Causal forests

A tutorial in high-dimensional causal inference

Ian Lundberg

General Exam
Frontiers of Causal Inference
12 October 2017



PC: Michael Schweppe via Wikimedia Commons CC BY-SA 2.0

Introductory note for those finding these slides online

These slides were prepared for the Sociology Statistics Reading Group at Princeton. Everyone read the following paper in advance:

Athey, Susan, and Guido Imbens. 2016. Recursive partitioning for heterogeneous causal effects. *Proceedings of the National Academy of Sciences*, 113(27):7353–7360. [link]

The aim was to discuss this paper so that together the group would leave with a good understanding of its contribution. Along the way, these slides touch on other related literature that uses tree-based methods for causal inference. In addition, these slides counted as one of several requirements for a general exam I completed in causal inference.

Disclaimer that I invented nothing in these slides, and there are likely places where I misread the original papers.



BART

Note: These slides assume randomized treatment assignment until the section labeled "confounding."

Potential employment

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	1	1
2	High school	1	0	1	1
3	College	0	1	1	0
4	College	1	1	1	0

Potential employment No job training Education Treated Job training Treatment effect W_i $Y_i(0)$ $Y_i(1)$ $\tau_i = Y_i(1) - Y_i(0)$ ID X_i 1 High school 0 High school College 0 4 College

$$ar{ au} = ar{Y}_{i:W_i=1}(1) - ar{Y}_{i:W_i=0}(0)$$

$$= 1 - 0.5$$

$$= 0.5$$

Potential employment

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	1	?	1	?
3	College	0	1	?	?
4	College	1	?	1	?

Potential employment

Causal inference: A missing data problem

			- Otential en		
	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	1	?	1	?
3	College	0	1	?	?
4	College	1	?	1	?

If
$$W_i \perp \{Y_i(0), Y_i(1)\}$$
, then

$$\hat{\bar{\tau}} = \bar{Y}_{i:W_i=1} - \bar{Y}_{i:W_i=0} = 1 - 0.5 = 0.5$$

Intro

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	1	?	1	?
3	College	0	1	?	?
4	College	1	?	1	?

Potential employment

What if we want to study $\tau_i = f(X_i)$?

$$\begin{split} \hat{\bar{\tau}}_{\mathsf{High school}} &= \bar{Y}_{i:W_i=1,X_i=\mathsf{High school}} \\ &- \bar{Y}_{i:W_i=0,X_i=\mathsf{High school}} \\ &= 1-0.5 \\ &= 0.5 \end{split} \qquad \qquad \begin{split} \hat{\bar{\tau}}_{\mathsf{College}} &= \bar{Y}_{i:W_i=1,X_i=\mathsf{College}} \\ &- \bar{Y}_{i:W_i=0,X_i=\mathsf{College}} \\ &= 1-1 \\ &= 0.5 \end{split}$$

4

College

No job training Education Treated Job training Treatment effect W_i $Y_i(0)$ $Y_i(1)$ $\tau_i = Y_i(1) - Y_i(0)$ ID X_i 1 High school 0 High school College

Potential employment

What if there are dozens of X variables?

	Education	Treated	No job training	Job training	Treatment effect	
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$	
1	High school	0	0	?	?	
2	High school	1	?	1	?	
3	College	0	1	?	?	
4	College	1	?	1	?	

Potential employment

What if there are dozens of *X* variables? What if *X* is continuous?

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	1	?	1	?
3	College	0	1	?	?
4	College	1	?	1	?

Potential employment

What if there are dozens of *X* variables? What if *X* is continuous?

It's hard to know which subgroups of X might show interesting effect heterogeneity

Sample split

Which subgroups of *X* have very different average outcomes?

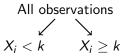
Prediction: One tree

$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2$$

All observations

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2$$



$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2$$

$$MSE_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i|\Pi_1)})^2$$

All observations
$$X_i < k$$
 $X_i \ge k$

BART

Choose *k* to minimize MSE₁

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2$$

All observations
$$X_i < 16$$
 $X_i \ge 16$

$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \quad X_i < k_1 \quad X_i \geq k_1 \qquad X_i < k_2 \quad X_i \geq k_2$$

Prediction: One tree

$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \quad X_i < k_1 \quad X_i \geq k_1 \qquad X_i < k_2 \quad X_i \geq k_2$$

Choose k_1 or k_2 to minimize MSE_2

BART

$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \quad X_i < 12 \quad X_i \geq 12$$

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \quad X_i < 12 \quad X_i \geq 12$$

$$\mathsf{MSE}_3 \qquad \qquad Z_i = \mathsf{White} \quad Z_i \neq \mathsf{White}$$

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \qquad X_i < 12 \qquad X_i \geq 12$$

$$\mathsf{MSE}_3 \qquad \qquad Z_i = \mathsf{White} \qquad Z_i \neq \mathsf{White}$$

$$\mathsf{MSE}_3 \qquad \qquad \mathsf{MSE}_3 \qquad \qquad \mathsf{MSE}_3 \qquad \mathsf{MSE}_3 \qquad \mathsf{MSE}_4 = \mathsf{MSE}_4 \qquad \mathsf{MSE}_5 = \mathsf{M$$

Prediction: One tree

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All \ observations}$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \qquad X_i < 12 \qquad X_i \geq 12$$

$$\qquad \qquad \mathsf{MSE}_3 \qquad \qquad Z_i = \mathsf{White} \qquad Z_i \neq \mathsf{White}$$

$$\qquad \qquad \mathsf{MSE}_3 \qquad \qquad \mathsf{MSE}_3 \qquad \qquad \mathsf{MSE}_3 \qquad \qquad \mathsf{MSE}_4 = \mathsf{White} \qquad \mathsf{MSE}_4 = \mathsf{White} \qquad \mathsf{MSE}_5 = \mathsf{White} \qquad \mathsf{MSE}_6 = \mathsf{White} \qquad \mathsf{MSE}_6 = \mathsf{MSE}_6 = \mathsf{MSE}_6 = \mathsf{White} \qquad \mathsf{MSE}_6 = \mathsf{$$

Could continue until all leaves had only one observation.

