Meta-learners for Estimating Heterogeneous Treatment Effects using Machine Learning

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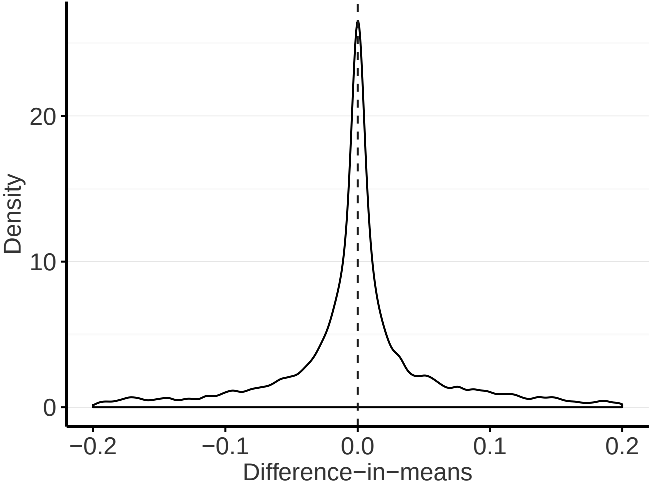
Heterogenous Treatment Effects

- 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

ML Prediction versus Causal Inference

- Causal Inference is like a prediction problem: but predicting something we don't directly observe and possibly cannot estimate well in a given sample
- ML algorithms are good at prediction, but have issues with causal inference:
  - Interventions imply counterfactuals: response schedule versus model prediction
  - Validation requires estimation in the case of causal inference
  - Identification problems not solved by large data
  - Predicting the outcome mistaken for predicting the causal effect
    - targeting based on the lagged outcome

Distribution of Treatment Effects



Sekhon and Shem-Tov (2017)

Conditional Average Treatment Effect (CATE)

Individual Treatment Effect (ITE): $D_i := Y_i(1) - Y_i(0)$

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:

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

Variance of Conditional Average Treatment Effect

$$CATE := \tau(x_i) := \mathbb{E}\Big[D\Big|X = x_i\Big] = \mathbb{E}\Big[Y(1) - Y(0)\Big|X_i = x_i\Big]$$

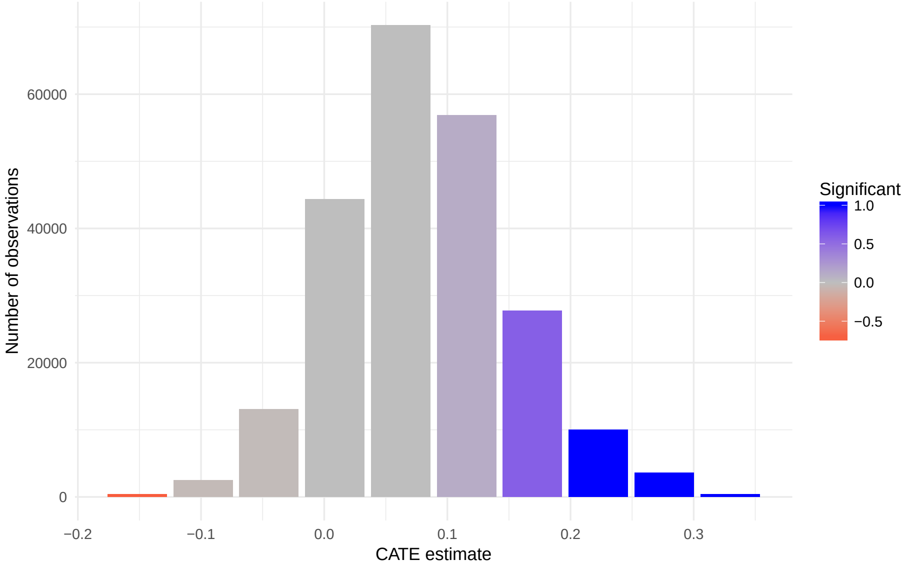
Decompose the MSE at x_i:

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

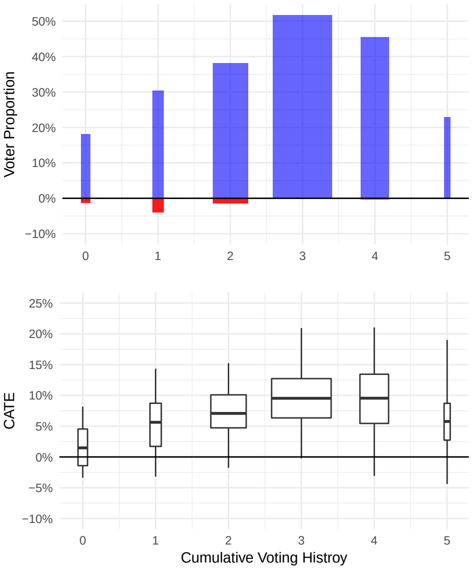
- Since we cannot estimate D_i, we estimate the CATE at x_i
- But the error for the CATE is not the same as the error for the ITE

