Meta-learners for Estimating Heterogeneous Treatment Effects using Machine Learning

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joint work with Sören R. Künzel, Peter Bickel, and Bin Yu

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October 19, 2017

Heterogenous Treatment Effects

- Measuring human activity has generated massive datasets with granular population data: e.g.,
  - Browsing, search, and purchase data from online platforms
  - Internet of things
  - Electronic medical records, genetic markers
  - Administrative data: schools, criminal justice, IRS
- Big in size and breadth: wide datasets
- Data can be used for personalization of treatments, creating markets, modeling behavior
- Many inferential issues: e.g., heterogeneity, targeting optimal treatments, interpretable results

Conditional Average Treatment Effect (CATE)

Individual Treatment Effect (ITE): $D_i := Y_i(t) - Y_i(c)$

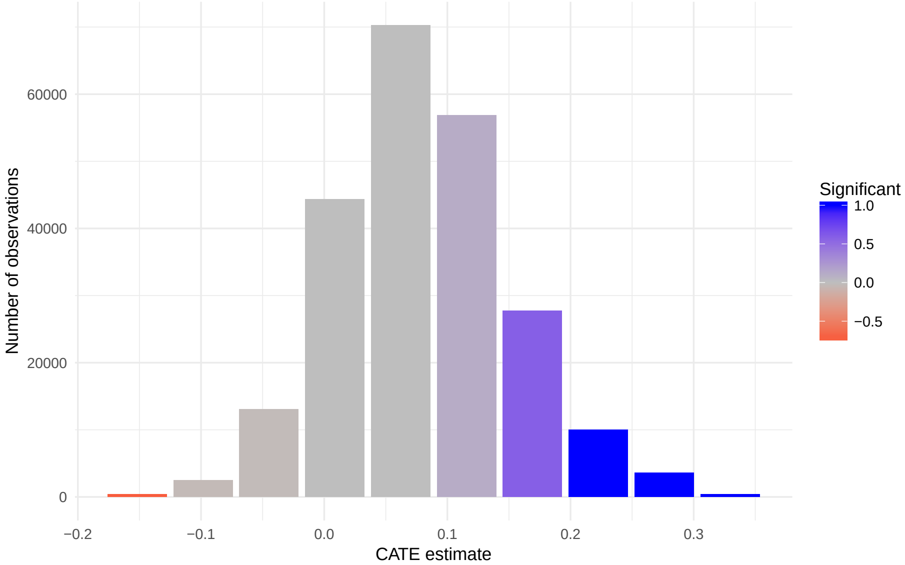
Let $\hat{\tau}_i$ be an estimator for D_i

$\tau(x_i)$ is the **CATE** for all units whose covariate vector is equal to x_i:

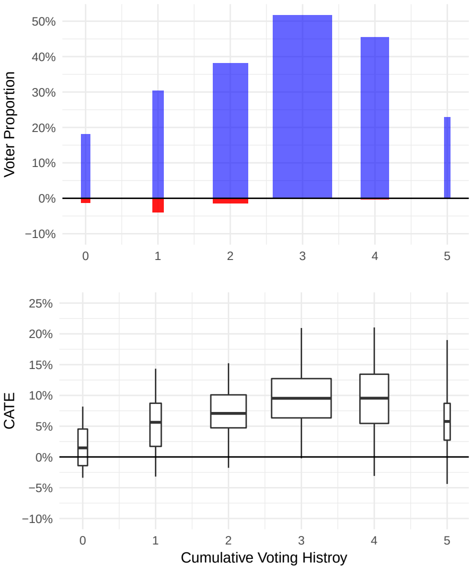
$$CATE := \tau(x_i) := \mathbb{E}\Big[D \Big| X = x_i\Big] = \mathbb{E}\Big[Y(t) - Y(c) \Big| X_i = x_i\Big]$$

Supplementary

GOTV: Social pressure (Gerber, Green, Lairmer, 2008)



GOTV: Social pressure (Gerber, Green, Lairmer, 2008)



How to estimate the CATE?

Meta–learners

A meta–learner decomposes the problem of estimating the CATE into several sub–regression problems. The estimator which solve those sub–problems are called **base–learners**

- Flexibility to choose base–learners which work well in a particular setting
- Deep Learning, (honest) Random Forests, BART, or other machine learning algorithms

Estimators for the CATE

$$\begin{aligned}\tau(x) &= \mathbb{E}[Y(1) - Y(0)|X = x] \\ &= \mathbb{E}[Y(1)|X = x] - \mathbb{E}[Y(0)|X = x]\end{aligned}$$

Estimators for the CATE

$$
\begin{aligned}
\tau(x) &= \mathbb{E}[Y(1) - Y(0)|X = x] \\
&= \mathbb{E}[Y(1)|X = x] - \mathbb{E}[Y(0)|X = x] \\
&= \mu_1(x) - \mu_0(x)
\end{aligned}
$$

T–learner

1.) Split the data into control and treatment group,

2.) Estimate the response functions separately,

$$
\begin{aligned}
\hat{\mu}_1(x) &= \hat{\mathbb{E}}[Y^{obs}|X = x, W = 1] \\
\hat{\mu}_0(x) &= \hat{\mathbb{E}}[Y^{obs}|X = x, W = 0],
\end{aligned}
$$

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

Estimators for the CATE

$$\begin{aligned}\tau(x) &= \mathbb{E}[Y(1) - Y(0)|X = x] \\ &= \mathbb{E}[Y(1)|X = x] - \mathbb{E}[Y(0)|X = x] \\ &= \mu_1(x) - \mu_0(x)\end{aligned}$$

T–learner

1.) Split the data into control and treatment group,

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$$\hat{\mu}_1(x) = \hat{\mathbb{E}}[Y^{obs}|X = x, W = 1]$$
$$\hat{\mu}_0(x) = \hat{\mathbb{E}}[Y^{obs}|X = x, W = 0],$$