Unbiased but uselessly high variance!

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All \ observations}$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{MSE}_2 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 \quad X_i < 12 \quad X_i \geq 12$$

$$\qquad \qquad \mathsf{MSE}_3 \qquad \qquad Z_i = \mathsf{White} \quad Z_i \neq \mathsf{White}$$

Could continue until all leaves had only one observation.

Unbiased but uselessly high variance!

$$\begin{split} \mathsf{MSE}_0 &= \tfrac{1}{n} \sum (Y_i - \bar{Y})^2 & \mathsf{All observations} \\ \mathsf{MSE}_1 &= \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 & X_i < 16 & X_i \geq 16 \\ \mathsf{MSE}_2 &= \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_2)})^2 & X_i < 12 & X_i \geq 12 \end{split}$$

Could continue until all leaves had only one observation.

Unbiased but uselessly high variance!

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2$$

All observations
$$X_i < 16$$
 $X_i \ge 16$

Could continue until all leaves had only one observation.

Unbiased but uselessly high variance!

$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2$$

All observations
$$X_i < 16$$
 $X_i > 16$

Partition
$$\Pi \in \mathbb{P} \longrightarrow \left\{ \ell_1 = \{x_i : x_i < 16\}, \ \ell_2 = \{x_i : x_i \ge 16\} \right\}$$



$$\mathsf{MSE}_0 = \frac{1}{2} \sum (Y_i - \bar{Y})^2$$

$$\mathsf{MSE}_1 = \frac{1}{n} \sum_{i} (Y_i - \bar{Y}_{i:x_i \in \ell(x_i \mid \Pi_1)})^2$$

All observations
$$X_i < 16$$
 $X_i \ge 16$

Partition
$$\Pi \in \mathbb{P} \longrightarrow \left\{ \ell_1 = \{x_i : x_i < 16\}, \ \ell_2 = \{x_i : x_i \ge 16\} \right\}$$



Prediction rule for new x:

$$\hat{\mu}(x) = \bar{Y}_{j:x_j \in \ell(x_i|\Pi)}$$

Prediction: One tree

$$\mathsf{MSE}_0 = \tfrac{1}{n} \sum (Y_i - \bar{Y})^2 \qquad \qquad \mathsf{All observations}$$

$$\mathsf{MSE}_1 = \tfrac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i \mid \Pi_1)})^2 \qquad \qquad X_i < 16 \qquad X_i \geq 16$$

$$\mathsf{Partition} \ \Pi \in \mathbb{P} \longrightarrow \left\{ \ell_1 = \{x_i : x_i < 16\}, \ \ell_2 = \{x_i : x_i \geq 16\} \right\}$$

$$\mathsf{Leaves}$$

$$\mathsf{Prediction rule for new } x_i$$

Could we use this method to find causal effects $\hat{\tau}(x)$ that are heterogeneous between leaves?

 $\hat{\mu}(x) = \bar{Y}_{j:x_i \in \ell(x_i|\Pi)}$

We do not observe the ground truth

- We do not observe the ground truth
- ② Honest estimation:
 - One sample to choose partition
 - One sample to estimate leaf effects

- We do not observe the ground truth
- ② Honest estimation:
 - One sample to choose partition
 - One sample to estimate leaf effects

Why is the split critical?

Fitting both on the training sample risks overfitting: Estimating many "heterogeneous effects" that are really just noise idiosyncratic to the sample.

- We do not observe the ground truth
- ② Honest estimation:
 - One sample to choose partition
 - One sample to estimate leaf effects

Why is the split critical?

Fitting both on the training sample risks overfitting: Estimating many "heterogeneous effects" that are really just noise idiosyncratic to the sample.

We want to search for true heterogeneity, not noise.

BART

Sample splitting

$$\mathsf{MSE}_{\mu}(S^{\mathsf{te}}, S^{\mathsf{est}}, \Pi) \equiv \frac{1}{\#(S^{\mathsf{te}})} \sum_{i \in S^{\mathsf{te}}} \left\{ \overbrace{(Y_i - \hat{\mu}(X_i; S^{\mathsf{est}}, \Pi))^2}^{\mathsf{MSE} \; \mathsf{criterion}} - \overbrace{Y_i^2}^{\mathsf{Authors} \; \mathsf{add}} \right\}$$

$$\mathsf{MSE}_{\mu}(S^{\mathsf{te}}, S^{\mathsf{est}}, \Pi) \equiv rac{1}{\#(S^{\mathsf{te}})} \sum_{i \in S^{\mathsf{te}}} \left\{ \overbrace{(Y_i - \hat{\mu}(X_i; S^{\mathsf{est}}, \Pi))^2}^{\mathsf{MSE} \; \mathsf{criterion}} - \overbrace{Y_i^2}^{\mathsf{Authors} \; \mathsf{add}}
ight\}$$

$$\mathsf{EMSE}_{\mu}(\Pi) \equiv \mathbb{E}_{\mathcal{S}^\mathsf{te}, \mathcal{S}^\mathsf{est}} igg[\mathsf{MSE}_{\mu}(\mathcal{S}^\mathsf{te}, \mathcal{S}^\mathsf{est}, \Pi) igg]$$