Supplementary

GOTV: Social pressure



GOTV: Social pressure



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

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

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

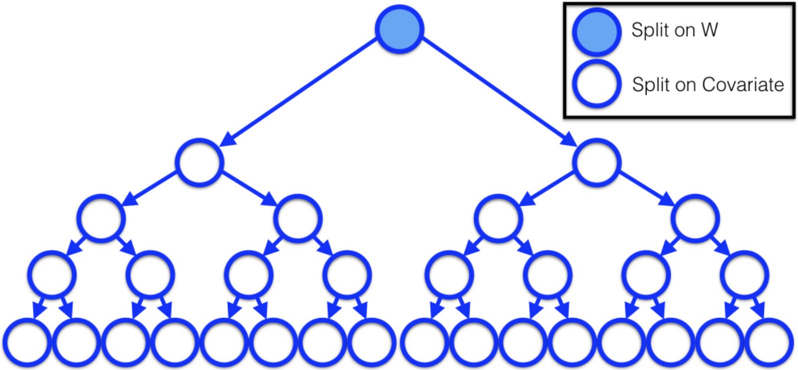
S–learner

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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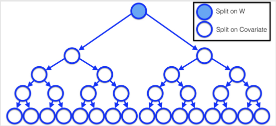

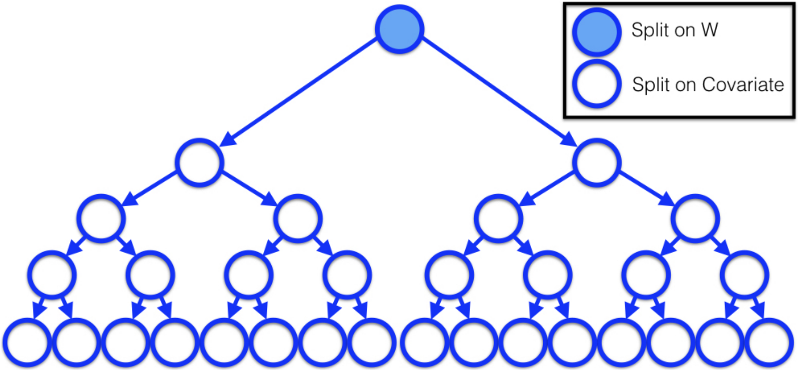

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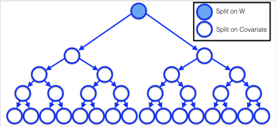

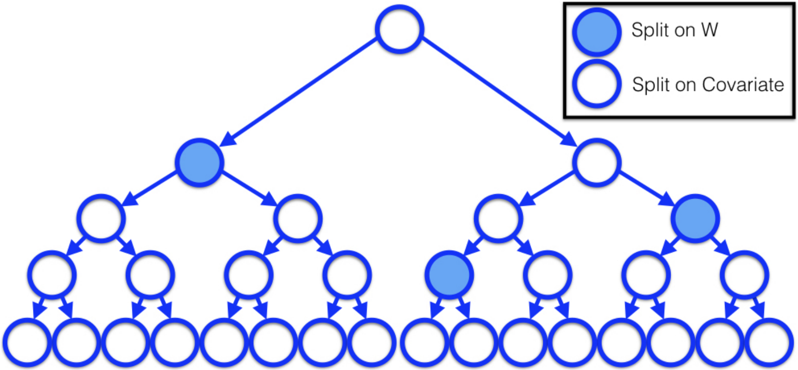

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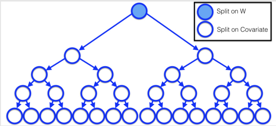
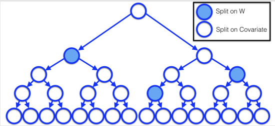
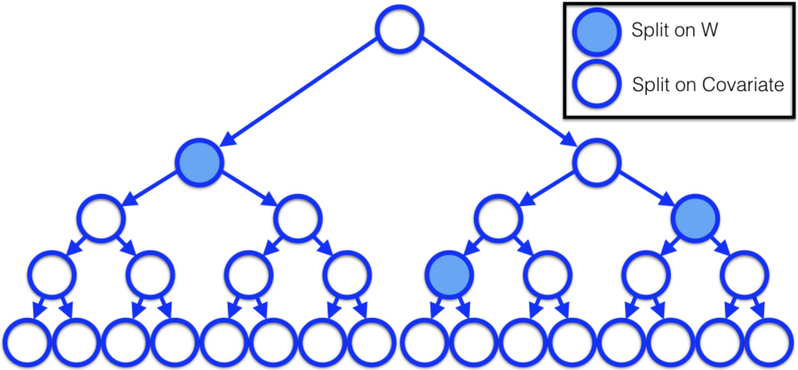


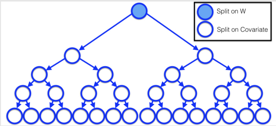
S–learner





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

T–learner



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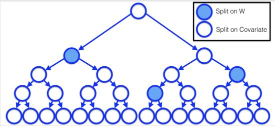