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

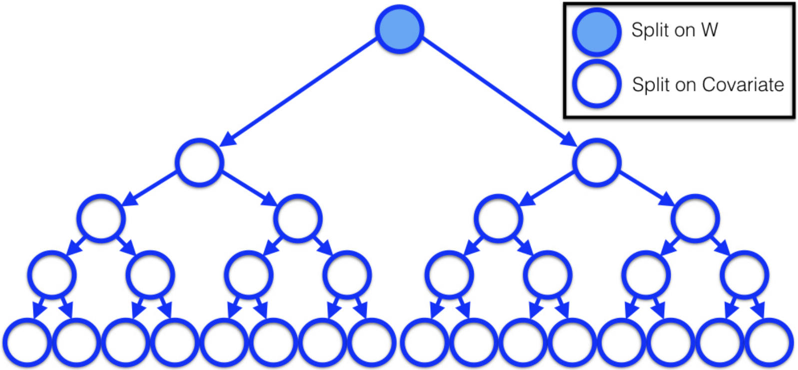
S–learner

1.) Use the treatment assignment as a usual variable without giving it any special role and estimate

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

2.) $\hat{\tau}(x) := \hat{\mu}(x, 1) - \hat{\mu}(x, 0)$

$$\hat{\tau}(x) = f(x, w = 1) - f(x, w = 0)$$



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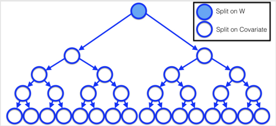
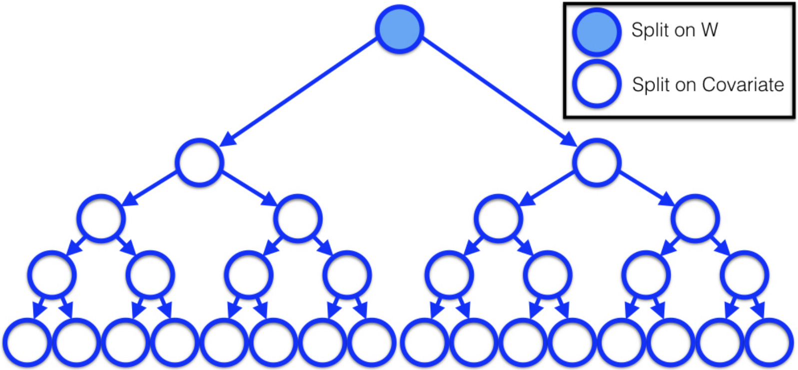
T–learner





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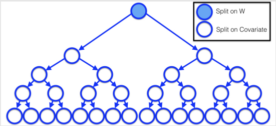

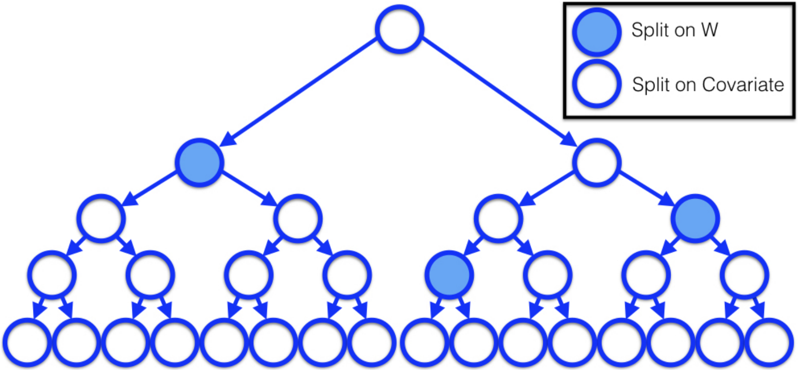

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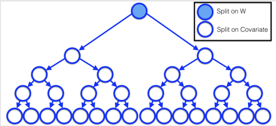

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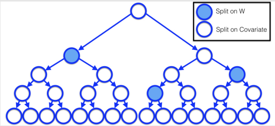

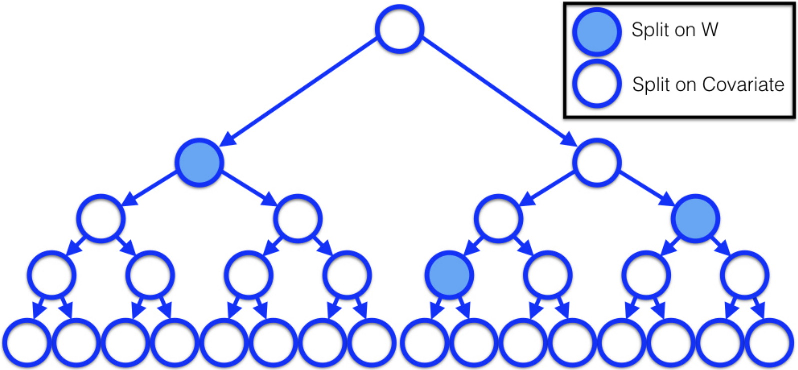

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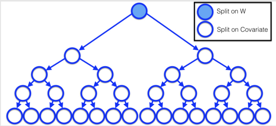

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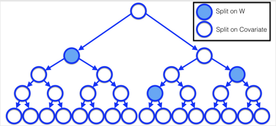

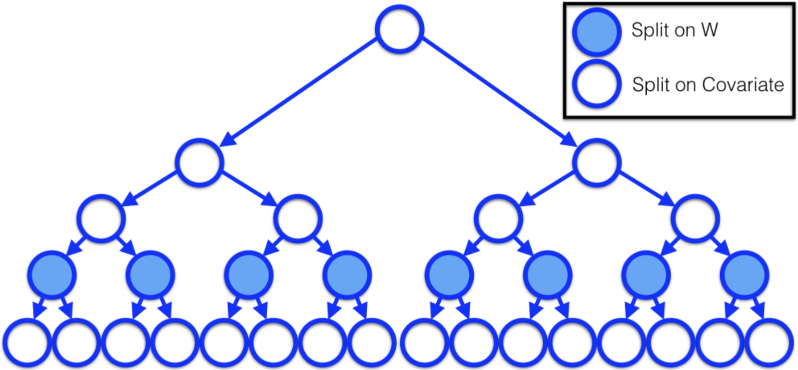

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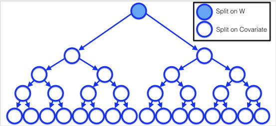

