I}} \mathbb{P}^w (X_i, Y_i) \in B_i).
\]

(18)

**Proof.** [Proof of Lemma 1]

\[
\mathbb{P} \left( \bigcap_{i \in \mathcal{I}} \{(X_i, Y_i) \in B_i \} \mid W = w \right)
\]

\[
= \mathbb{P} \left( \left( \bigcap_{i \in \mathcal{I}} \{(X_i, Y_i) \in B_i \} \right) \cap \left( \bigcap_{j \in S} \{W_j = 1\} \cap \bigcap_{k \in S^c} \{W_k = 0\} \right) \right) / \mathbb{P}(W = w)
\]
= \mathbb{P}\left(\bigcap_{i \in \mathcal{I}} \{(X_i, Y_i, W_i) \in B_i \times \{1\}\} \cap \left( \bigcap_{j \in S \setminus \{i\}} \{W_j = 1\} \cap \bigcap_{k \in S^c} \{W_k = 0\} \right) \right) / \mathbb{P}(W = w)
= \prod_{i \in \mathcal{I}} \mathbb{P}\left((X_i, Y_i, W_i) \in B_i \times \{1\}\right) \mathbb{P}\left(\bigcap_{j \in S \setminus \{i\}} \{W_j = 1\} \cap \bigcap_{k \in S^c} \{W_k = 0\} \right) / \mathbb{P}(W = w) = (*)

The last equality holds because, \((X_i, Y_i, W_i)_{i=1}^N\) are mutually independent. The second term can be rewritten in the following way,

\[
\mathbb{P}\left(\bigcap_{j \in S \setminus \{i\}} \{W_j = 1\} \cap \bigcap_{k \in S^c} \{W_k = 0\} \right) / \mathbb{P}(W = w) = \prod_{j \in S \setminus \{i\}} \mathbb{P}(W_j = 1) \prod_{k \in S^c} \mathbb{P}(W_k = 0) / \mathbb{P}(W = w)
= \prod_{j \in S \setminus \{i\}} \mathbb{P}(W_j = 1) \prod_{k \in S^c} \mathbb{P}(W_k = 0) / \mathbb{P}(W = w)
\]

Thus,

\[
(*) = \prod_{i \in \mathcal{I}} \mathbb{P}\left((X_i, Y_i, W_i) \in B_i \times \{1\}\right) \mathbb{P}\left(\bigcap_{j \in S \setminus \{i\}} \{W_j = 1\} \cap \bigcap_{k \in S^c} \{W_k = 0\} \right) / \mathbb{P}(W = w) = \prod_{i \in \mathcal{I}} \mathbb{P}\left((X_i, Y_i) \in B_i \cap \{W = w\}\right) / \mathbb{P}(W = w)
\]

which finishes the proof.

Next, we are concerned with showing that all treated units have the same distribution.

**Lemma 2 (identical distribution)** Assume the same assumptions as Lemma 1 and let \(i \neq j \in S\). Under the conditional distribution of \(W = w\), \((X_i, Y_i)\) and \((X_j, Y_j)\) have the same distribution, \(P_1\).

**Proof.** Let \(B \subset \mathbb{R}^p \times \mathbb{R}\), then

\[
\mathbb{P}\left((X_i, Y_i) \in B \mid W = w\right) = \mathbb{P}\left((X_i, Y_i, W_i) \in B \cap \{1\}\right) / \mathbb{P}(W = w)
= \mathbb{P}\left((X_i, Y_i, W_i) \in B \times \{1\}\right) / \mathbb{P}(W = 1)
= \mathbb{P}\left((X_j, Y_j, W_j) \in B \times \{1\}\right) / \mathbb{P}(W = 1)
= \mathbb{P}\left((X_j, Y_j) \in B \mid W = 1\right)
\]
\[= \mathbb{P}\left((X_j, Y_j) \in B \bigg| W = w\right).\]

Here * follows from \((X_i, Y_i, W_i)_{i=1}^N\) being mutually independent, and * follows, because \((X_i, Y_i, W_i)_{i=1}^N\) are indetically distributed under \(P\).

### F. Convergence Rates Results for the T–learner

In this section, we want to prove Theorem 1 of the main paper. We start with a short lemma which will be useful for the proof of the theorem.

**Lemma 3** Let \(P\) be defined as in \(\text{[4]}\) with \(0 \leq e_{\min} < e(x) < e_{\min} < 1\). Furthermore, let \(X, W\) be distributed according to \(P\), and let \(g\) be a positive function such that the expectations below exist, then

\[
\begin{align*}
\frac{e_{\min}}{e_{\max}} \mathbb{E}[g(X)] & \leq \mathbb{E}[g(X)|W = 1] \leq \frac{e_{\max}}{e_{\min}} \mathbb{E}[g(X)], \\
\frac{1 - e_{\max}}{1 - e_{\min}} \mathbb{E}[g(X)] & \leq \mathbb{E}[g(X)|W = 0] \leq \frac{1 - e_{\min}}{1 - e_{\max}} \mathbb{E}[g(X)].
\end{align*}
\]

(19)

**Proof.** [Proof of Lemma 3] Let us prove \(19\) first. The the lower bound follows from

\[
\mathbb{E}[g(X)|W = 1] \geq \mathbb{E}[g(X)] \frac{\inf_x e(x)}{E[W]} \geq \frac{e_{\min}}{e_{\max}} \mathbb{E}[g(X)],
\]

and for the upper bound, note that

\[
\mathbb{E}[g(X)|W = 1] \leq \mathbb{E}[g(X)] \frac{\sup_x e(x)}{E[W]} \leq \frac{e_{\max}}{e_{\min}} \mathbb{E}[g(X)].
\]

(20)

follows from a symmetrical argument.

Let us now restate Theorem 1. Let \(m, n \in \mathbb{N}^+\) and \(N = m + n\) and let \(P\) be a distribution of \((X, W, Y)\) according to \(\text{[4]}\) with propensity score bounded away from 0 and 1. That is, there exists \(e_{\min}\) and \(e_{\max}\) such that \(0 < e_{\min} < e(x) < e_{\max} < 1\). Furthermore, let \((X_i, W_i, Y_i)_{i=1}^N\) be i.i.d. from \(P\) and define \(P^{nm}\) to be the conditional distribution of \((X_i, W_i, Y_i)_{i=1}^N\) given that we observe \(n\) treated units, \(\sum_{i=1}^{N} W_i = n\).

Note that \(n\) and \(m\) are not random under \(P^{nm}\). We are interested in the performance of the T–learner, \(\hat{T}_{P^{nm}}\), under \(P^{nm}\) as measured by the EMSE,

\[
\text{EMSE}(\hat{T}_{P^{nm}}, P^{nm}) \overset{\text{def}}{=} \mathbb{E}\left[ (\hat{T}^{nm}(X) - \tau(X))^2 \bigg| \sum_{i=1}^{N} W_i = n \right].
\]

The expectation is here taken over the training data set \((X_i, W_i, Y_i)_{i=1}^N\) which is distributed according to \(P^{nm}\) and \(X\) which is distributed according to the marginal distribution of \(X\) in \(P\).