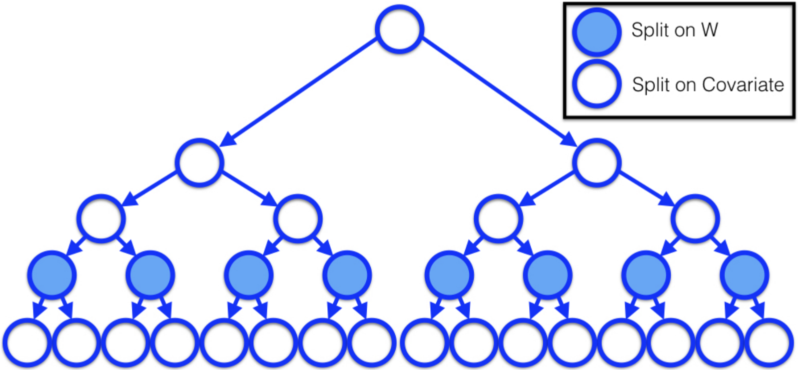

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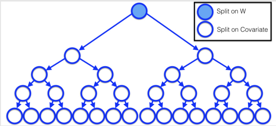
T–learner



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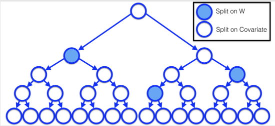
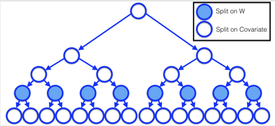
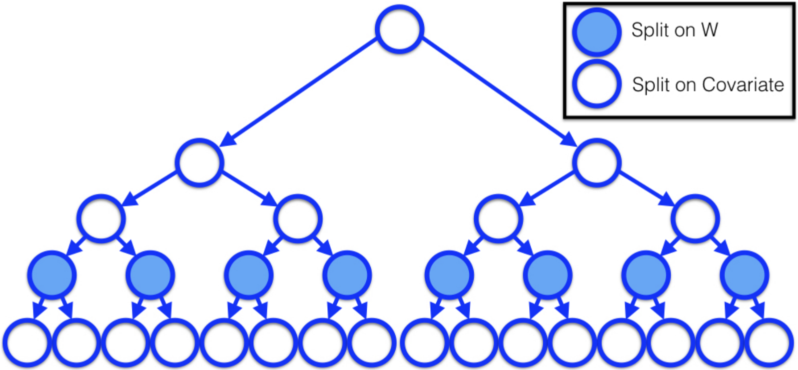
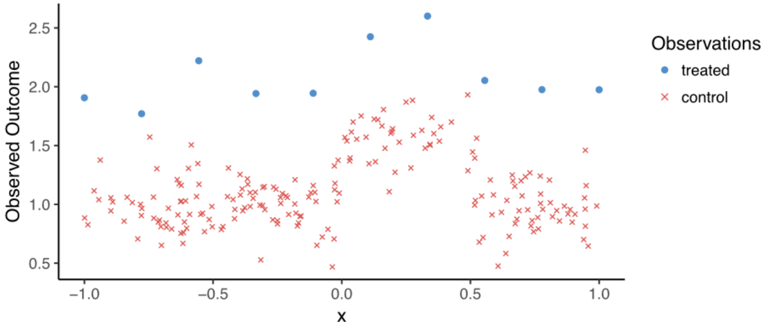