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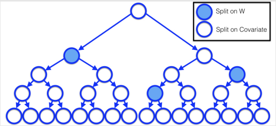
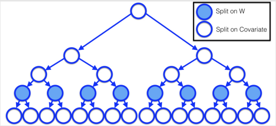
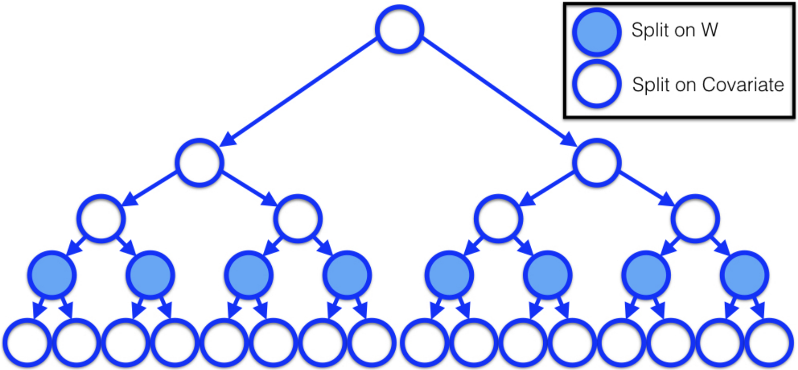
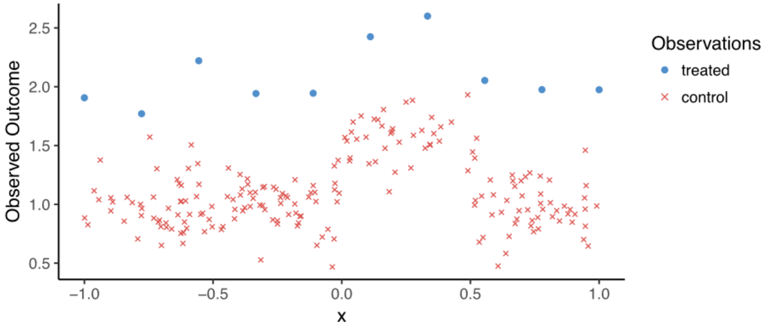


Causal Forest





Motivating X



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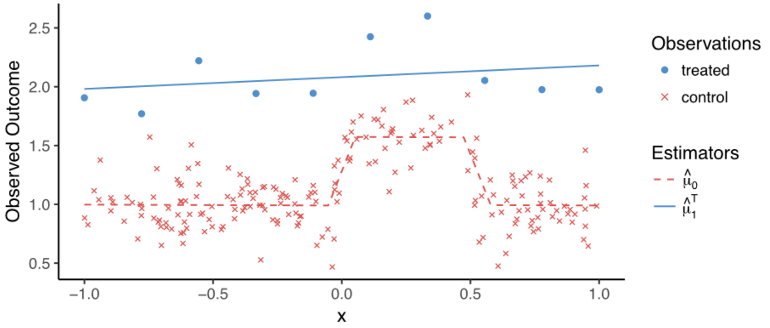

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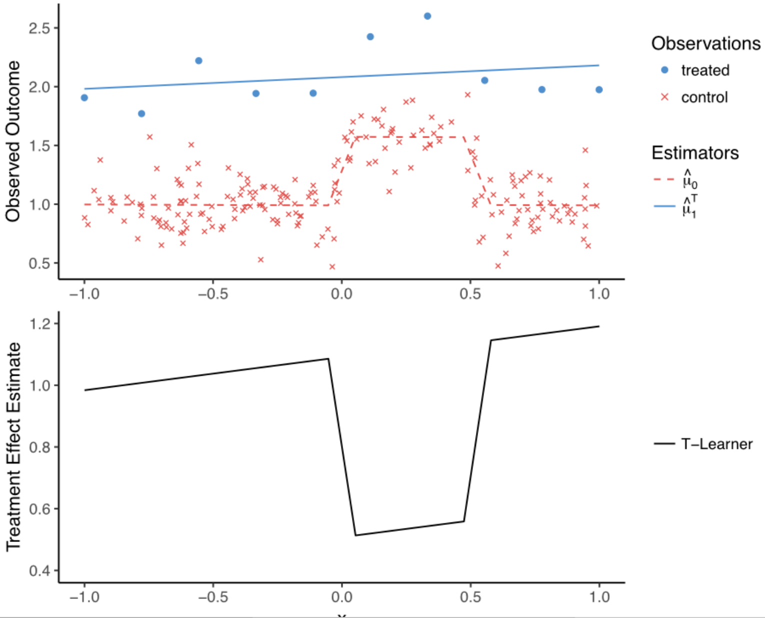

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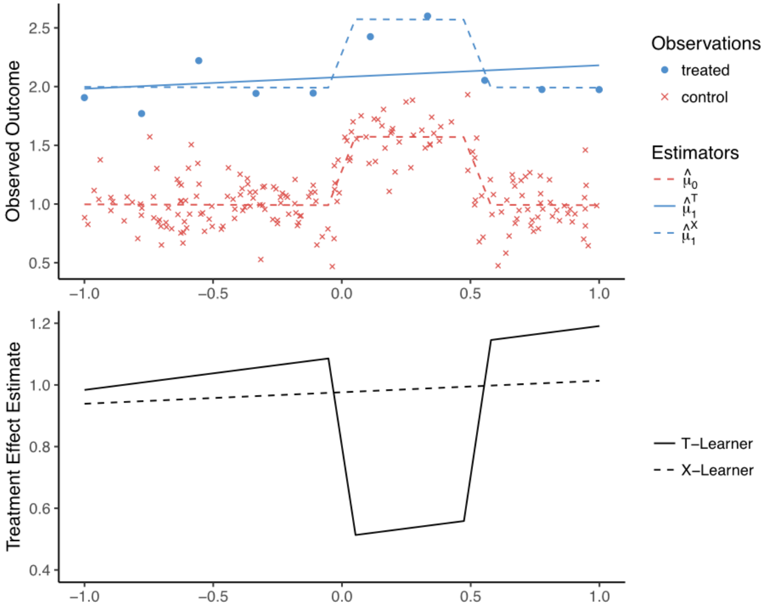


Definition of the X–learner

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

with $\mu_c(x) = \mathbb{E}[Y(0)|X = x]$.