For a family of superpopulations, \(F \in S(a_\mu, a_\tau)\), we want to show that the T–learner with an optimal choice of base learners achieves a rate of

\[
\mathcal{O}(m^{-a_\mu} + n^{-a_\mu}).
\]

An optimal choice of base learners are estimators which achieve the minimax rate of \(n^{-a_\tau}\) and \(m^{-a_\tau}\) in \(F\).

**Proof.** [Proof of Theorem 1] The EMSE can be upper bounded by the errors of the single base learners,

\[
\begin{align*}
\text{EMSE}(\hat{T}_{P^{nm}}, P^{nm}) &= \mathbb{E}\left[ (\hat{T}^{nm}(X) - \tau(X))^2 \bigg| \sum_{i=1}^{N} W_i = n \right] \\
&\leq 2 \mathbb{E}\left[ (\hat{\mu}^m_a(X) - \mu_1(X))^2 \bigg| \sum_{i=1}^{N} W_i = n \right] + 2 \mathbb{E}\left[ (\hat{\mu}^m_0(X) - \mu_0(X))^2 \bigg| \sum_{i=1}^{N} W_i = n \right].
\end{align*}
\]

(21)
Hence, it follows that,

\[(\hat{r}_T^{mn}(X) - \tau(X))^2 \leq 2(\hat{\mu}_1^n(X) - \mu_1(X))^2 + 2(\hat{\mu}_0^n(X) - \mu_0(X))^2.\]

Let us look only at the first term. We can write,

\[A = \mathbb{E}\left[ (\hat{\mu}_1^n(X) - \mu_1(X))^2 \bigg| \sum_{i=1}^N W_i = n \right]\]

\[= \mathbb{E}\left[ (\hat{\mu}_1^n(X) - \mu_1(X))^2 \bigg| W_i, \sum_{i=1}^N W_i = n \right] \left| \sum_{i=1}^N W_i = n \right]. \quad (21)\]

It is, of course, not necessary to condition on \(\sum_{i=1}^N W_i = n\) in the inner expectation, and we only do this to keep track that there are \(n\) treated units.

For \(i \in \{1, \ldots, n\}\), let \(q_i\) be the \(i\)th smallest number in \(\{k : W_k = 1\}\). That is \(\{q_i : i \in \{1, \ldots, n\}\}\) are the indexes of the treated units. To emphasize that \(\hat{\mu}_1^n(X)\) only depends on the treated observations, \((X_{q_i}, Y_{q_i})_{i=1}^n\), we write \(\hat{\mu}_1^n((X_{q_i}, Y_{q_i})_{i=1}^n, X)\). Furthermore, we define \(\mathcal{P}_1\) to be the conditional distribution of \((X, Y)\) given \(W = 1\). Conditioning on \(W\), Theorem 2 implies that \((X_{q_i}, Y_{q_i})_{i=1}^n\) is i.i.d. from \(\mathcal{P}_1\). Let us define \(\tilde{X}\) to be distributed according to \(\mathcal{P}_1\). Then we can apply Lemma 3 and use the definition of \(S(a_{\mu}, a_r)\) to conclude that the inner expectation in (21) is in \(O(n^{-a_\mu})\),

\[\mathbb{E}\left[ (\hat{\mu}_1^n((X_{q_i}, Y_{q_i})_{i=1}^n, X) - \mu_1(X))^2 \bigg| W_i, \sum_{i=1}^N W_i = n \right] \leq \frac{e_{\max}}{e_{\min}} \mathbb{E}\left[ (\hat{\mu}_1^n((X_{q_i}, Y_{q_i})_{i=1}^n, \tilde{X}) - \mu_1(\tilde{X}))^2 \bigg| W_i, \sum_{i=1}^N W_i = n \right] \leq \frac{e_{\max}}{e_{\min}} Cn^{-a_\mu}.\]

Hence, it follows that,

\[A \leq 2\mathbb{E}\left[ \frac{e_{\max}}{e_{\min}} Cn^{-a_\mu} \bigg| \sum_{i=1}^n W_i = n \right] \leq 2\frac{e_{\max}}{e_{\min}} Cn^{-a_\mu}.\]

By a symmetrical argument, it also holds that

\[B \leq 2\frac{1}{1 - e_{\max}} Cm^{-a_\mu},\]

and we can conclude that

\[\text{EMSE}(\hat{r}_T^{mn}, \mathcal{P}) \leq 2C \left[ \frac{1}{1 - e_{\max}} + \frac{e_{\max}}{e_{\min}} \right] (n^{-a_\mu} + m^{-a_\mu}).\]

**G. Convergence Rates Results for the X–learner**

In the following section, we are concerned with the convergence rate of the X–learner. As motivated in the main paper, we believe that \(\tau_0\) of the X–learner should achieve a rate of \(O(m^{-a_r} + n^{-a_\mu})\) and \(\hat{\tau}_1\) should achieve a rate of \(O(m^{-a_\mu} + n^{-a_r})\). In the following, we will prove this for two cases, and we show that for those cases the rate is optimal. In the first, we assume that the CATE is linear and thus \(a_r = 1\). We don’t assume any regularity conditions on the response functions, and we show that the X–learner with an OLS estimator in the second stage and an appropriate estimator in the first stage will achieve the optimal convergence rate. We show this first for the MSE (Theorem 4) and then for the EMSE (Theorem 5). We then focus on the case when we don’t have any extra regularity conditions on the CATE, but the response functions are Lipschitz continuous (Theorem 7). The optimal convergence rate is here not obvious, and we will first prove a minimax lower bound for the EMSE, and we then show that the X–learner with the KNN estimates achieve this optimal performance.
G.1. MSE and EMSE convergence rate for the linear CATE

Theorem 4 (Rate for the pointwise MSE) 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 \(P\) given in equation \([3]\) and assume that the following assumptions are satisfied:

**B1** Ignorability holds.

**B2** The treatment effect is linear, \(\tau(x) = x^T \beta\), with \(\beta \in \mathbb{R}^d\).

**B3** There exists an estimator \(\hat{\mu}_0\) such that for all \(x\),

\[
\mathbb{E} \left[ (\mu(x) - \hat{\mu}_0 \parallel x)^2 \right] \leq C_0 m^{-a}\]

**B4** The error terms \(\varepsilon_i\) are independent given \(X\), with \(\mathbb{E}[\varepsilon_i|X=x] = 0\) and \(\text{Var}[\varepsilon_i|X=x] \leq \sigma^2 < \infty\).

**B5** 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

\[
\sup_{n > n_0} \mathbb{E} \left[ \gamma_{\max}(\hat{\Sigma}_n) \sum_{i=1}^N W_i = n \right] < c_1 \quad \text{and} \quad \sup_{n > n_0} \mathbb{E} \left[ \gamma_{\min}(\hat{\Sigma}_n) / \gamma_{\max}(\hat{\Sigma}_n) \sum_{i=1}^N W_i = n \right] < c_2,
\]

where \(\hat{\Sigma}_n = \frac{1}{n} (X^1)' X^1\) and \(X^1\) is the matrix consisting of the features of the treated units.