Causal Forest

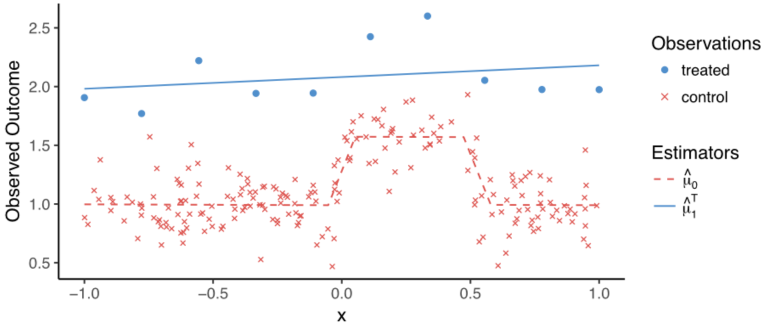




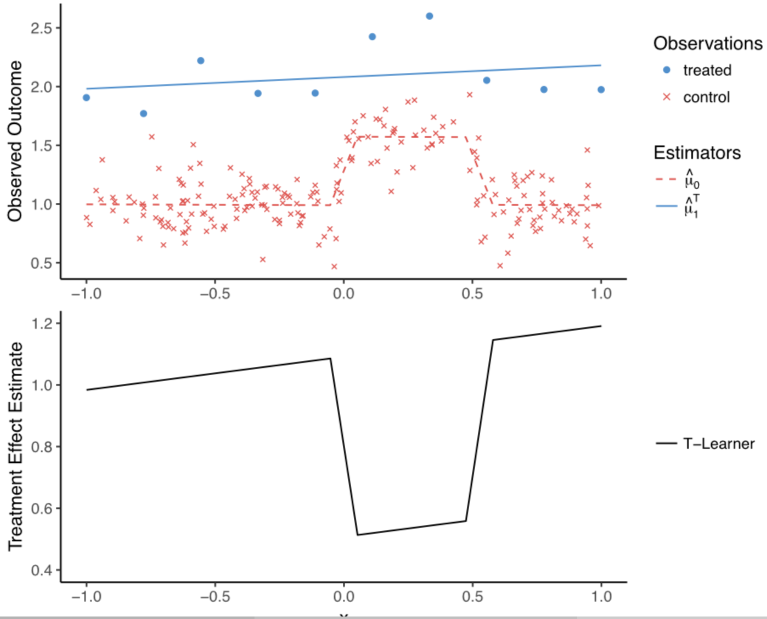
Motivating X



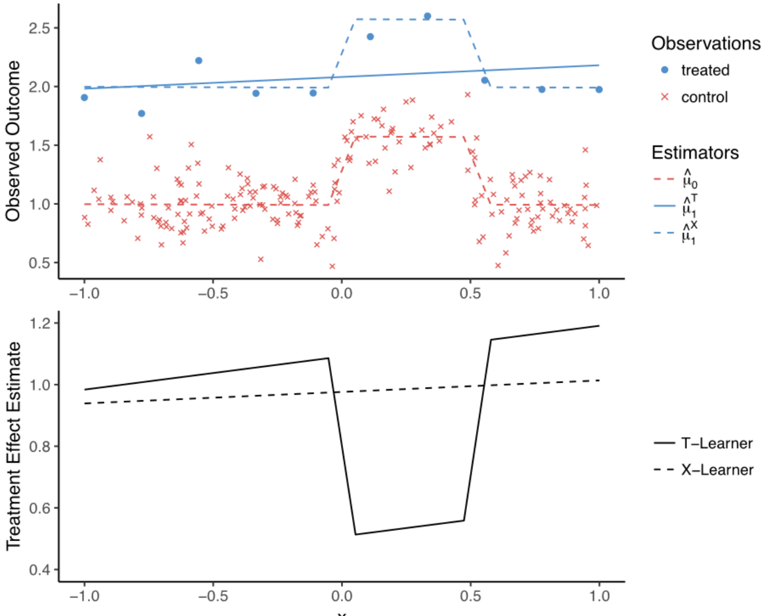
Motivating X



Motivating X



Motivating X



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

$\tilde{D}^1_i := Y^1_i - \hat{\mu}_c(X^1_i)$ ▷ Impute 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
$\hat{\mu}_t = M_2(Y^1 \sim X^1)$

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

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

- 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 $i \neq j$

Theorem 1

Künzel, Sekhon, Bickel, Yu 2017

Assume we observe m control and n treatment units,

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

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

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

Conjecture

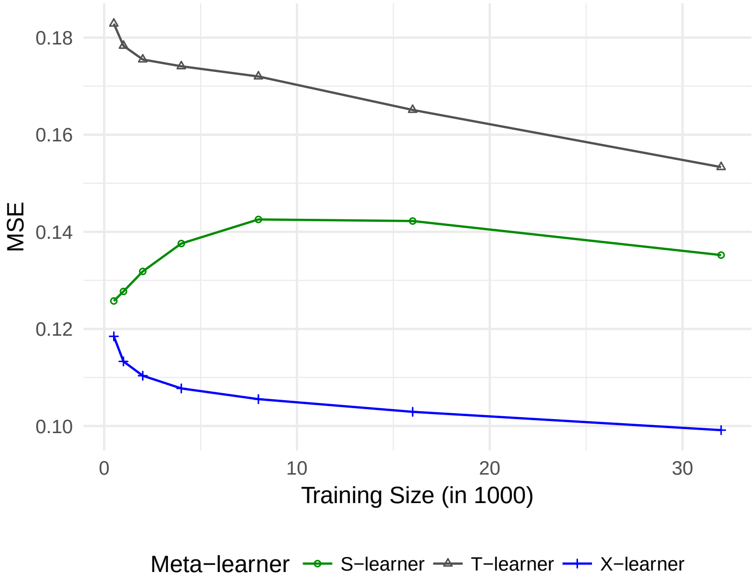
Conjecture about the Minimax rates of the X–learner

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 will achieve the rates of:

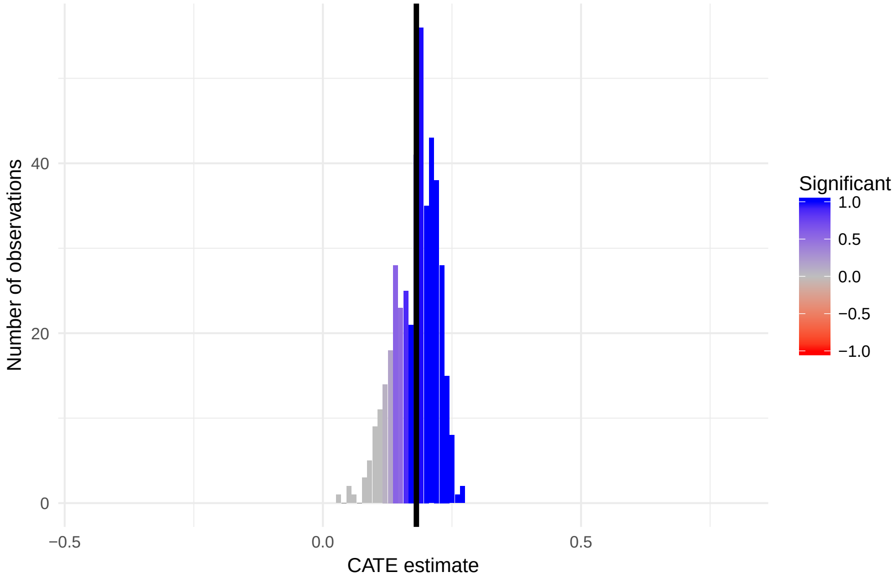
$$\hat{\tau}_0 \in \mathcal{O}\left(m^{-a_\tau} + n^{-a_\mu}\right)$$

$$\hat{\tau}_1 \in \mathcal{O}\left(m^{-a_\mu} + n^{-a_\tau}\right)$$

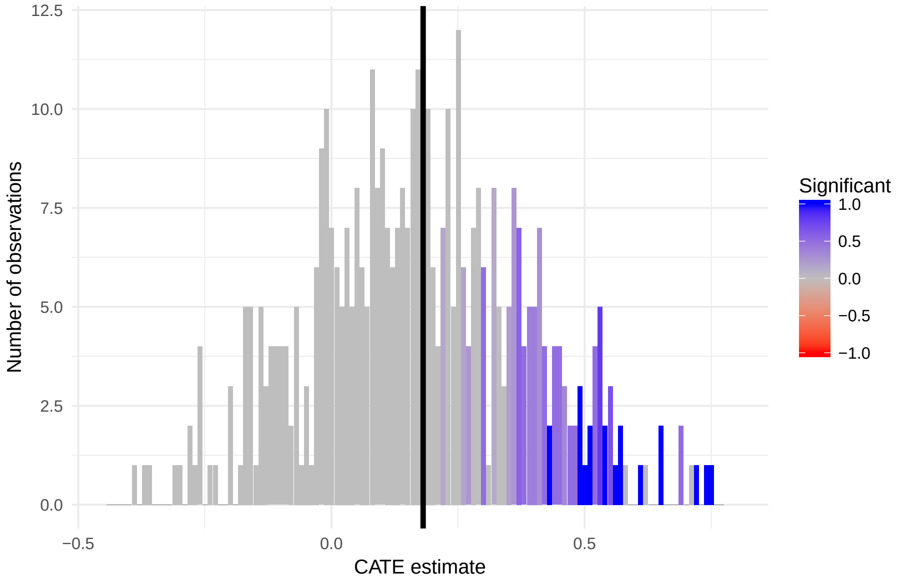
Data Simulation: Social pressure and Voter Turnout