X–learner

1.) Estimate the control response function:

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

2.) Define the **imputed ITE**:

$$\tilde{D}_i^1 := Y_i(1) - \hat{\mu}_c(X_i(1)),$$

3.) Estimate the CATE:

$$\hat{\tau}(x) = \hat{\mathbb{E}}[\tilde{D}^1|X = x].$$

Definition of the X–learner

Algorithm 1 X–learner

procedure X–LEARNER(X, Y, W)

$\hat{\mu}_c = {\color{blue}M_1}(Y^0 \sim X^0)$ ▷ Estimate response function

$\tilde{D}^1_i := Y^1_i - \hat{\mu}_c(X^1_i)$ ▷ Imputed ITE

$\hat{\tau}_1 = {\color{blue}M_3}(\tilde{D}^1 \sim X^1)$ ▷ Estimate CATE

end procedure

Definition of the X–learner

Algorithm 2 X–learner

procedure X–LEARNER(X, Y, W)

$\hat{\mu}_c = M_1(Y^0 \sim X^0)$ ▷ Estimate response function

$\hat{\mu}_t = M_2(Y^1 \sim X^1)$

$\tilde{D}_i^1 := Y_i^1 - \hat{\mu}_c(X_i^1)$ ▷ Imputed ITE

$\tilde{D}_i^0 := \hat{\mu}_t(X_i^0) - Y_i^0$

$\hat{\tau}_1 = M_3(\tilde{D}^1 \sim X^1)$ ▷ Estimate CATE

$\hat{\tau}_0 = M_4(\tilde{D}^0 \sim X^0)$

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

end procedure

Properties of the X–learner: Setup for Theory

A model for estimating the CATE

$$X \sim \lambda$$
$$W \sim \text{Bern}(e(X))$$
$$Y(0) = \mu_0(X) + \varepsilon(0)$$
$$Y(1) = \mu_1(X) + \varepsilon(1)$$

- If τ satisfies some regularity conditions (e.g. sparsity or smoothness), it can be directly exploited in the second base–learner
- This effect is in particular strong when μ_0 can be estimated very well
- Or when the error when estimating $\mu_0(x_i)$ is uncorrelated from the error when estimating $\mu_0(x_j)$ for $i \neq j$

Conjecture

Conjecture about the Minimax rates of the X–learner

If the response functions can be estimated at a particular rate a_μ, the CATE can be estimated at a rate of a_τ, the right choice of base learners, and some additional assumptions, then the two parts of the X–learner, $\hat{\tau}_0$ and $\hat{\tau}_1$, will achieve a rate of

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

respectively.

Theorem 1

Theorem covers the case when estimating the base functions is not beneficial

Künzel, Sekhon, Bickel, Yu 2017

Assume we observe m control and n treatment units,

1.) Strong Ignorability holds: $(Y(0), Y(1)) \perp W|X \quad 0 < e(X) < 1$

2.) The treatment effect is linear, $\tau(x) = x^T\beta$

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

Then the X-learner with $\hat{\mu}_0$ in the first stage, OLS in the second stage, achieves the parametric rate in n,

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

If there are a many control units, such that $m \asymp n^{1/a}$, then

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

Theorem 2

Theorem covers the case when estimating the CATE function is not beneficial

Künzel, Sekhon, Bickel, Yu 2017

X–learner is minimax optimal for a class of estimators using KNN as the base leaner. Assume:

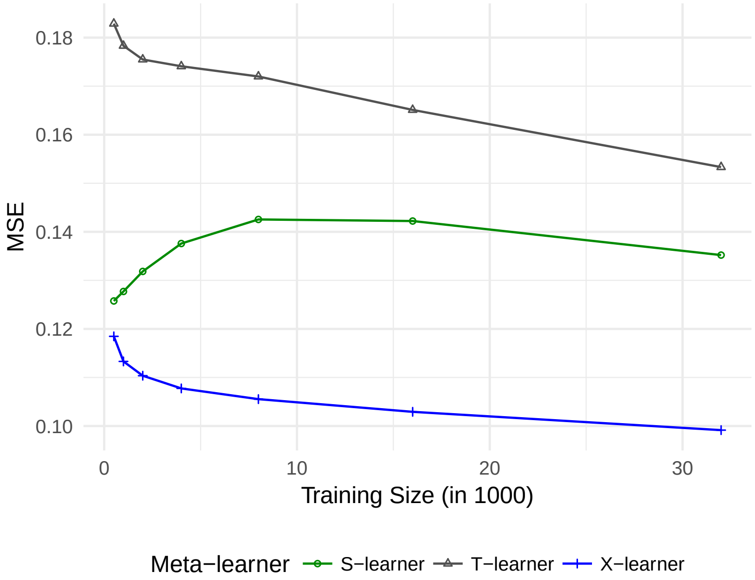
- Outcome functions are Lipschitz continuous
- CATE function has no simplification
- Features are uniformly distributed $[0, 1]^d$

The fastest possible rate of convergence for this class of problems is:

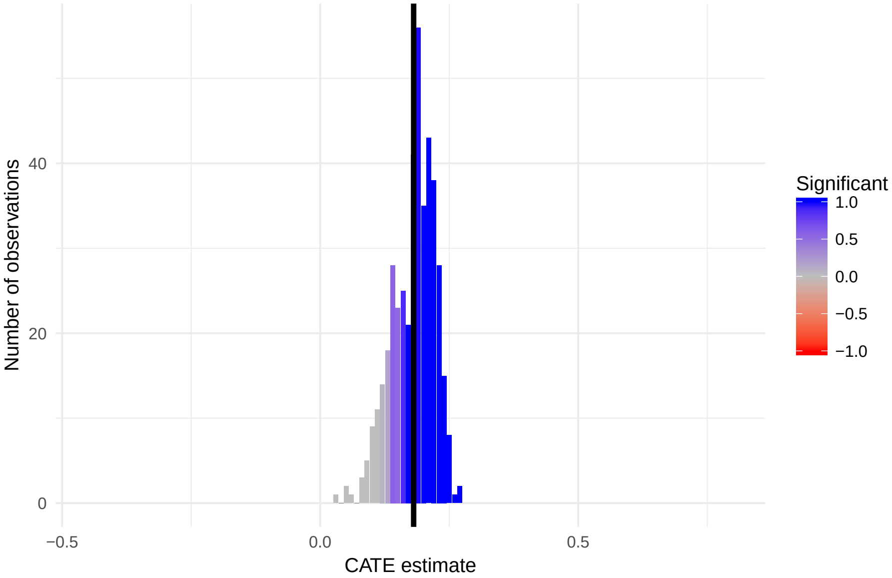
$$\mathcal{O}\left(\min(n_0, n_1)^{-\frac{1}{2+d}}\right)$$

- The speed of convergence is dominated by the size of the smaller assignment group
- In the worst case, there is nothing to learn from the other assignment group

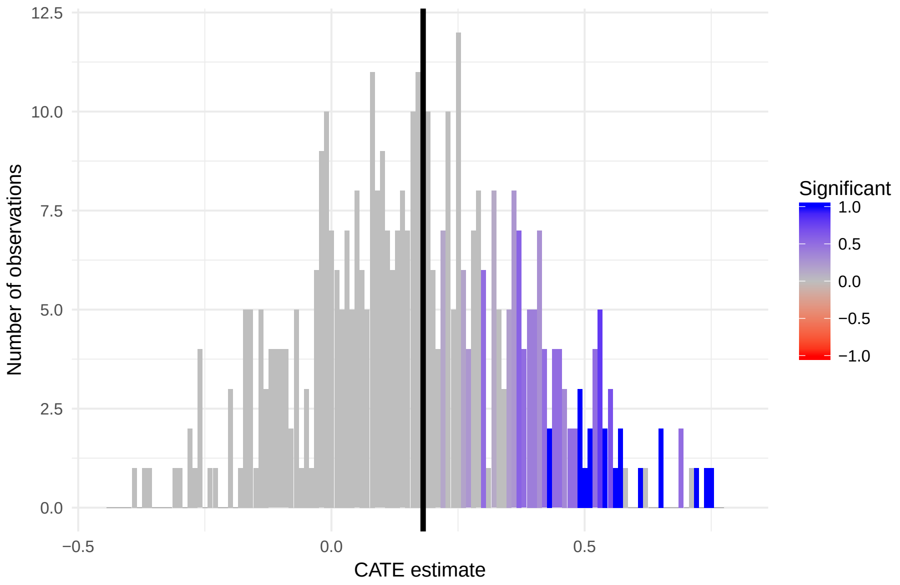
Data Simulation: Social pressure and Voter Turnout