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 \(n > n_0\),

\[
\mathbb{E} \left[ (\tau(x) - \hat{\tau}_X(x))^2 \right] \left( \sum_{i=1}^N W_i = n \right) \leq C_x (m^{-a} + n^{-1})
\]

with \(C_x = \max(c_2 C_0, \sigma^2 d c_1) \|x\|^2\).

**Proof.** [Proof of Theorem 4] In the following, we will write \(X\) instead of \(X^1\) for the observed features of the treated units to simplify the notation. Furthermore, we denote that when \(g \equiv 0\) in \([9]\) in the main paper, the X–learner will be equal to \(\hat{\tau}_1\) and we only have to analyze the performance of \(\hat{\tau}_1\).

The imputed treatment effects for the treated group can be written as

\[
D_i^1 = Y_i - \hat{\mu}_0(X_i) = X_i \beta + \delta_i + \varepsilon_i,
\]

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

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

To simplify the notation, we define the event of observing \(n\) treated units as \(E_n = \{\sum_{i=1}^N W_i = n\}\). We decompose the MSE of \(\hat{\tau}(x)\) into two orthogonal error terms,

\[
\mathbb{E} \left[ (\tau(x) - \hat{\tau}_X(x))^2 \sum_{i=1}^N W_i = n \right] = \mathbb{E} \left[ (x' (\beta - \hat{\beta}))^2 \right] \leq \|x\|^2 \mathbb{E} \left[ \| (X' X)^{-1} X' \delta \|^2 + \| (X' X)^{-1} X' \varepsilon \|^2 \right] (E_n).
\]

Throughout the proof, we assume that \(n > n_0\) such assumption [B5] can be used. We will show that the second term decreases according to the parametric rate, \(n^{-1}\), while the first term decreases at a rate of \(m^{-a}\).

\[
\mathbb{E} \left[ \| (X' X)^{-1} X' \varepsilon \|^2 \right] (E_n) = \mathbb{E} \left\{ \text{tr} \left( X(X' X)^{-1} (X' X)^{-1} X' E \left[ \varepsilon \varepsilon' | X, E_n \right] \right) \right\} (E_n)
\]

\[
\leq \sigma^2 d \mathbb{E} \left[ \gamma_{\min}(\hat{\Sigma}_n) \left| E_n \right. \right] n^{-1}
\]

\[
\leq \sigma^2 d c_1 n^{-1}.
\]
For the last inequality we used assumption B5. Next, we are concerned with bounding the error coming from not perfectly predicting μ0:

\[
E \left[ \|(X'X)^{-1}X'\delta\|^2 \right]_{E_n} \leq E \left[ \gamma_{\text{max}}(\hat{\Sigma}_n)^2/\gamma_{\text{min}}(\hat{\Sigma}_n)^2 \right]_{E_n} n^{-1} \\
\leq E \left[ \gamma_{\text{max}}(\hat{\Sigma}_n)^2/\gamma_{\text{min}}(\hat{\Sigma}_n)^2 \right]_{E_n} C^0 m^{-\alpha} \\
\leq c_2 C^0 m^{-\alpha}.
\]

here we used that \(\gamma_{\text{max}}(\hat{\Sigma}^{-2}_n) = \gamma_{\text{min}}^2(\hat{\Sigma}_n)\), and \(E \left[ \|\delta\|^2 \right]_{X, E_n} = E \left[ \sum_{i=1}^{n} \delta^2(X_i) \right]_{X, E_n} \leq n C^0 m^{-\alpha}\). For the last statement, we used assumption B5. This leads to 23.

**Bounding the EMSE**

*Proof. [Proof of Theorem 2]* This proof is very similar to the proof of Theorem 4. The difference is that here we bound the EMSE instead of the pointwise MSE, and we have a somewhat weaker assumptions, because \(\hat{\mu}_0\) only satisfies that its EMSE converges at a rate of \(a\), but not necessary the MSE at every \(x\). We introduce \(X\) here to be a random variable with the same distribution as the feature distribution such that the EMSE can be written as \(E[(\tau(X) - \hat{\tau}_X(X))^2 | E_n]\). Recall that we use the notation that \(E_n\) is the event that we observe exactly \(n\) treated and \(m = N - n\) control units,

\[
E_n = \left\{ \sum_{i=1}^{N} W_i = n \right\}.
\]

We start with a similar decomposition as 24,

\[
E \left[ (\tau(X) - \hat{\tau}_X(X))^2 | E_n \right] \leq E \left[ \|X\|^2 \right] E \left[ \|\beta - \hat{\beta}\|^2 | E_n \right] \\
= E \left[ \|X\|^2 \right] E \left[ \|X(X'X)^{-1}X'\delta\|^2 + \|X'X\|^{-1}X'\delta\|^2 | E_n \right].
\]

Following exactly the same steps as in 25, we receive

\[
E \left[ \|X(X'X)^{-1}X'\delta\|^2 | E_n \right] \leq \sigma^2 d \Sigma^{-1} n^{-1}.
\]

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

\[
E \left[ \|X(X'X)^{-1}X'\delta\|^2 | E_n \right] \leq E \left[ \gamma_{\text{min}}(X'X) \|X(X'X)^{-1}X'\delta\|^2 | E_n \right] \\
\leq E \left[ \gamma_{\text{min}}(X'X) \|\delta\|^2 | E_n \right] \\
\leq E \left[ \gamma_{\text{min}}(\Sigma) \frac{1}{n} \|\delta\|^2 | E_n \right] \\
\leq C \Sigma \leq \frac{1}{n} \|\delta\|^2 | E_n \right] \\
\leq C \Sigma \leq \frac{1}{n} \|\delta\|^2 | E_n \right] \\
\leq C \Sigma \leq \frac{1}{n} \|\delta\|^2 | E_n \right].
\]

Here the last inequality follows from Condition 6.

We now apply 19 20 and Condition 4 to conclude that

\[
E \left[ \|\delta_1\|^2 | E_n \right] = E \left[ \|\mu_0(X_1) - \hat{\mu}_0(X_1)\|^2 | E_n, W_1 = 1 \right] \\
\leq \frac{\epsilon_{\text{max}} - \epsilon_{\text{max}} \epsilon_{\text{min}}}{\epsilon_{\text{min}} - \epsilon_{\text{max}} \epsilon_{\text{min}}} E \left[ \|\mu_0(X_1) - \hat{\mu}_0(X_1)\|^2 | E_n, W_1 = 0 \right] \\
\leq \frac{\epsilon_{\text{max}} - \epsilon_{\text{max}} \epsilon_{\text{min}}}{\epsilon_{\text{min}} - \epsilon_{\text{max}} \epsilon_{\text{min}}} C \Sigma \Sigma^{-1} n^{-\alpha}.
\]

Lastly, we use the assumption that \(E \left[ \|X\|^2 | E_n \right] \leq C \Sigma\) and conclude that

\[
E \left[ (\tau(X) - \hat{\tau}_X(X))^2 | E_n \right] \leq C \Sigma \left( \frac{\epsilon_{\text{max}} - \epsilon_{\text{max}} \epsilon_{\text{min}}}{\epsilon_{\text{min}} - \epsilon_{\text{max}} \epsilon_{\text{min}}} C \Sigma \Sigma^{-1} n^{-\alpha} + \sigma^2 d \Sigma^{-1} n^{-1} \right).
\]

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G.2. Achieving the parametric rate

When there are a lot of control units, such that \( m \geq n^{1/a} \), then we have seen that the X–learner achieves the parametric rate. However, in some situations the X–learner also achieves the parametric rate even if the number of control units is of the same order as the number of treated units. To illustrate this, we consider an example in which the conditional average treatment effect and the response functions depend on disjoint and independent subsets of the features.