Note: The authors include the final Y_i^2 term to simplify the math; it just shifts the estimator by a constant.

$$\mathsf{MSE}_{\mu}(S^{\mathsf{te}}, S^{\mathsf{est}}, \Pi) \equiv \frac{1}{\#(S^{\mathsf{te}})} \sum_{i \in S^{\mathsf{te}}} \left\{ \overbrace{(Y_i - \hat{\mu}(X_i; S^{\mathsf{est}}, \Pi))^2}^{\mathsf{MSE} \; \mathsf{criterion}} - \overbrace{Y_i^2}^{\mathsf{Authors} \; \mathsf{add}} \right\}$$

$$\mathsf{EMSE}_{\mu}(\mathsf{\Pi}) \equiv \mathbb{E}_{S^\mathsf{te},S^\mathsf{est}}igg[\mathsf{MSE}_{\mu}(S^\mathsf{te},S^\mathsf{est},\mathsf{\Pi})igg]$$

Honest criterion: Maximize

This is
$$S^{\mathsf{tr}}$$
 in the classical approach $Q^H(\pi) \equiv -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}},S^{\mathsf{tr}}} \bigg[\mathsf{MSE}_{\mu}(S^{\mathsf{te}},\overset{\bullet}{S^{\mathsf{est}}},\pi(S^{\mathsf{tr}})) \bigg]$

where $\pi: \mathbb{R}^{p+1} \to \mathbb{P}$ is a function that takes a training sample $S^{\text{tr}} \in \mathbb{R}^{p+1}$ and outputs a partition $\Pi \in \mathbb{P}$.

Note: The authors include the final Y_i^2 term to simplify the math; it just shifts the estimator by a constant.

Analytic estimator for EMSE_{μ}(Π) (p. 7356)

Goal: Estimate expected MSE using only the training sample.

This will be used to place splits when training a tree.

$$\begin{split} -\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \left[\left(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) \right)^2 - Y_i^2 \right] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \left[\left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 \right] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \left[2 \left(Y_i - \mu(X_i \mid \Pi) \right) \left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right) \right] \end{split}$$

Expected mean squared error for a partition Π

$$\begin{split} -\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 \bigg] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[2 \bigg(Y_i - \mu(X_i \mid \Pi) \bigg) \bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg) \Bigg] \end{split}$$

Expected mean squared error for a partition Π

$$-\mathsf{EMSE}_{\mu}(\Pi) = -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \left[\left(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right]$$

Over estimation sets used to estimate the leaf-specific $\hat{\mu}$ and test sets to evaluate those

$$\begin{split} &= - \mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right)^2 - Y_i^2 \right] \\ &= - \mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) \right)^2 - Y_i^2 \right] \\ &- \mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right)^2 \right] \\ &- \mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[2 \left(Y_i - \mu(X_i \mid \Pi) \right) \left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right) \right] \end{split}$$

4□ > 4□ > 4 = > 4 = > = 9 < 0</p>

Expected mean squared error for a partition Π Prediction based on S^{est} from the leave $\ell(X_i)$ containing X_i

$$-\mathsf{EMSE}_{\mu}(\Pi) = -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \left[\left(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right]$$

Over estimation sets used to estimate the leaf-specific $\hat{\mu}$ and test sets to evaluate those

$$\begin{split} &= - \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right)^2 - Y_i^2 \right] \\ &= - \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) \right)^2 - Y_i^2 \right] \\ &- \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[\left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right)^2 \right] \\ &- \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[2 \left(Y_i - \mu(X_i \mid \Pi) \right) \left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right) \right] \end{split}$$

$$\begin{split} -\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 - Y_i^2 \bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 - Y_i^2 \bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) \bigg)^2 - Y_i^2 \bigg] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg)^2 \bigg] \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[2 \bigg(Y_i - \mu(X_i \mid \Pi) \bigg) \bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}},\Pi) \bigg) \bigg] \end{split}$$

$$\begin{split} -\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[\bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg)^2 \Bigg] \\ &= 2 \Big(\mathsf{First term} \Big) \Big(\mathsf{Second term} \Big) \\ &- \mathbb{E}_{S^{\mathsf{te}},S^{\mathsf{est}}} \Bigg[2 \Big(Y_i - \mu(X_i \mid \Pi) \Big) \bigg(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg) \Bigg] \end{split}$$

E(A) = 0 by assumption

$$\begin{aligned}
-\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \left[\left(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right] \\
&= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - Y_i^2 \right] \\
&= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \left[\left(Y_i - \mu(X_i \mid \Pi) \right)^2 - Y_i^2 \right] \end{aligned}$$

$$-\mathbb{E}_{S^{\text{te}},S^{\text{est}}}\left[\begin{pmatrix}\mu(X_i\mid\Pi)-\hat{\mu}(X_i\mid S^{\text{est}},\Pi)\end{pmatrix}^2\right]$$

$$Cov(A,B)=0 \text{ because } Y_i \text{ is from a sample independent of } S^{\text{est}}$$

$$Cov(AB)=E(AB)-E(A)E(B) -\mathbb{E}_{S^{\text{te}},S^{\text{est}}}\left[2\begin{pmatrix}Y_i-\mu(X_i\mid\Pi)\end{pmatrix}\begin{pmatrix}\mu(X_i\mid\Pi)-\hat{\mu}(X_i\mid S^{\text{est}},\Pi)\end{pmatrix}\right]$$