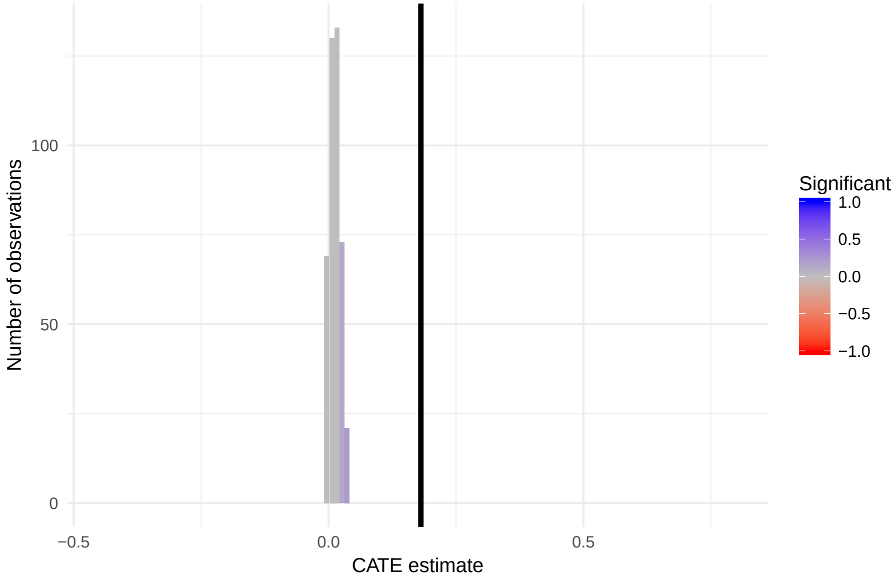
Reducing Transphobia: X–RF



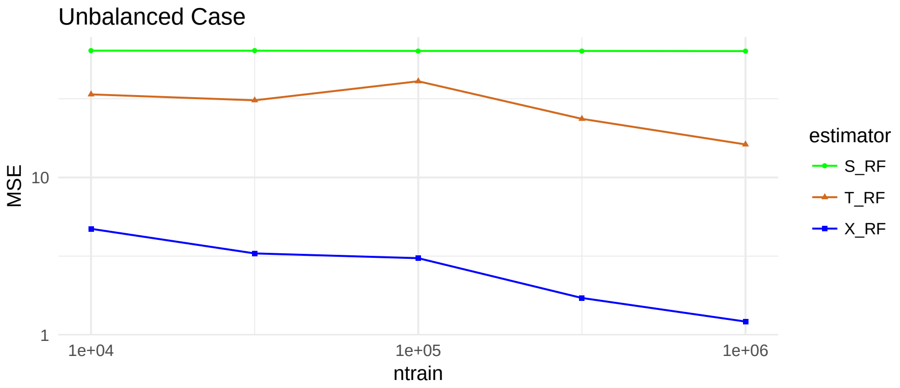
Reducing Transphobia: T–RF



Reducing Transphobia: S–RF

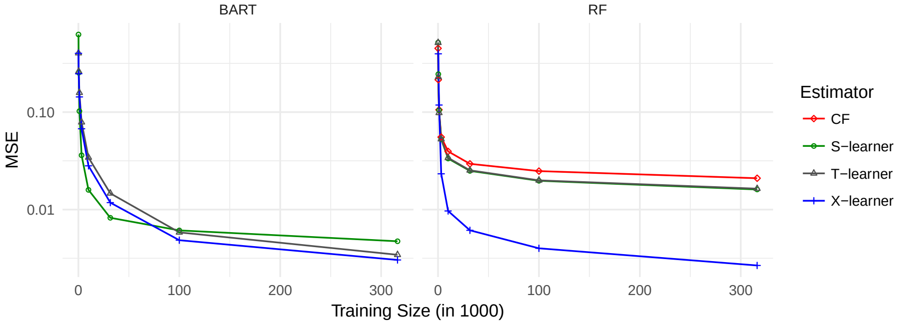


The Unbalanced Case



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

Complex Treatment Effect



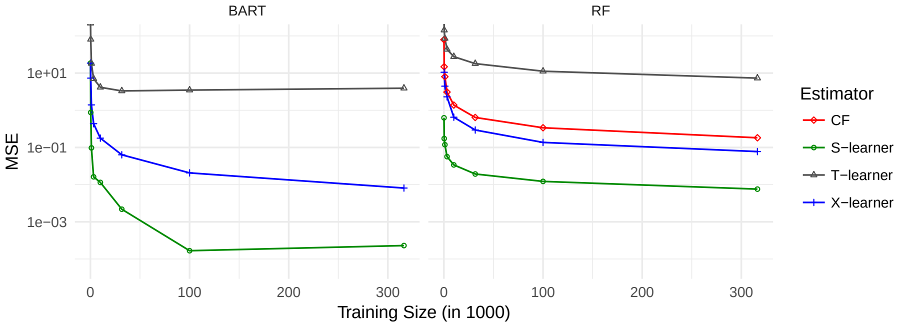
Complex Setting (WA, 2)

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

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

$$e(x) = 0.5$$

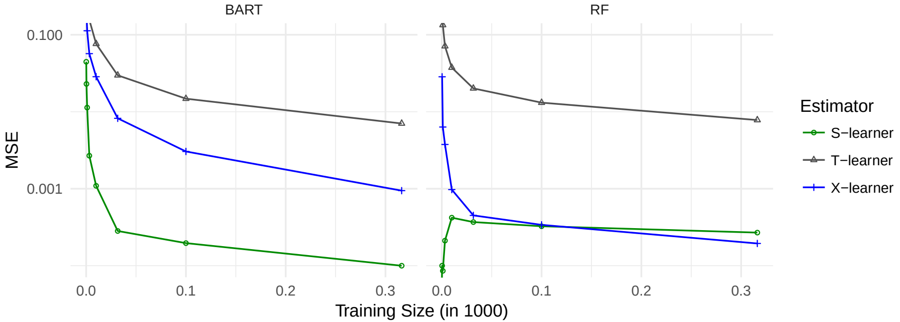
No Treatment Effect



Simple Setting

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

Resisting Confounding

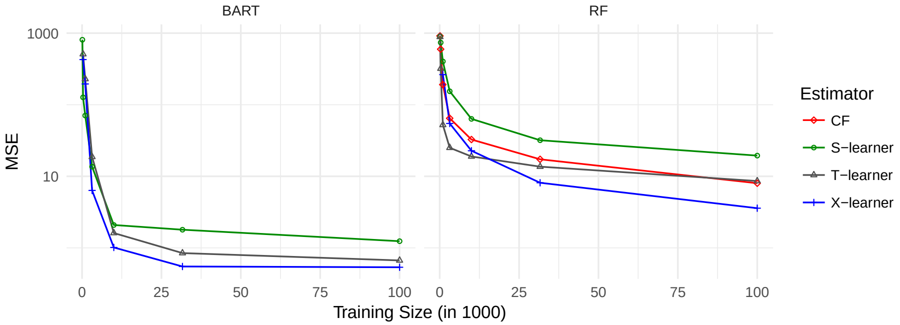


Confounded without TE (WA, 1)