Specifically, we assume that we observe \( m \) control units and \( n \) treated units according to Model 1. We assume the same setup and the same conditions as in Theorem 2. In particular, we assume that there exists an estimator \( \hat{\mu}_0 \) which only depends on the control observations and estimates the control response function at a rate of at most \( m^{-a} \). In addition to these conditions we also assume the following independence condition.

**Condition 7** There exists subsets, \( S, \bar{S} \subset \{1, \ldots, d\} \) with \( S \cap \bar{S} = \emptyset \), such that

- \((X_i)_{i \in S} \) and \((X_i)_{i \in \bar{S}} \) are independent,
- For all \( i \in S \), \( E[X_i|W_i = 1] = 0 \),
- There exists a function \( \tilde{\mu}_0 \), and a vector \( \beta \) with \( \mu_0(x) = \tilde{\mu}_0(x_{\bar{S}}) \) and \( \tau(x) = x_T \tilde{\beta} \).

For technical reasons, we also need bounds on the fourth moments of the feature vector and the error of the estimator for the control response.

**Condition 8** The fourth moments of the feature vector are bounded,

\[
E[\|X\|_4^4|W = 1] \leq C_X.
\]

**Condition 9** There exists an \( m_0 \) such that for all \( m > m_0 \),

\[
E \left[ (\mu_0(X) - \hat{\mu}_0^m(X))^4 | W = 1 \right] \leq C_\delta.
\]

Here \( \hat{\mu}_0^m \) is defined in Condition 4.

This condition is for example satisfied when \( \mu_0 \) is bounded.

Under these additional assumptions, the EMSE of the X–learner achieves the parametric rate in \( n \), given that \( m > m_0 \).

**Theorem 5** Assume that Conditions 7–9 hold. Then the X–learner with \( \hat{\mu}_0^m \) in the first stage and OLS in the second stage achieves the parametric rate in \( n \). That is, there exists a constant \( C \) such that for all \( m > m_0 \) and \( n > 1 \),

\[
E \left[ (\tau(X) - \hat{\tau}_X^mn(X))^2 \left| \sum_i W_i = n \right. \right] \leq Cn^{-1}.
\]

We will proof the following lemma first, because it will be useful for the proof of Theorem 5.

**Lemma 4** Under the assumption of Theorem 5 there exists a constant \( C \) such that for all \( n > n_0 \), \( m > m_0 \), and \( s > 0 \),

\[
P \left( \|X'^{-1}X\|_2 \delta_n \geq s \left| \sum_i W_i = n \right. \right) \leq C \frac{1}{s^2},
\]

where \( \delta_n = \mu_0(X_1^n) - \hat{\mu}_0^m(X_1^n) \).

**Proof.** [Proof of Lemma 4] To simplify the notation, we write \( X \) instead of \( X^1 \) for the feature matrix of the treated units, and we define the event of observing exactly \( n \) treated units as

\[
E_n = \left\{ \sum_{i=1}^n W_i = n \right\}
\]

to shorten the notation.
We use Condition 6 and then Chebyshev’s inequality to conclude that for all \( n > n_0 \) (\( n_0 \) is determined by Condition 0),

\[
P \left( \|X'X\|^{-1} X' \delta \|_2^2 \geq s \big| E_n \right) = P \left( \frac{1}{n} \|\Sigma_n^{-1} X' \delta\|_2^2 \geq s \big| E_n \right)
\]

\[
\leq P \left( \frac{1}{n} \gamma^{-2}_n (\|\Sigma_n\| \|X' \delta\|_2^2 \geq s \big| E_n \right)
\]

\[
\leq E \left[ P \left( \frac{1}{n} C^2_2 \|X' \delta\|_2^2 \geq s \big| E_n, \delta \right) \big| E_n \right]
\]

Next we apply the Efron–Stein inequality to bound the variance term,

\[
\text{Var} \left( \|X' \delta\|_2^2 \big| E_n, \delta \right) \leq \frac{1}{2} \sum_{i=1}^n E \left[ (f(X) - f(X^{(i)}))^2 \big| E_n, \delta \right].
\]

Here \( f(x) = \|x' \delta\|_2^2 \), \( X^{(i)} = \{X_1, \ldots, X_{i-1}, \tilde{X}_i, X_{i+1}, \ldots, X_n\} \), and \( \tilde{X} \) is an independent copy of \( X \).

Let us now bound the summands:

\[
E \left[ (f(X) - f(X^{(i)}))^2 \big| E_n, \delta \right]
\]

\[
= E \left[ \|X' \delta\|_2^2 - \|X' \delta - (X_i - \tilde{X}_i) \delta_i\|_2^2 \big| E_n, \delta \right]
\]

\[
= E \left[ \left( 2 \delta' X_i (X_i - \tilde{X}_i) \delta_i \right)^2 + \sum_{i \neq j} \left( (X_i - \tilde{X}_i) \delta_i \right)^2 \big| E_n, \delta \right]
\]

Let us first bound \( E[A|E_n, \delta] \).

\[
E \left[ \left( 2 \delta' X_i (X_i - \tilde{X}_i) \delta_i \right)^2 \big| E_n, \delta \right] = E \left[ \sum_{j=1}^n \delta_j X_j'(X_i - \tilde{X}_i) \delta_i X_k'(X_i - \tilde{X}_i) \delta_i \big| E_n, \delta \right]
\]

\[
= \left( A \right) \sum_{j=1}^n \delta_j (X_j'(X_i - \tilde{X}_i) \delta_i)^2 \big| E_n, \delta \right]
\]

\[
\leq 4 \delta^4(n - 1) E \left[ (X'_1(X_2 - \tilde{X}_2))^2 \big| E_n, \delta \right] + 4 \delta^4 E \left[ (X'_1(X_1 - \tilde{X}_1))^2 \big| E_n, \delta \right]
\]

\[
\leq C_A \delta^4 n
\]

Here

\[
C_A = 4 \max \left( E \left[ (X'_1(X_2 - \tilde{X}_2))^2 \big| E_n \right], E \left[ (X'_1(X_1 - \tilde{X}_1))^2 \big| E_n \right] \right),
\]

which is bounded by Condition 8. For equation (a) we used that for \( k \neq j \), we have that either \( k \) or \( j \) is not equal to \( i \). Without loss of generality let \( j \neq i \). Then

\[
E \left[ \delta_j X_j'(X_i - \tilde{X}_i) \delta_i X_k'(X_i - \tilde{X}_i) \delta_i \big| E_n, \delta \right]
\]

\[
= \delta_j E \left[ X_j' \big| W, E_n, \delta \right] E \left[ (X_i - \tilde{X}_i) \delta_i X_k'(X_i - \tilde{X}_i) \delta_i \big| W, E_n, \delta \big| E_n, \delta \right]
\]

\[
= 0,
\]

because \( E \left[ X'_j W \big| E_n, \delta \right] = 0 \) per assumption.