$$0=E(AB)-0$$

$$\begin{split} -\mathsf{EMSE}_{\mu}(\Pi) &= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) + \mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi) \bigg)^2 - Y_i^2 \Bigg] \\ &= -\mathbb{E}_{S^{\mathsf{te}}, S^{\mathsf{est}}} \Bigg[\bigg(Y_i - \mu(X_i \mid \Pi) \bigg)^2 - Y_i^2 \Bigg] \end{split}$$

$$E(A) = 0 \text{ by assumption} - \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[\left(\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \right)^2 \right]$$

$$Cov(A, B) = 0 \text{ because } Y_i \text{ is from a sample independent of } S^{\text{est}}$$

$$Cov(AB) = E(AB) - E(A)E(B) - \mathbb{E}_{S^{\text{te}},S^{\text{est}}} \left[2 \left(\frac{X_i \mid \Pi}{\mu(X_i \mid \Pi)} \right) \left(\frac{\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi)}{\mu(X_i \mid \Pi) - \hat{\mu}(X_i \mid S^{\text{est}}, \Pi)} \right) \right]$$

Sample split

BART

$$\begin{split} &= -\mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \Big[(Y_i - \mu(X_i \mid \Pi))^2 - Y_i^2 \Big] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \Big[(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi) - \mu(X_i \mid \Pi))^2 \Big] \\ \\ &= -\mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \Big[Y_i^2 + \mu^2(X_i \mid \Pi) - 2Y_i\mu(X_i \mid \Pi) - Y_i^2 \Big] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \Big[(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi) - \mu(X_i \mid \Pi))^2 \Big] \\ \\ &= - \mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \Big[\mu^2(X_i \mid \Pi) - 2\mu(X_i \mid \Pi)\mu(X_i \mid \Pi) \Big] \end{split}$$

 $-\mathbb{E}_{X_i,S^{\mathsf{est}}}\bigg[(\hat{\mu}(X_i\mid S^{\mathsf{est}},\Pi)-\mu(X_i\mid \Pi))^2\bigg]$

 $= \mathbb{E}_{X_i} \left[\mu^2(X_i \mid \Pi) \right] - \mathbb{E}_{S^{\text{est}}, X_i} \left[\mathbb{V}(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi)) \right]$

Athey & Imbens 2016, p. 7356

$$\begin{split} &= -\mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \left[(Y_{i} - \mu(X_{i} \mid \Pi))^{2} - Y_{i}^{2} \right] \\ &- \mathbb{E}_{X_{i},S^{\text{est}}} \left[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \right] \\ &- \mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \left[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - 2Y_{i}\mu(X_{i} \mid \Pi) - Y_{i}^{2} \right] \\ &- \mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \left[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \right] \\ &= - \mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \left[\mu^{2}(X_{i} \mid \Pi) - 2\mu(X_{i} \mid \Pi)\mu(X_{i} \mid \Pi) \right] \\ &- \mathbb{E}_{X_{i},S^{\text{est}}} \left[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \right] \\ &= \mathbb{E}_{X_{i}} \left[\mu^{2}(X_{i} \mid \Pi) \right] - \mathbb{E}_{S^{\text{est}},X_{i}} \left[\mathbb{V}(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi)) \right] \end{split}$$

Sample split

$$\begin{split} &= -\mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \Big[(Y_{i} - \mu(X_{i} \mid \Pi))^{2} - Y_{i}^{2} \Big] \\ &- \mathbb{E}_{X_{i},S^{\text{est}}} \Big[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \Big] \qquad \mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} (Y_{i}) \\ &= -\mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \Big[Y_{i}^{2} + \mu^{2}(X_{i} \mid \Pi) - 2Y_{i}\mu(X_{i} \mid \Pi) - Y_{i}^{2} \Big] \\ &- \mathbb{E}_{X_{i},S^{\text{est}}} \Big[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \Big] \\ &= -\mathbb{E}_{(Y_{i},X_{i}),S^{\text{est}}} \Big[\mu^{2}(X_{i} \mid \Pi) - 2\mu(X_{i} \mid \Pi)\mu(X_{i} \mid \Pi) \Big] \\ &- \mathbb{E}_{X_{i},S^{\text{est}}} \Big[(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) - \mu(X_{i} \mid \Pi))^{2} \Big] \\ &= \mathbb{E}_{X_{i}} \Big[\mu^{2}(X_{i} \mid \Pi) \Big] - \mathbb{E}_{S^{\text{est}},X_{i}} \Big[\mathbb{V}(\hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi)) \Big] \end{split}$$

$$\begin{split} &= -\mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \bigg[(Y_i - \mu(X_i \mid \Pi))^2 - Y_i^2 \bigg] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \bigg[(\hat{\mu}(X_i \mid S^{\text{est}},\Pi) - \mu(X_i \mid \Pi))^2 \bigg] \\ &= -\mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \bigg[Y_i^2 + \mu^2(X_i \mid \Pi) - 2Y_i\mu(X_i \mid \Pi) - Y_i^2 \bigg] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \bigg[(\hat{\mu}(X_i \mid S^{\text{est}},\Pi) - \mu(X_i \mid \Pi))^2 \bigg] \\ &= - \mathbb{E}_{(Y_i,X_i),S^{\text{est}}} \bigg[\mu^2(X_i \mid \Pi) - 2\mu(X_i \mid \Pi)\mu(X_i \mid \Pi) \bigg] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \bigg[(\hat{\mu}(X_i \mid S^{\text{est}},\Pi) - \mu(X_i \mid \Pi))^2 \bigg] \\ &- \mathbb{E}_{X_i,S^{\text{est}}} \bigg[(\hat{\mu}(X_i \mid S^{\text{est}},\Pi) - \mu(X_i \mid \Pi))^2 \bigg] \\ &- \mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg] \bigg] \bigg] \bigg] \bigg] \\ &= \mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg] \bigg] \bigg] \bigg] \bigg] \\ &- \mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg[\mathbb{E}_{X_i} \bigg] \bigg] \bigg] \bigg] \bigg] \bigg] \bigg] \bigg] \\ &= \mathbb{E}_{X_i} \bigg[\mathbb{E}$$