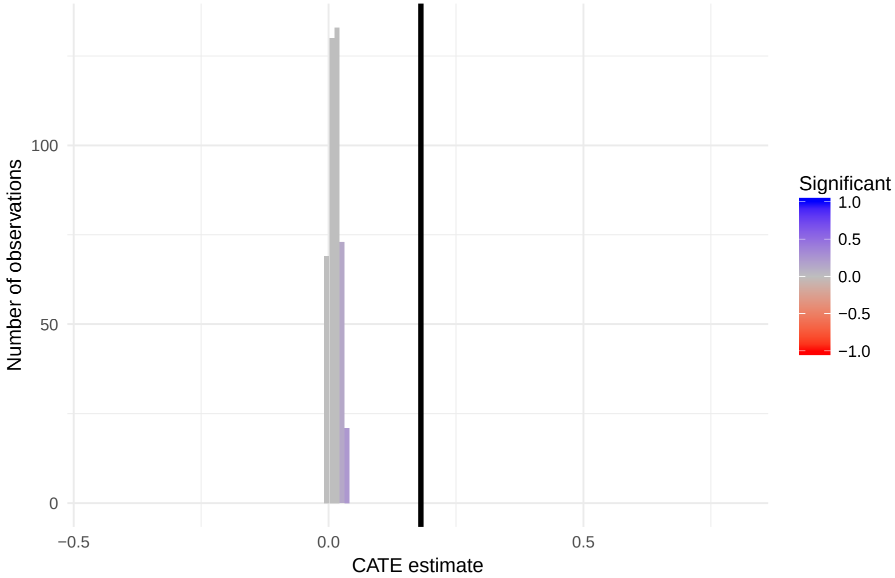
Reducing Transphobia: X–RF



Reducing Transphobia: T–RF



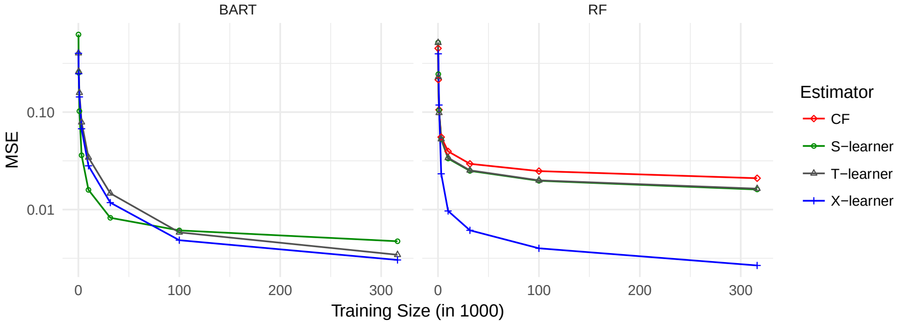
Reducing Transphobia: S–RF



Reducing Transphobia: Simulation

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

Complex Treatment Effect



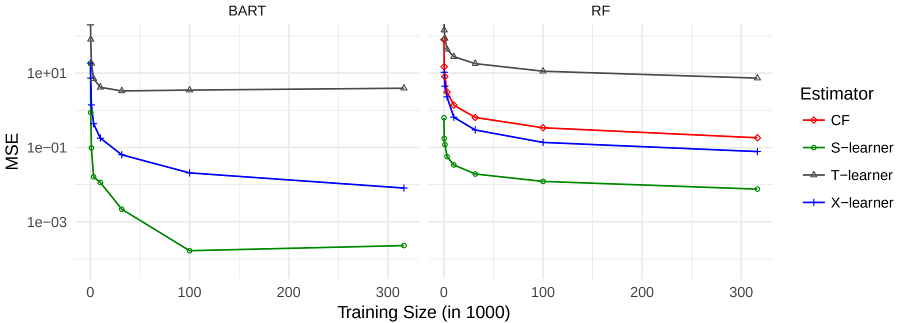
Complex Setting (WA, 2)

$$\mu_1(x) = \frac{1}{2}\eta(x_1)\eta(x_2) \text{ with } \eta(x) = 1 + \frac{1}{1+e^{-20(x-1/3)}}$$

$$\mu_0(x) = -\mu_1(x)$$

$$e(x) = 0.5$$

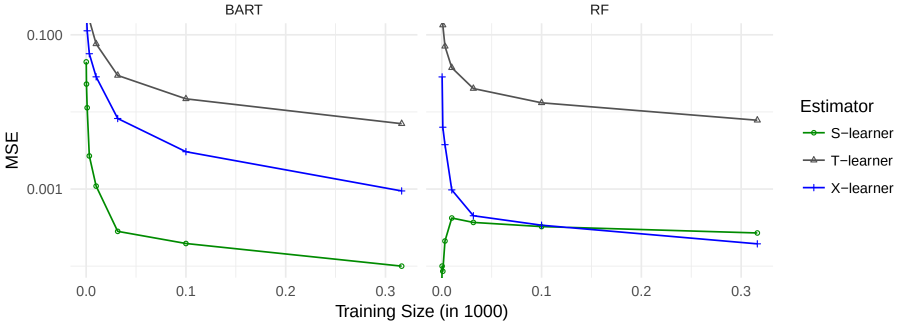
No Treatment Effect



Simple Setting

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

Resisting Confounding

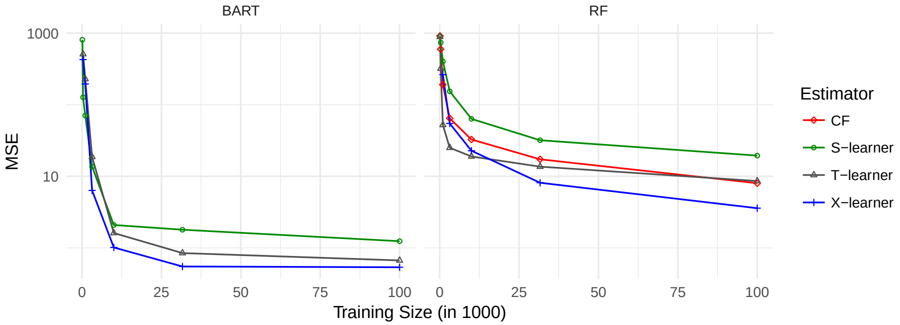


Confounded without TE (WA, 1)

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

More Estimators

Flexibility of Base Learners is Needed



Complicated Setting

$$\mu_1(x) = x^T\beta_1, \text{ with } \beta_1 \sim \text{Unif}([1,30]^d)$$
$$\mu_0(x) = x^T\beta_0, \text{ with } \beta_0 \sim \text{Unif}([1,30]^d)$$
$$e(x) = .5$$

Conclusion

- We expect more from our experiments than ever before
- We should protect the Type I error rate—e.g., honest Random Forests, cross-fitting
- Power is a significant concern
- Somethings are easier to validate than others: experiments estimating average sample effects versus CATE
- Observational data?
- Validation, validation, and validation

My Collaborators

Sören R. Künzel

Peter Bickel

Bin Yu

Variance of Conditional Average Treatment Effect

$$CATE := \tau(x_i) := \mathbb{E}\Big[D\Big|X = x_i\Big] = \mathbb{E}\Big[Y(t) - Y(c)\Big|X_i = x_i\Big]$$

Decompose the MSE at x_i:

$$\mathbb{E}\left[(D_i - \hat{\tau}_i)^2 | X_i = x_i\right] =$$
$$\underbrace{\mathbb{E}\left[(D_i - \tau(x_i))^2 | X_i = x_i\right]}_{\text{Approximation Error}} + \underbrace{\mathbb{E}\left[(\tau(x_i) - \hat{\tau}_i)^2 | X_i = x_i\right]}_{\text{Estimation Error}}$$

- Since we cannot estimate D_i, we estimate the CATE at x_i
- But the error for the CATE is not the same as the error for the ITE

Supplementary

Individual Treatment Effects: Information Theory Bound

$Y_u \sim P = N(\mu, \sigma^2)$, and we want to predict a new Y_i.
Our expected risk with infinite data is:

$$\mathbb{E}(\mu - Y_i)^2 =$$

Individual Treatment Effects: Information Theory Bound

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Our expected risk with infinite data is:

$$\mathbb{E}(\mu - Y_i)^2 = \sigma^2 = \alpha$$

With one data point?