In order to bound \( E[B|E_n, \delta] \), note that all the forth moments of \( X \) are bounded and thus,

\[
E \left[ \|X_i - \tilde{X}_i\|_2^4 \big| E_n, \delta \right] \leq C_B \delta^4.
\]
Finally, we bound $\mathbb{E}[C| E_n, \delta]$. 

$$
\mathbb{E} \left[ 4\delta' X (X_i - \tilde{X}_i)\delta_i (X_i - \tilde{X}_i) \delta_i \| X_i - \tilde{X}_i \|_2^2 | E_n, \delta \right] = \mathbb{E} \left[ \sum_{j=1}^{n} \delta_j X'_j (X_i - \tilde{X}_i) \delta_i (X_i - \tilde{X}_i) \delta_i \| X_i - \tilde{X}_i \|_2^2 | E_n, \delta \right] 
= \mathbb{E} \left[ \delta_i X'_i (X_i - \tilde{X}_i) \| X_i - \tilde{X}_i \|_2^2 | E_n, \delta \right] 
= C \delta_i^4
$$

Where the second equality follows from the same argument as in [30] and the last equality is implied by Condition 8.

Plugging Term A, B, and C in, we have that for all $n > n_0$, 

$$
\text{Var} \left( \| X' \|_2^2 | E_n, \delta \right) \leq \frac{1}{2} \sum_{t=1}^{n} \mathbb{E} \left[ (f(X, \delta) - f(X^{(i)}, \delta^{(i)}))^2 \right] \leq C \delta^4 n^2,
$$

with $C = C_A + C_B + C_C$. Thus for $n > n_0$, 

$$
\mathbb{P} \left( n\| (X'X)^{-1} X' \|_2^2 \geq s | E_n \right) \leq \mathbb{E} \left[ \frac{CC_2^4 \delta^4}{s^2} | E_n \right] \leq CC_2^4 C_\delta \frac{1}{s^2}.
$$

**Proof.** (Proof of Theorem 5) We start with the same decomposition as [27] 

$$
\mathbb{E} \left[ (\tau(\mathcal{X}) - \hat{\tau}_m(\mathcal{X}))^2 | E_n \right] \leq \mathbb{E} \left[ \| X' \|_2^2 \right] \mathbb{E} \left[ \| (X'X)^{-1} X' \|_2^2 + \| (X'X)^{-1} X' \|_2 \right] | E_n \right],
$$

and we follow the same steps to conclude that 

$$
\mathbb{E} \left[ \| (X'X)^{-1} X' \|_2^2 | E_n \right] \leq \sigma^2 d C_2 n^{-1} \quad \text{and} \quad \mathbb{E} \left[ \| X' \|_2^2 \right] \leq C_\chi.
$$

From Lemma 4, we can conclude that there exists a constant $C$ such that 

$$
\lim_{n \to \infty} \mathbb{E} \left[ n\| (X'X)^{-1} X' \|_2^2 | E_n \right] = \lim_{n \to \infty} \int_{0}^{\infty} \mathbb{P} \left( n\| (X'X)^{-1} X' \|_2^2 \geq s | E_n \right) ds 
\leq \lim_{n \to \infty} \int_{0}^{\infty} \max(1, C \frac{1}{s^2}) ds 
\leq 1 + C.
$$

Thus there exists a $\tilde{C}$ such that for all $n > 1$, 

$$
\mathbb{E} \left[ \| (X'X)^{-1} X' \|_2^2 | E_n \right] \leq \tilde{C} n^{-1}.
$$

**G.3. EMSE convergence rate for Lipschitz continuous response functions**

In Section [G.1] we considered an example when the distribution of $(Y(0), Y(1), W, X)$ was assumed to be in some family $F \in S(\alpha_{\mu}, \alpha_{\tau})$ with $\alpha_{\tau} > \alpha_{\mu}$, 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 $\alpha_{\tau} \leq \alpha_{\mu}$.

Let us first consider the case, when $\alpha_{\tau} < \alpha_{\mu}$. This is a somewhat artificial case, since having response functions which can be estimated at a rate of $N^{-\alpha_{\mu}}$ implies that the CATE cannot be too complicated. For example, if $\mu_0$ and $\mu_1$ is Lipschitz continuous, then the CATE is Lipschitz continuous as well, and we would expect $\alpha_{\tau} \approx \alpha_{\mu}$. Even though it is hard to construct a case with $\alpha_{\tau} < \alpha_{\mu}$, we cannot exclude such a situation, and we would expect in such a case the T–learner to perform better than the X–learner.

We, therefore, believe that the case when $\alpha_{\tau} \approx \alpha_{\mu}$ is a more reasonable assumption than the case when $\alpha_{\tau} < \alpha_{\mu}$. In this case, we would expect the T and X learner to perform similarly when compared to their worst–case convergence rate. Let us try to backup this intuition with a specific example. Theorem 2 already confirms that $\tilde{\tau}_1$ achieves the expected rate, 

$$
O \left( m^{-\alpha_{\mu}} + n^{-\alpha_{\tau}} \right),
$$

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. We assume to have some noise level $\sigma$ which is fixed, and we start by introducing a family, $F_L$ of distributions with Lipschitz continuous regression functions.
Definition 4 (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 $Y_i = \mu(X_i) + \varepsilon_i$,
   where the $\varepsilon_i$ is independent and normally distributed with mean 0 and variance $\sigma^2$,
3. $X_i$ and $\varepsilon_i$ are independent, and
4. $\mu$ is Lipschitz continuous with parameter $L$.

Remark 4 The optimal rate of convergence for the regression problem of estimating $x \mapsto E[Y|X=x]$ in Definition 4 is $N^{-2/(2+d)}$. Furthermore, the KNN algorithm with the right choice of the number neighbors and the Nadaraya-Watson estimator with the right kernels achieve this rate, and they are thus minimax optimal for this regression problem.

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

Definition 5 Let $D^L_{mn}$ be the family of distributions of $(Y(0), Y(1), W, X) \in \mathbb{R}^N \times \mathbb{R}^N \times \{0,1\}^N \times [0,1]^d \times \mathbb{R}$ 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 $(\varepsilon_{0i}, \varepsilon_{1i})$ is independent normally distributed with mean 0 and marginal variances $\sigma^2$,
5. $X, W$ and $\varepsilon = (\varepsilon_{0i}, \varepsilon_{1i})$ are independent, and
6. $\mu_0, \mu_1$ are Lipschitz continuous with parameter $L$.