Regularization + confounding

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{\mathsf{S}^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid \mathsf{S}^{\mathsf{est}}, \Pi)) \bigg]$$

Regularization + confounding

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

Estimate with
$$\hat{\mathbb{V}}\left(\hat{\mu}(x\mid S^{\text{est}},\Pi)\right) \equiv \frac{S_{\text{Str}}^2(\ell(x|\Pi))}{N^{\text{est}}(\ell(x|\Pi))}$$

$$\hat{\mathbb{E}}_{X_i} \bigg[\hat{\mathbb{V}}_{S^{\text{est}}} \bigg(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \bigg) \mid i \in S^{\text{te}} \bigg] = \sum_{\ell} p_{\ell} \frac{S_{S^{\text{tr}}}^2(\ell)}{N^{\text{est}}(\ell)}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

Estimate with
$$\hat{\mathbb{V}}\left(\hat{\mu}(x\mid S^{\text{est}},\Pi)\right) \equiv \frac{S_{\text{Str}}^2(\ell(x|\Pi))}{N^{\text{est}}(\ell(x|\Pi))}$$

$$\begin{split} \hat{\mathbb{E}}_{X_i} \bigg[\hat{\mathbb{V}}_{S^{\text{est}}} \bigg(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \bigg) \mid i \in S^{\text{te}} \bigg] &= \sum_{\ell} p_{\ell} \frac{S_{\mathsf{S}^{\text{tr}}}^2(\ell)}{\mathsf{N}^{\text{est}}(\ell)} \\ & \text{(assuming } \approx \text{ equal leaf sizes)} \approx \sum_{\ell} \frac{1}{\#\ell} \frac{S_{\mathsf{S}^{\text{tr}}}^2(\ell)}{\mathsf{N}^{\text{est}}/\#\ell} \end{split}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

$$\begin{split} \hat{\mathbb{E}}_{X_i} \Big[\hat{\mathbb{V}}_{S^{\text{est}}} \Big(\hat{\mu}(X_i \mid S^{\text{est}}, \Pi) \Big) \mid i \in S^{\text{te}} \Big] &= \sum_{\ell} p_\ell \frac{S_{S^{\text{tr}}}^2(\ell)}{N^{\text{est}}(\ell)} \\ &\text{(assuming } \approx \text{ equal leaf sizes) } \approx \sum_{\ell} \frac{1}{\#\ell} \frac{S_{S^{\text{tr}}}^2(\ell)}{N^{\text{est}}/\#\ell} \\ &= \frac{1}{N^{\text{est}}} \sum_{\ell \in \mathcal{P}} S_{S^{\text{tr}}}^2(\ell) \end{split}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

Regularization + confounding

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

$$\mathbb{V}(\hat{\mu}\mid x,\Pi) = \mathbb{E}(\hat{\mu}^2\mid x,\Pi) - \left[\mathbb{E}(\hat{\mu}\mid x,\Pi)
ight]^2$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \left[\mu^2(X_i \mid \Pi) \right] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \left[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \right]$$

Sample split

$$\begin{split} \mathbb{V}(\hat{\mu} \mid x, \Pi) &= \mathbb{E}(\hat{\mu}^2 \mid x, \Pi) - \left[\mathbb{E}(\hat{\mu} \mid x, \Pi) \right]^2 \\ \frac{S_{\mathcal{S}^{\text{tr}}}^2(\ell(x \mid \Pi))}{N^{\text{tr}}(\ell(x \mid \Pi))} &\approx \hat{\mu}^2(x \mid S^{\text{tr}}\Pi) - \mu^2(x \mid \Pi) \\ \mu^2(x \mid \Pi) &\approx \hat{\mu}^2(x \mid S^{\text{tr}}, \Pi) - \frac{S_{\mathcal{S}^{\text{tr}}}^2(\ell(x \mid \Pi))}{N^{\text{tr}}(\ell(x \mid \Pi))} \end{split}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

$$\begin{split} \mathbb{V}(\hat{\mu} \mid x, \Pi) &= \mathbb{E}(\hat{\mu}^2 \mid x, \Pi) - \left[\mathbb{E}(\hat{\mu} \mid x, \Pi)\right]^2 \\ \frac{S_{\mathcal{S}^{\text{tr}}}^2(\ell(x \mid \Pi))}{N^{\text{tr}}(\ell(x \mid \Pi))} &\approx \hat{\mu}^2(x \mid S^{\text{tr}}\Pi) - \mu^2(x \mid \Pi) \\ \mu^2(x \mid \Pi) &\approx \hat{\mu}^2(x \mid S^{\text{tr}}, \Pi) - \frac{S_{\mathcal{S}^{\text{tr}}}^2(\ell(x \mid \Pi))}{N^{\text{tr}}(\ell(x \mid \Pi))} \\ \hat{\mathbb{E}}_{X_i}(\mu^2(X_i \mid \Pi)) &\approx \frac{1}{N^{\text{tr}}} \sum_{i \in S^{\text{tr}}} \hat{\mu}^2(x_i \mid S^{\text{tr}}, \Pi) - \sum_{\ell} \frac{1}{\#\ell} \frac{S_{\mathcal{S}^{\text{tr}}}^2(\ell)}{N^{\text{tr}}/\#\ell} \\ &= \frac{1}{N^{\text{tr}}} \sum_{i \in S} \hat{\mu}^2(x_i \mid S^{\text{tr}}, \Pi) - \frac{1}{N^{\text{tr}}} \sum_{i \in S^{\text{tr}}} S_{\mathcal{S}^{\text{tr}}}^2(\ell) \end{split}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \left[\mu^2(X_i \mid \Pi) \right] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \left[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \right]$$