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

More Estimators

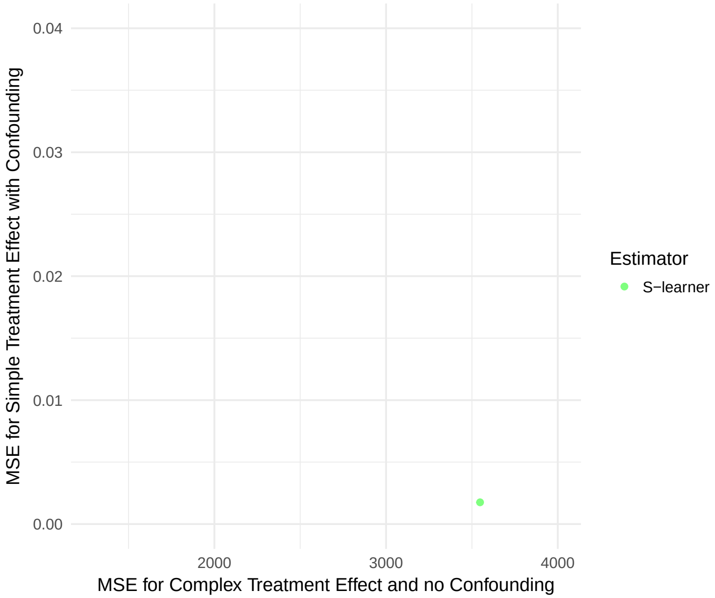
Flexibility of Base Learners is Needed



Complicated Setting

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

Adaptivity



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

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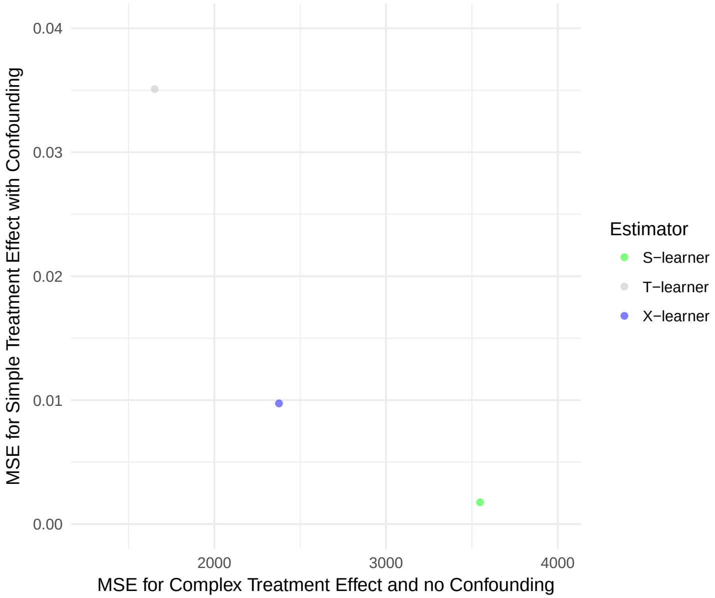
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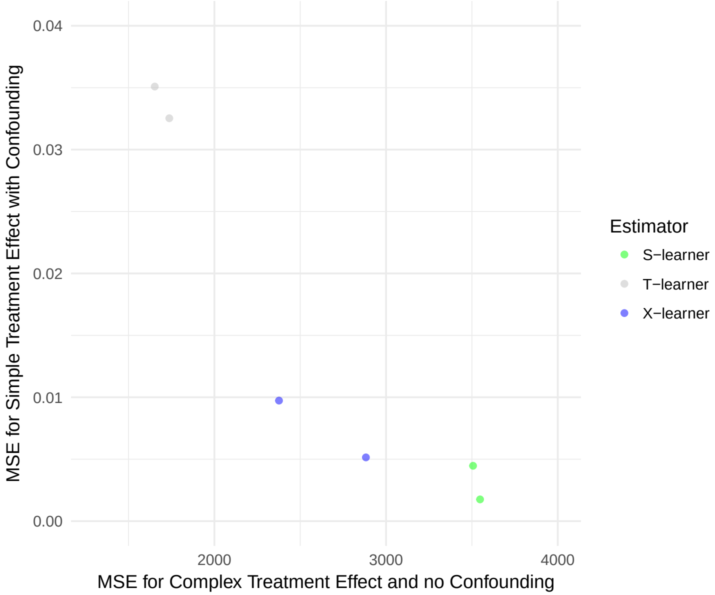
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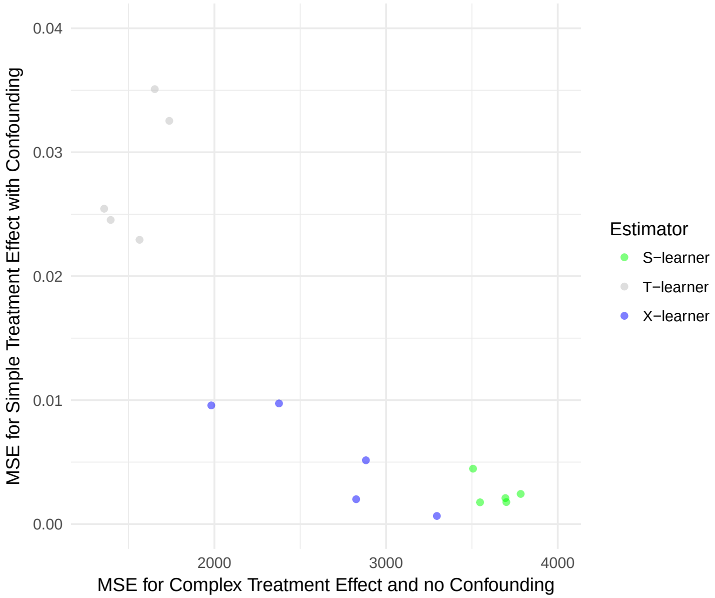