Note that if $(Y(0), Y(1), W, X)$ is distributed according to a distribution in $D^L_{mn}$, then $(Y(0), X)$ given $W = 0$ and $(Y(1), X)$ given $W = 1$ have marginal distributions in $F^L$, and $(X, \mu_1(X) - Y(0))$ given $W = 0$ and $(X, Y(1) - \mu_0(X))$ given $W = 1$ have distributions in $F^{2L}$, and thus we therefore conclude that $D^L_{mn} \in S\left(\frac{2}{2+d}, \frac{2}{2+d}\right)$.

We will first prove in Theorem 6 that the best possible rate which can be uniformly achieved for distributions in this family is $O(n^{2/(2+d)} + m^{2/(2+d)})$.

This is precisely the rate the T-learner with the right base learners achieves (c.f. Theorem 1). In Theorem 7 we will then show that the X-learner with the KNN estimator for both stages achieves this optimal rate as well, and we conclude that both the T and X learner achieve the optimal minimax rate for this class of distributions.

Minimax Lower Bound

In this section, we will derive a lower bound on the best possible rate for $D^L_{mn}$.

Theorem 6 (Minimax Lower Bound) Let $\hat{\tau}$ be an arbitrary estimator, $a_1, a_2 > 0$, and $c$ such that for all $n, m \geq 1$,

$$\sup_{P \in D^L_{mn}} \text{EMSE}(P, \hat{\tau}^{mn}) \leq c(m^{-a_0} + n^{-a_1}),$$

(31)

then $a_1$ and $a_2$ are at most $2/(2+d)$, $a_0, a_1 \leq 2/(2+d)$.

---

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

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Proof. [Proof of Theorem 6] To shorten the notation, we define $\mu_n = 2/(2 + d)$. We will show by contradiction that $a_1 \leq a$. The proof for $a_0$ is mathematically symmetric. We assume $a_1$ was bigger than $a$, and we will show that this implies that there exists a sequence of estimators $\hat{\mu}_n$, such that

$$\sup_{p_i \in F_L} \mathbb{E}_{D_1^p \sim P_1^n} \left[ (\mu_1(X) - \hat{\mu}_n(X; D_1^n))^2 \right] \leq 2cn^{-a_1}$$

which is a contradiction, since per definition of $D_L^{mn}$, $\mu_1$ cannot be estimated at a rate faster than $n^{-a}$ (c.f., (20)). Note that we write here $\hat{\mu}_n$ because we want to be explicit that $\hat{\mu}_n$ only depends on the treated observations.

Similiar to $\hat{\mu}_1^1(D_1^p, I_1^p)$, we will use the notation $\hat{\mu}_1^m(D_1^p, I_1^p)$ to be explicit about the dependence of the estimator $\hat{\mu}_1^m$ on the data in the control group, $D_1^m$, and the data in the treated group, $D_1^t$. Furthermore, note that in Definition 3 each distribution in $D_1^{mn}$ is fully specified by the distribution of $W$, $\varepsilon$, and the functions $\mu_1$ and $\mu_2$. Define $\mathcal{C}_L$ to be the set of all functions $f : [0, 1]^d \rightarrow \mathbb{R}$ that are L-Lipschitz continuous. For $f_1 \in \mathcal{C}_L$, define $D(f_1)$ to be the distribution in $D_1^{mn}$ with $\mu_0 = 0$, $\mu_1 = f_1$, $\varepsilon_0 \perp \varepsilon_1$, and $W$ defined componentwise by

$$W_i = \begin{cases} 1 & \text{if } i \leq n \\ 0 & \text{else.} \end{cases}$$

Then (31) implies that

$$c(m^{-a_0} + n^{-a_1}) \geq \sup_{p \in D_L^{mn}} \mathbb{E}_{D_0^m \times D_1^p \sim P} \left[ (\tau_{D_0^m} \tau_{D_1^p} - \hat{\tau}_{mn}^{D_0^m, D_1^p})^2 \right] \geq \sup_{f_1 \in \mathcal{C}_L} \mathbb{E}_{D_0^m \times D_0^m \sim D(f_1)} \left[ (\mu_1^{D_1^p}(X) - \hat{\tau}_{mn}^{D_0^m, D_1^p})^2 \right].$$

This follows, because in $D(f_1)$, $\hat{\tau}_{D_0^m}^{D_1^p} = \mu_1^{D_1^p} = f_1$. We use here the notation $\tau_{D_0^m}$, $\tau_{D_1^p}$, and $\mu_1^{D_1^p}$ to emphasize that those terms depend on the distribution of $P$ and $D(f_1)$, respectively.

Let $\mathcal{P}_0$ be the distribution of $D_0^m = (X_0^m, Y_0^m)^n_{i=1}$ under $D(f_1)$. Note that under $\mathcal{P}_0$, $X_i \overset{iid}{\sim} [0, 1]$, and $Y_0 \overset{iid}{\sim} \mathbb{N}(0, \sigma^2)$, and $X_0$ and $Y_0$ are independent. In particular $\mathcal{P}_0$ does not depend on $f_1$. We can thus write

$$c(m^{-a_0} + n^{-a_1}) \geq \sup_{f_1 \in \mathcal{C}_L} \mathbb{E}_{D_0^m \sim \mathcal{D}(f_1)} \left[ \left( \mu_1^{D_1^p}(X) - \hat{\tau}_{mn}^{D_0^m, D_1^p} \right)^2 \right] \geq \sup_{f_1 \in \mathcal{C}_L} \mathbb{E}_{D_0^m \sim \mathcal{D}(f_1)} \mathbb{E}_{D_0^m \sim \mathcal{P}_0} \left[ \left( \mu_1^{D_1^p}(X) - \hat{\tau}_{mn}^{D_0^m, D_1^p} \right)^2 \right].$$

$\mathcal{D}(f_1)$ is here the distribution of $D_1^p$ under $D(f_1)$. For the last step we used Jensen’s inequality.

Now choose a sequence $m_n$ in such a way that $m_n^{-a_1} + n^{-a_2} \leq 2n^{-a_1}$, and define

$$\hat{\mu}_1^m(x; D_1^n) = \mathbb{E}_{D_0^m \sim \mathcal{P}_0^n} [\hat{\tau}_{mn}(x; D_0^m, D_1^n)].$$

Furthermore, note that

$$\{D_1(f_1) : f_1 \in \mathcal{C}_L\} = \{P_i \in F_L\},$$

to conclude that

$$2cn^{-a_1} \geq c(m_n^{-a_0} + n^{-a_1}) \geq \sup_{f_1 \in \mathcal{C}_L} \mathbb{E}_{D_1^p \sim \mathcal{D}(f_1)} \left[ \left( \mu_1^{D_1^p}(X) - \hat{\mu}_1^m(D_1^n; X) \right)^2 \right] \geq \sup_{P_i \in F_L} \mathbb{E}_{D_1^p \sim P_1^n} \left[ \left( \mu_1^m(X) - \hat{\mu}_1^m(D_1^n; X) \right)^2 \right].$$

This is, however, a contradiction, because we assumed $a_1 > a$. 