Intro

Regularization + confounding

$$\begin{split} -\widehat{\mathsf{EMSE}}_{\mu}(\mathcal{S}^{\mathsf{tr}}, \mathcal{N}^{\mathsf{est}}, \Pi) &= \frac{1}{\mathit{N}^{\mathsf{tr}}} \sum_{i \in \mathcal{S}^{\mathsf{tr}}} \hat{\mu}^2(X_i \mid \mathcal{S}^{\mathsf{tr}}, \Pi) - \frac{1}{\mathit{N}^{\mathsf{tr}}} \sum_{\ell \in \Pi} \mathcal{S}^2_{\mathcal{S}^{\mathsf{tr}}}(\ell) \\ &- \frac{1}{\mathit{N}^{\mathsf{est}}} \sum_{\ell \in \Pi} \mathcal{S}^2_{\mathcal{S}^{\mathsf{tr}}}(\ell) \end{split}$$

$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

Intro

$$\begin{split} -\widehat{\mathsf{EMSE}}_{\mu}(S^{\mathsf{tr}}, \mathcal{N}^{\mathsf{est}}, \Pi) &= \frac{1}{\mathcal{N}^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\mu}^2(X_i \mid S^{\mathsf{tr}}, \Pi) - \frac{1}{\mathcal{N}^{\mathsf{tr}}} \sum_{\ell \in \Pi} S^2_{S^{\mathsf{tr}}}(\ell) \\ &- \frac{1}{\mathcal{N}^{\mathsf{est}}} \sum_{\ell \in \Pi} S^2_{S^{\mathsf{tr}}}(\ell) \\ &= \underbrace{\frac{1}{\mathcal{N}^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\mu}^2(X_i \mid S^{\mathsf{tr}}, \Pi) - \underbrace{\left(\frac{1}{\mathcal{N}^{\mathsf{tr}}} + \frac{1}{\mathcal{N}^{\mathsf{est}}}\right) \sum_{\ell \in \Pi} S^2_{S^{\mathsf{tr}}}(\ell)}_{\mathsf{Uncertainty about leaf means}} \end{split}$$

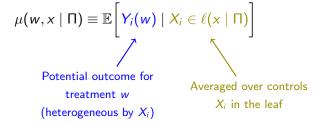
$$-\mathsf{EMSE}_{\mu}(\Pi) = \mathbb{E}_{X_i} \bigg[\mu^2(X_i \mid \Pi) \bigg] - \mathbb{E}_{S^{\mathsf{est}}, X_i} \bigg[\mathbb{V}(\hat{\mu}(X_i \mid S^{\mathsf{est}}, \Pi)) \bigg]$$

Note: We still assume randomized treatment assignment

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E}\Big[Y_i(w) \mid X_i \in \ell(x \mid \Pi)\Big]$$

Population-average potential outcomes within leaves:



Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E} \left[Y_i(w) \mid X_i \in \ell(x \mid \Pi) \right]$$

Average causal effect:

$$\tau(x\mid \Pi) \equiv \mathbb{E}\bigg[Y_i(1) - Y_i(0)\mid X_i \in \ell(x\mid \Pi)\bigg] = \mu(1,x\mid \Pi) - \mu(0,x\mid \Pi)$$

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E} \left[Y_i(w) \mid X_i \in \ell(x \mid \Pi) \right]$$

Average causal effect:

$$\tau(x \mid \Pi) \equiv \mathbb{E}\left[Y_i(1) - Y_i(0) \mid X_i \in \ell(x \mid \Pi)\right] = \mu(1, x \mid \Pi) - \mu(0, x \mid \Pi)$$

Average effect evaluated at (potentially moderating) covariate value *x*

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E}\left[Y_i(w) \mid X_i \in \ell(x \mid \Pi)\right]$$

Average causal effect:

$$\tau(x\mid\Pi)\equiv\mathbb{E}\bigg[Y_i(1)-Y_i(0)\mid X_i\in\ell(x\mid\Pi)\bigg]=\mu(1,x\mid\Pi)-\mu(0,x\mid\Pi)$$

Difference in potential outcomes

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E} \left[Y_i(w) \mid X_i \in \ell(x \mid \Pi) \right]$$

Average causal effect:

$$\tau(x \mid \Pi) \equiv \mathbb{E}\bigg[Y_i(1) - Y_i(0) \mid X_i \in \ell(x \mid \Pi)\bigg] = \mu(1, x \mid \Pi) - \mu(0, x \mid \Pi)$$

Among observations in the leaf ℓ

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E}\left[Y_i(w) \mid X_i \in \ell(x \mid \Pi)\right]$$

Average causal effect:

$$\tau(x \mid \Pi) \equiv \mathbb{E}\Big[Y_i(1) - Y_i(0) \mid X_i \in \ell(x \mid \Pi)\Big] = \mu(1, x \mid \Pi) - \mu(0, x \mid \Pi)$$