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Our expected risk with infinite data is:

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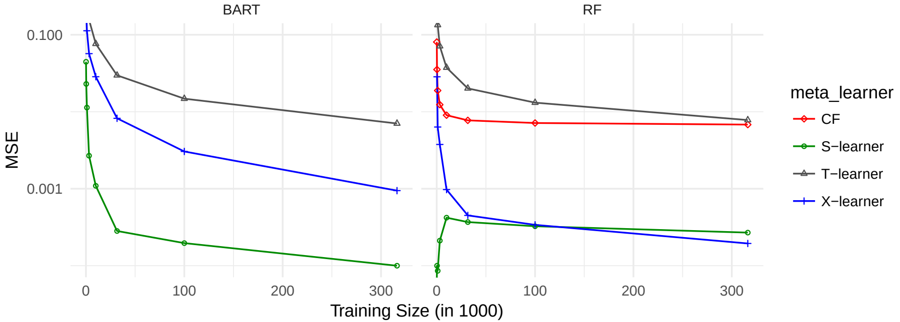
With one data point?

$$\begin{aligned} E(Y_i - Y_u)^2 &= E(Y_i - \mu + Y_u - \mu)^2 \\ &= E(Y_i - \mu)^2 + E(Y_u - \mu)^2 \\ &= 2\sigma^2 \\ &= 2\alpha \end{aligned}$$

General results for Cover-Hart class, which is a convex cone (Gneiting, 2012)
Back to CATE

Resisting Confounding: different base learners, same effect



Confounded without TE (WA, 1)

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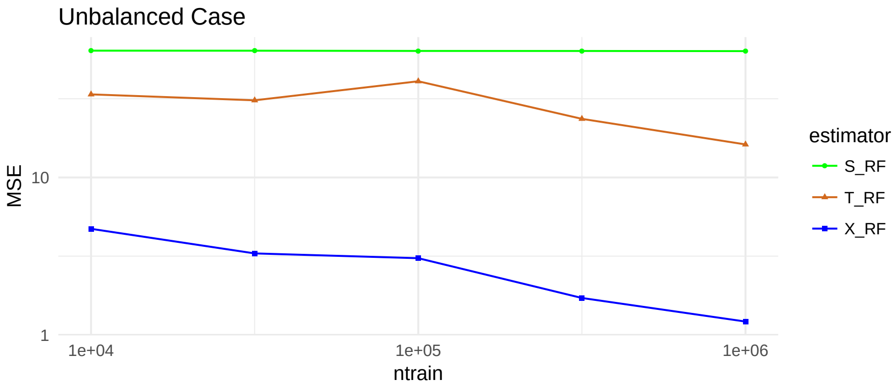
$$e(x) = \frac{1}{4}(1 + \beta_{2,4}(x_1))$$

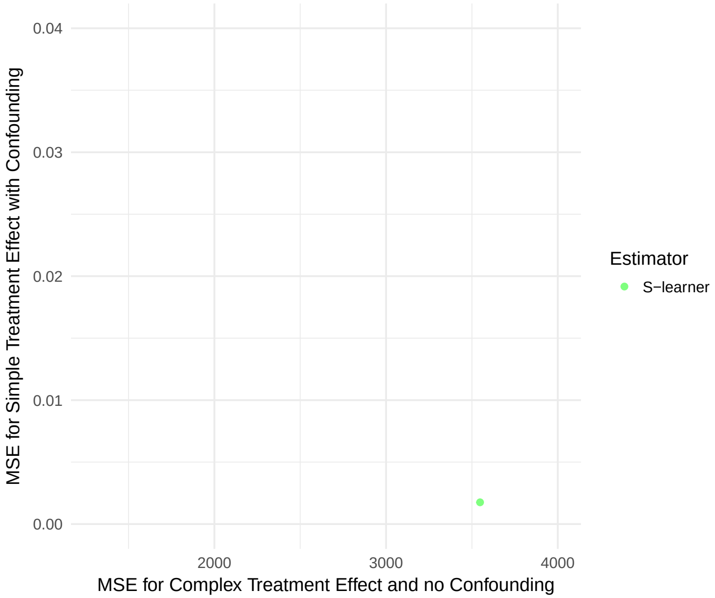
Back

The Unbalanced Case



$$\mu_0(x) = x^T\beta + 5 * 1(x1 > .5), \quad \text{with} \quad \beta \sim \text{Unif}\left([1,5]^d\right)$$
$$\mu_1(x) = \mu_1(x) + 8$$
$$e(x) = 0.01$$

Adaptivity



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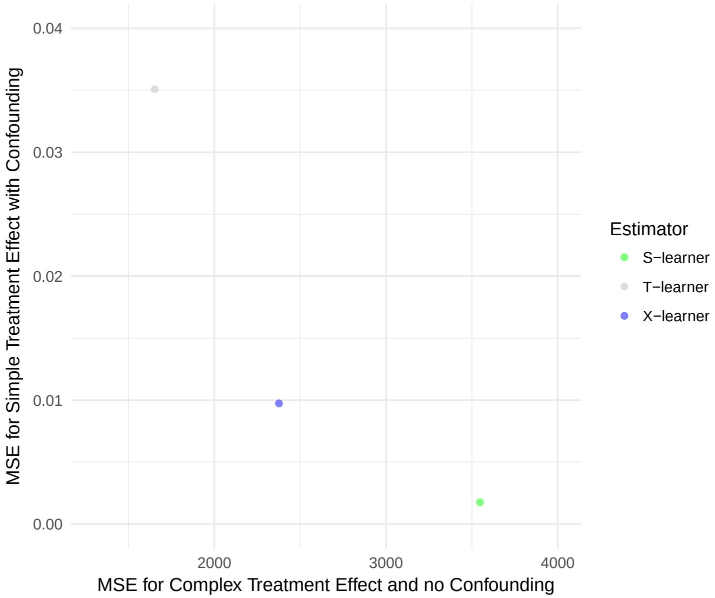
MSE for Simple Treatment Effect with Confounding
MSE for Complex Treatment Effect and no Confounding
Estimator
S−learner