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EMSE convergence of the X–learner

Finally, we can show that the X–learner with the right choice of base learners will achieve this minimax lower bound.

**Theorem 7** Let \( d > 2 \) and assume \((X, W, Y(0), Y(1)) \sim \mathcal{P} \in \mathcal{D}_{mn}^L\). In particular, \( \mu_0 \) and \( \mu_1 \) are Lipschitz continuous with constant \( L \),

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

and \( X \sim \text{Unif}([0,1]^d) \).

Furthermore, let \( \hat{\tau}^{mn} \) be the X–learner with

- \( g \equiv 0 \),
- the base learner of the fist stage for the control, \( \hat{\mu}_0 \), is a KNN estimator with constant \( k_0 = \left \lceil (\sigma^2/L^2)^{2} m^{2/d} \right \rceil \),
- the base learner of the second stage for the treated group, \( \hat{\tau}_1 \), is a KNN estimator with constant \( k_1 = \left \lceil (\sigma^2/L^2)^{2} n^{2/d} \right \rceil \).

Then \( \hat{\tau}^{mn} \) achieves the optimal rate as given in Theorem 6. That is, there exists a constant \( C \) such that

\[
E[\|\tau - \hat{\tau}^{mn}\|^2] \leq C\sigma^2 L^2 \left( \frac{d}{\sqrt{mn}} \right) \left( m^{-2/(2+d)} + n^{-2/(2+d)} \right).
\] (32)

Note that in the third step of the X–learner, Equation 9, the \( \hat{\tau}_0 \) and \( \hat{\tau}_1 \) are averaged,

\[
\hat{\tau}^{mn}(x) = g(x)\hat{\tau}_0^{mn}(x) + (1 - g(x))\hat{\tau}_1^{mn}(x).
\]

By choosing \( g \equiv 0 \), we are analyzing \( \hat{\tau}_0^{mn} \). Per symmetry it is straightforward to show that with the right choice of base learners, \( \hat{\tau}_0^{mn} \) also achieves a rate of \( O(m^{-2/(2+d)} + n^{-2/(2+d)}) \). With this choice of base learners the X–learner achieves this optimal rate for every choice of \( g \).

We will first state two useful lemminata which we will need in the proof of this theorem.

**Lemma 5** Let \( \hat{\mu}_0^m \) be a KNN estimator only based on the control group with constant \( k_0 \), and let \( \hat{\mu}_1^n \) be a KNN estimator based on the treated group with constant \( k_1 \), then under the assumption of Theorem 6

\[
E[\|\hat{\mu}_0^m - \mu_0\|^2] \leq \frac{\sigma^2}{k_0} + cL^2 \left( \frac{k_0}{m} \right)^{2/d},
\]

\[
E[\|\hat{\mu}_1^n - \mu_1\|^2] \leq \frac{\sigma^2}{k_1} + cL^2 \left( \frac{k_1}{n} \right)^{2/d},
\]

for some constant \( c \).

**Proof.** [Proof of Lemma 5] This is a direct implication of Theorem 6.2 in [20].

**Lemma 6** Let \( x \in [0,1]^d \), \( X_1, \ldots, X_n \overset{iid}{\sim} \text{Unif}([0,1]^d) \) and \( d > 2 \). Define \( \bar{X}(x) \) to be the nearest neighbor of \( x \), then there exists a constant \( c \) such that for all \( n > 0 \),

\[
E[\|\bar{X}(x) - x\|^2] \leq \frac{c}{n^{2d}}.
\]

**Proof.** [Proof of Lemma 6] First of all we consider

\[
P(\|\bar{X}(x) - x\| \geq \delta) = (1 - P(\|X_1 - x\| \leq \delta))^n \leq (1 - \delta^d)^n \leq e^{-\delta^d n}
\]

Now we can compute the expectation,

\[
E[\|\bar{X}(x) - x\|^2] = \int_0^\infty P(\|\bar{X}(x) - x\| \geq \sqrt{\delta})d\delta \leq \int_0^d e^{-\delta^d / 2} d\delta \leq \frac{1}{(cn)^{2/d} d}.\]
Proof. Many ideas of this proof are motivated by [20] and [22]. Furthermore, note that we restrict our analysis here only on \( \hat{\tau}_1^{mn} \), but the analysis for \( \hat{\tau}_0^{mn} \) follows the same steps.

We decompose \( \hat{\tau}_1^{mn} \) as

\[
\hat{\tau}_1^{mn}(x) = \frac{1}{k_1} \sum_{i=1}^{k_1} \left[ Y_{i,n}^1(x) - \hat{\mu}_0^m \left( X_{i,n}^1(x) \right) \right] = \hat{\mu}_1^n(x) - \frac{1}{k_1} \sum_{i=1}^{k_1} \hat{\mu}_0^m \left( X_{i,n}^1(x) \right)
\]

with the notation that \( \left( (X_{1,n,w}^m(x), Y_{1,n,w}^m(x)), \ldots, (X_{n,w,n,w}^m(x), Y_{n,w,n,w}^m(x)) \right) \) is a reordering of the touples \( (X_j^w(x), Y_j^w(x)) \) such that \( \|X_j^w(x) - x\| \) is increasing in \( i \). With this notation we can write the estimators of the first stage as

\[
\hat{\mu}_0^m(x) = \frac{1}{k_0} \sum_{i=1}^{k_0} Y_{i,m}^0(x), \quad \text{and} \quad \hat{\mu}_1^n(x) = \frac{1}{k_1} \sum_{i=1}^{k_1} Y_{i,n}^1(x),
\]

and we can upper bound the EMSE with the following sum.

\[
\mathbb{E} \left[ \| \tau(\mathcal{X}) - \hat{\tau}_1^{mn}(\mathcal{X}) \|^2 \right]
\]

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

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

The first term is the regression problem for the first step of the X-learner and we can control this term with Lemma 9.

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

The second term is more challenging:

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

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

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

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

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

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Next we find an upper bound for (33).

\[
(33) \leq E\left(\frac{1}{k_1k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} \left\| \mu_0(\mathcal{X}) - \mu_0\left(X^0_{(j,m)}(X^1_{(i,n)}(\mathcal{X}))\right) \right\|^2 \right) \\
\leq E\left(\frac{1}{k_1k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} L \left\| X - X^0_{(j,m)}(X^1_{(i,n)}(\mathcal{X})) \right\|^2 \right) \\
\leq L^2 \frac{1}{k_1k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} E \left\| X - X^0_{(j,m)}(X^1_{(i,n)}(\mathcal{X})) \right\|^2 \\
\leq L^2 \frac{1}{k_1k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} E \left\| X^1_{(i,n)}(\mathcal{X}) - X^0_{(j,m)}(X^1_{(i,n)}(\mathcal{X})) \right\|^2 \quad (35) \\
+ L^2 \frac{1}{k_1k_0} \sum_{i=1}^{k_1} \sum_{j=1}^{k_0} E \left\| X^1_{(i,n)}(\mathcal{X}) - X_{(j,m)}(X^1_{(i,n)}(\mathcal{X})) \right\|^2 \quad (36)
\]

where (35) follows from Jensen’s inequality.