Compact notation

$$\hat{\mu}(w, x \mid S, \Pi) \equiv \frac{1}{\#(\{i \in S_w : X_i \in \ell(x \mid \Pi)\}\}} \sum_{i \in S_w : X_i \in \ell(x \mid \Pi)} Y_i^{\text{obs}}$$

$$\hat{\mu}(w, x \mid S, \Pi) \equiv \frac{1}{\#(\{i \in S_w : X_i \in \ell(x \mid \Pi)\}\}} \sum_{i \in S_w : X_i \in \ell(x \mid \Pi)} Y_i^{\text{obs}}$$

MSE for treatment effects:

$$\mathsf{MSE}_{ au}(S^\mathsf{te}, S^\mathsf{est}, \Pi) \equiv \frac{1}{\#(S^\mathsf{te})} \sum_{i \in S^\mathsf{te}} \left\{ \left(au_i - \hat{ au}(X_i \mid S^\mathsf{est}, \Pi) \right)^2 - au_i^2 \right\}$$

Intro

$$\hat{\mu}(w, x \mid S, \Pi) \equiv \frac{1}{\#(\{i \in S_w : X_i \in \ell(x \mid \Pi)\})} \sum_{i \in S_w : X_i \in \ell(x \mid \Pi)} Y_i^{\text{obs}}$$

MSE for treatment effects:

$$\mathsf{MSE}_{\tau}(S^{\mathsf{te}}, S^{\mathsf{est}}, \Pi) \equiv \frac{1}{\#(S^{\mathsf{te}})} \sum_{i \in S^{\mathsf{te}}} \left\{ \left(\tau_i - \hat{\tau}(X_i \mid S^{\mathsf{est}}, \Pi) \right)^2 - \tau_i^2 \right\}$$

Challenge! τ_i is *never* observed.

Adapt EMSE_{μ} to estimate EMSE_{τ}

$$-\widehat{\mathsf{EMSE}}_{\mu}(S^{\mathsf{tr}}, N^{\mathsf{est}}, \Pi) = \underbrace{\frac{1}{N^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\mu}^2(X_i \mid S^{\mathsf{tr}}, \Pi) - \underbrace{\left(\frac{1}{N^{\mathsf{tr}}} + \frac{1}{N^{\mathsf{est}}}\right) \sum_{\ell \in \Pi} S^2_{S^{\mathsf{tr}}}(\ell)}_{\mathsf{Uncertainty about leaf means}}$$

Conventional CART criterion Uncertainty about leaf means

$$\begin{split} -\widehat{\mathsf{EMSE}}_\tau(S^{\mathsf{tr}}, N^{\mathsf{est}}, \Pi) &= \underbrace{\frac{1}{N^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\tau}^2(X_i \mid S^{\mathsf{tr}}, \Pi)}_{\substack{\mathsf{Variance of treatment effects across leaves}} \\ &- \underbrace{\left(\frac{1}{N^{\mathsf{tr}}} + \frac{1}{N^{\mathsf{est}}}\right) \sum_{\ell \in \Pi} \left(\frac{S^2_{\mathsf{treat}}(\ell)}{p} + \frac{S^2_{\mathsf{gr}}(\ell)}{1 - p}\right)}_{\substack{\ell \in \Pi}} \end{split}$$

Uncertainty about leaf treatment effects

Adapt EMSE_{μ} to estimate EMSE_{τ}

$$-\widehat{\mathsf{EMSE}}_{\mu}(S^{\mathsf{tr}}, \mathsf{N}^{\mathsf{est}}, \mathsf{\Pi}) = \underbrace{\frac{1}{\mathsf{N}^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\mu}^2(X_i \mid S^{\mathsf{tr}}, \mathsf{\Pi}) - \underbrace{\left(\frac{1}{\mathsf{N}^{\mathsf{tr}}} + \frac{1}{\mathsf{N}^{\mathsf{est}}}\right) \sum_{\ell \in \mathsf{\Pi}} S^2_{\mathsf{Str}}(\ell)}_{\mathsf{Uncertainty about leaf means}}$$

Variance of treatment

$$-\widehat{\mathsf{EMSE}}_\tau(S^{\mathsf{tr}}, \mathsf{N}^{\mathsf{est}}, \Pi) = \frac{1}{\mathsf{N}^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\tau}^2(X_i \mid S^{\mathsf{tr}}, \Pi)$$

Prefers leaves with heterogeneous effects

effects across leaves
$$-\left(\frac{1}{\mathit{N}^{\mathsf{tr}}} + \frac{1}{\mathit{N}^{\mathsf{est}}}\right) \sum_{\ell \in \mathcal{P}} \left(\frac{S_{\mathsf{S}^{\mathsf{tr}}_{\mathsf{treat}}}^2(\ell)}{p} + \frac{S_{\mathsf{S}^{\mathsf{tr}}_{\mathsf{control}}}^2(\ell)}{1-p}\right)$$

Uncertainty about leaf treatment effects

Prefers leaves with good fit (leaf-specific effects estimated precisely)