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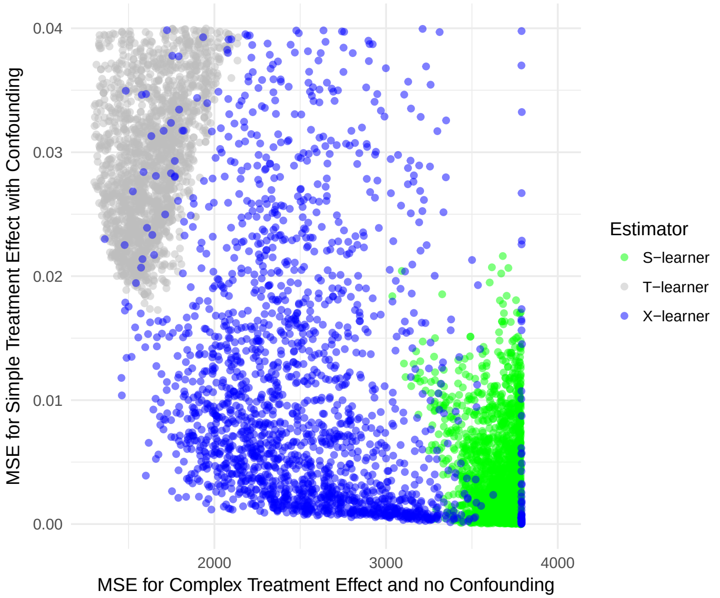

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Tuning

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:

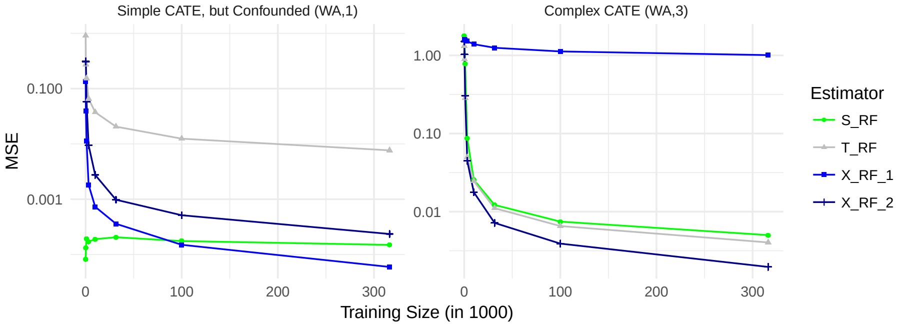
1.) Pre-specified tuning

2.) Gaussian Process

3.) Hyperband

Supplementary

Tuning



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

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

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

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

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:

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

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With one data point?

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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)
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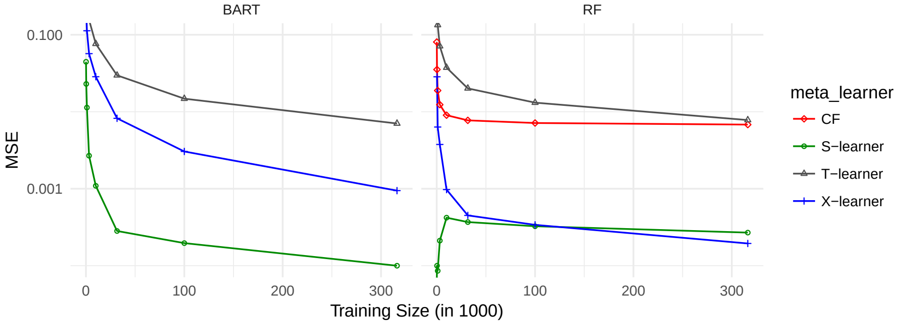
Resisting Confounding: different base learners, same effect



Confounded without TE (WA, 1)

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

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Reducing Transphobia: Simulation

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