Let’s consider (36): We partition the data into \(A_1, \ldots, A_{k_1}\) sets, where the first \(k_1 - 1\) sets have \(\lceil \frac{n}{k_1} \rceil\) elements and we define \(\tilde{X}_{i,1}(x)\) to be the nearest neighbor of \(x\) in \(A_i\). Then we can conclude that

\[
\frac{1}{k_1} \sum_{i=1}^{k_1} E \left\| X - X^1_{(i,n)}(\mathcal{X}) \right\|^2 \leq \frac{1}{k_1} \sum_{i=1}^{k_1} E \left\| X - \tilde{X}_{i,1}(\mathcal{X}) \right\|^2 \\
= \frac{1}{k_1} \sum_{i=1}^{k_1} E \left[ E \left\| X - \tilde{X}_{i,1}(\mathcal{X}) \right\|^2 \left| \mathcal{X} \right. \right] \leq \frac{\tilde{c}}{\lceil \frac{n}{k_1} \rceil^{2/d}}. 
\]

Here the last inequality follows from Lemma 6. With exactly the same argument, we can bound (37) and we thus have:

\[
(33) \leq L^2 \tilde{c} \ast \left( \frac{1}{\lceil \frac{n}{k_1} \rceil^{2/d}} + \frac{1}{\lceil \frac{k_0}{k_1} \rceil^{2/d}} \right) \leq 2L^2 \ast \left( \left( \frac{k_1}{n} \right)^{2/d} + \left( \frac{k_0}{m} \right)^{2/d} \right). 
\]

Plugging everything in, we have

\[
E[\tau(\mathcal{X}) - \tilde{\tau}^{\text{nn}}(\mathcal{X})]^2 \leq 2\frac{\sigma^2}{k_1} + 2(\sigma_c + 2\tilde{c})L^2 \left( \frac{k_1}{n} \right)^{2/d} + 2\frac{\sigma^2}{k_0} + 4\tilde{c}L^2 \left( \frac{k_0}{m} \right)^{2/d} \\
\leq C \left( \frac{\sigma^2}{k_1} + L^2 \left( \frac{k_1}{n} \right)^{2/d} + \frac{\sigma^2}{k_0} + \left( \frac{k_0}{m} \right)^{2/d} \right)
\]

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

### H. Pseudo Code

In this section, we will present pseudo code for the algorithms in this paper. We denote by \(Y^0\) and \(Y^1\) the observed outcomes for the control and the treated group. For example, \(Y^1_i\) 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, \(X^1_i\) corresponds to the feature vector of the \(i\)th unit in the treated group. \(M_k(Y \sim X)\) is the notation for a regression estimator, which estimates \(x \mapsto E[Y|X = x]\). It can be any regression/machine learning estimator. In particular, it can be a black box algorithm.
Algorithm 1 T-learner
1: procedure T-Learner($X,Y,W$)
2: \[ \hat{\mu}_0 = M_0(Y^0 \sim X^0) \]
3: \[ \hat{\mu}_1 = M_1(Y^1 \sim X^1) \]
4: \[ \hat{\tau}(x) = \hat{\mu}_1(x) - \hat{\mu}_0(x) \]

$M_0$ and $M_1$ are here some, possibly different machine learning/regression algorithms.

Algorithm 2 S-learner
1: procedure S-Learner($X,Y,W$)
2: \[ \hat{\mu} = M(Y \sim (X,W)) \]
3: \[ \hat{\tau}(x) = \hat{\mu}(x,1) - \hat{\mu}(x,0) \]

$M(Y \sim (X,W))$ is the notation for estimating $(x,w) \mapsto \mathbb{E}[Y|X=x,W=w]$ while treating $W$ as a 0,1–valued feature.

Algorithm 3 X-learner
1: procedure X-Learner($X,Y,W,g$)
2: \[ \hat{\mu}_0 = M_1(Y^0 \sim X^0) \quad \triangleright \text{Estimate response function} \]
3: \[ \hat{\mu}_1 = M_2(Y^1 \sim X^1) \]
4: \[ \tilde{D}_i^1 = Y_i^1 - \hat{\mu}_0(X_i^1) \quad \triangleright \text{Compute imputed treatment effects} \]
5: \[ \tilde{D}_i^0 = \hat{\mu}_1(X_i^0) - Y_i^0 \]
6: \[ \hat{\tau}_1 = M_3(\tilde{D}_i \sim X^1) \quad \triangleright \text{Estimate CATE for treated and control} \]
7: \[ \hat{\tau}_0 = M_4(\tilde{D}_i \sim X^0) \]
8: \[ \hat{\tau}(x) = g(x) \hat{\tau}_0(x) + (1 - g(x)) \hat{\tau}_1(x) \quad \triangleright \text{Average the estimates} \]

$g(x) \in [0,1]$ is a weighting 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, but also choosing it to be constant and equal to the ratio of treated units usually leads to a good estimator of the CATE.

Algorithm 4 F-learner
1: procedure F-Learner($X,Y,W$)
2: \[ \hat{e} = M_e[W \sim X] \]
3: \[ Y_i^* = Y_i - \frac{\hat{e}(X_i)}{\hat{e}(X_i)} \]
4: \[ \hat{\tau} = M_4(Y^* \sim X) \]

Algorithm 5 U-learner
1: procedure U-Learner($X,Y,W$)
2: \[ \hat{\mu}_{obs} = M_{obs}(Y_{obs} \sim X) \]
3: \[ \hat{e} = M_e[W \sim X] \]
4: \[ R_i = (Y_i - \hat{\mu}_{obs}(X_i))/(W_i - \hat{e}(X_i)) \]
5: \[ \hat{\tau} = M_4(R \sim X) \]
Algorithm 6 Bootstrap Confidence intervals

1: procedure computeCI(
    x: features of the training data,
    w: treatment assignments of the training data,
    y: observed outcomes of the training data,
    p: point of interest )
2:     for b in \{1, \ldots, B\} do
3:         s = sample(1 : n, replace = T, size = ⌈n/2⌉)
4:         x_\ast_b = x_s
5:         w_\ast_b = w_s
6:         y_\ast_b = y_s
7:         \hat{\tau}_\ast_b(p) = learner(x_\ast_b, w_\ast_b, y_\ast_b)[p]
8:     \hat{\tau}(p) = learner(x, w, y)[p]
9:     \sigma = sd(\{\hat{\tau}_\ast_b(p)\}_b=1^B)
10:    return (\hat{\tau}(p) - q_{\alpha/2}\sigma, \hat{\tau}(p) + q_{1-\alpha/2}\sigma)