Adaptivity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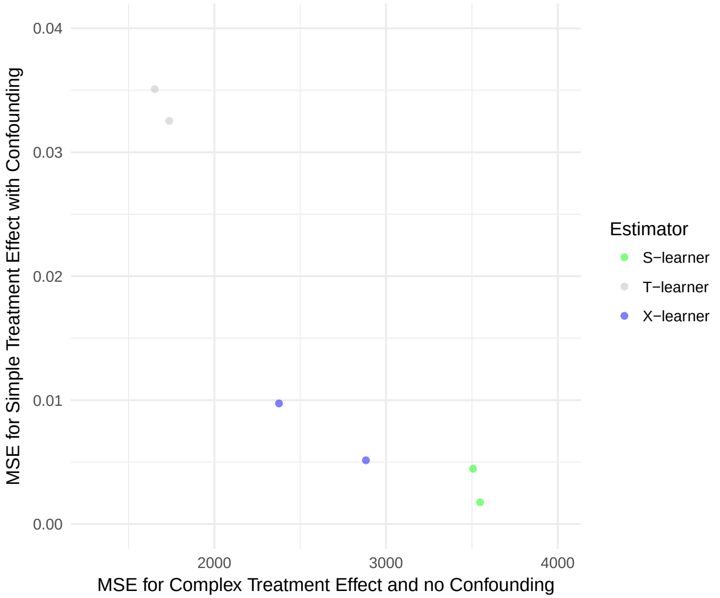
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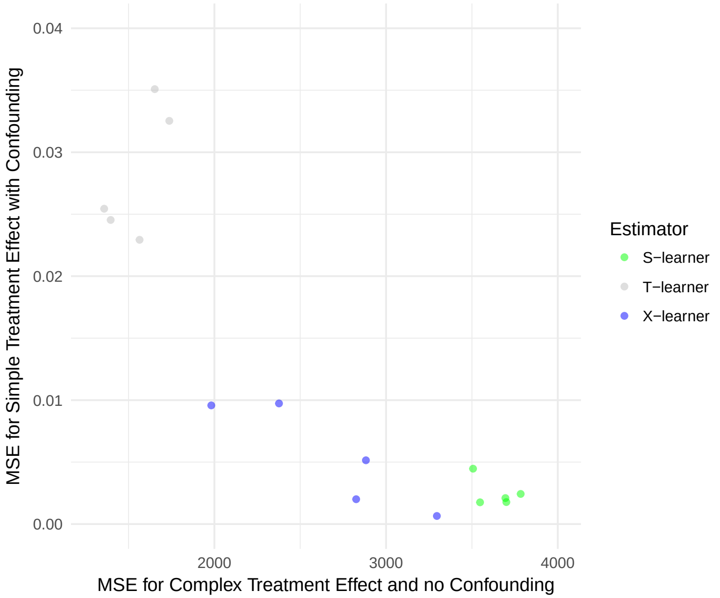
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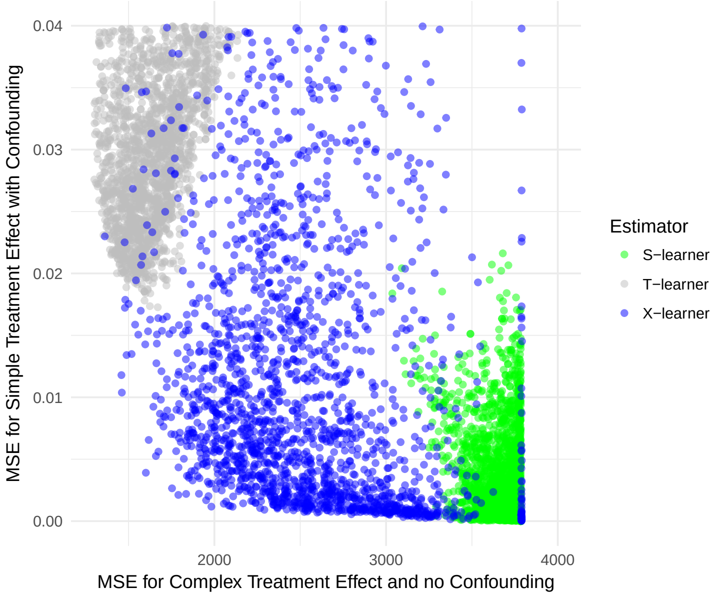

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0.01
0.00
MSE for Simple Treatment Effect with Confounding
2000
3000
4000
MSE for Complex Treatment Effect and no Confounding
Estimator
S−learner
T−learner
X−learner

Tuning

All meta–learners can be separated into several small regression problems, and we tune them separately using tuning methods which are specific for each of the learner

We have implemented a package combining the X–learner with honest Random Forests and it currently implements three tuning methods:

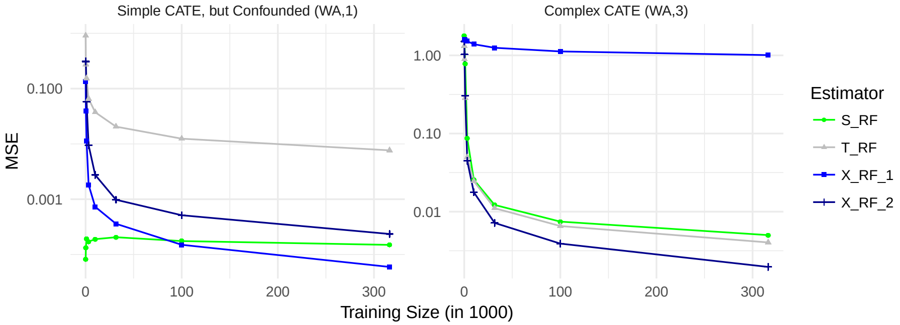
1.) Pre-specified tuning

2.) Gaussian Process

3.) Hyperband

Supplementary

Tuning



$$\mu_1(x) = 2x_1 - 1,$$
$$\mu_0(x) = 2x_1 - 1,$$
$$e(x) = \frac{1}{4}(1 + \beta_{2,4}(X_1))$$

$$\mu_1(x) = \zeta(X_1)\zeta(X_2),$$
$$\mu_0(x) = -\zeta(X_1)\zeta(X_2),$$
$$e(x) = 0.5,$$
$$\zeta(x) = \frac{2}{1 + e^{-12(x-1/2)}}$$