BART

1. Causal trees

Split by

$$-\widehat{\mathsf{EMSE}}_\tau(S^{\mathsf{tr}}, N^{\mathsf{est}}, \Pi) = \underbrace{\frac{1}{N^{\mathsf{tr}}} \sum_{i \in S^{\mathsf{tr}}} \hat{\tau}^2(X_i \mid S^{\mathsf{tr}}, \Pi)}_{\text{Variance of treatment effects across leaves}}$$

$$-\underbrace{\left(\frac{1}{N^{\mathsf{tr}}} + \frac{1}{N^{\mathsf{est}}}\right) \sum_{\ell \in \Pi} \left(\frac{S^2_{\mathsf{Str}}}{p} + \frac{S^2_{\mathsf{control}}}{1 - p}\right)}_{\mathsf{Uncertainty about leaf treatment effects}}$$

$$-\underbrace{\left(\frac{1}{N^{\mathsf{tr}}} + \frac{1}{N^{\mathsf{est}}}\right) \sum_{\ell \in \Pi} \left(\frac{S^2_{\mathsf{Str}}}{p} + \frac{S^2_{\mathsf{control}}}{1 - p}\right)}_{\mathsf{Uncertainty about leaf treatment effects}}$$

- Benefit: Prioritizes heterogeneity ($\hat{\tau}$ varies a lot) and fit (within-leaf precision)
- Drawback: Cannot be done with off-the-shelf CART methods

BART

2. Transformed outcome trees

Transform the outcome

$$Y_{i}^{*} = Y_{i} \frac{W_{i} - p}{p(1 - p)} \rightarrow \mathbb{E}(Y_{i}^{*} \mid X_{i} = x) = \tau(x)$$

$$\mathbb{E}(Y_{i}^{*}) = \mathbb{E}\left[Y_{i} \frac{W_{i} - p}{p(1 - p)}\right]$$

$$= \mathbb{E}\left[Y_{i} \frac{W_{i}}{p(1 - p)}\right] - \mathbb{E}\left[Y_{i} \frac{p}{p(1 - p)}\right]$$

$$= \mathbb{E}\left[Y_{i}(1) \frac{W_{i}}{p(1 - p)}\right] - \mathbb{E}\left[\left(Y_{i}(1)W_{i} + Y_{i}(0)(1 - W_{i})\right) \frac{p}{p(1 - p)}\right]$$

$$= Y_{i}(1) \frac{1}{p(1 - p)} \mathbb{E}[W_{i}] - Y_{i}(1) \frac{p}{p(1 - p)} \mathbb{E}[W_{i}] - Y_{i}(0) \frac{p}{p(1 - p)} \mathbb{E}[1 - W_{i}]$$

$$= Y_{i}(1) \frac{1 - p}{p(1 - p)} \mathbb{E}[W_{i}] - Y_{i}(0) \frac{p}{p(1 - p)} \mathbb{E}[1 - W_{i}]$$

$$= Y_{i}(1) \frac{p(1 - p)}{p(1 - p)} - Y_{i}(0) \frac{p(1 - p)}{p(1 - p)}$$

$$= Y_{i}(1) - Y_{i}(0) = \tau_{i}$$

2. Transformed outcome trees

- Benefit: Can use off-the-shelf CART methods for prediction
- Drawbacks: Inefficient. Treatment is ignored after transforming outcome. If within a leaf $\bar{W} \neq p$ (by chance), then sample average within leaf is a poor estimator of $\hat{\tau}$.

BART

3. Fit-based trees

Replace

$$\mathsf{MSE}_{\mu}(S^\mathsf{te}, S^\mathsf{est}, \mathsf{\Pi}) \equiv rac{1}{\#(S^\mathsf{te})} \sum_{i \in S^\mathsf{te}} \left\{ (Y_i - \hat{\mu}(X_i; S^\mathsf{est}, \mathsf{\Pi}))^2 - Y_i^2
ight\}$$

with the fit-based split rule

$$\mathsf{MSE}_{\mu,W}(S^\mathsf{te},S^\mathsf{est},\Pi) \equiv \sum_{i \in S^\mathsf{te}} \left\{ (Y_i - \hat{\mu}_w(W_iX_i;S^\mathsf{est},\Pi))^2 - Y_i^2
ight\}$$

which loss by model fit within each leaf: the difference from the expected value for the treatment group of observation *i*.

Benefit: Prefers splits that lead to better fit.

Drawback: Does not prefer splits that lead to variation in treatment effects.

Zeileis et al. 2008



4. Squared T-statistic trees

Split based on:

$$\hat{ au}$$
 in left leaf \int in right leaf $T^2\equiv Nrac{\left(ar{Y}_L-ar{Y}_R
ight)^2}{S^2/N_L+S^2/N_R}$

Benefit: Prefers splits that lead to variation in treatment effects.

Drawback: Missed opportunity to improve fit: ignores useful splits between leaves with similar treatment effects but very different average values.

BART

From trees to forests: Double-sample trees

An individual tree can be noisy. Instead, we might fit a forest.

- ① Draw a sample of size s
- 2 Split into an $\mathcal I$ and $\mathcal J$ sample.
- 4 Estimate leaf-specific $\hat{ au}_\ell$ using the $\mathcal I$ sample

Repeat many times.

Advantages of forests:

- Consistent for true $\tau(x)$
- Asymptotic normality
- Asymptotic variance is estimable

Why double-sample forests:

- Advantage: Trees search for heterogeneous effects
- Disadvantage: Requires sample splitting



From trees to forests: Propensity trees

An individual tree can be noisy. Instead, we might fit a forest.

- ① Draw a sample of size s
- ② Grow a tree on the ${\mathcal J}$ sample to predict W
 - Each leaf must have at least k observations of each treatment class
- 3 Estimate $\hat{ au}_\ell$ on each leaf

Repeat many times.

Advantages of forests:

- Consistent for true $\tau(x)$
- Asymptotic normality
- Asymptotic variance is estimable

Why propensity forests:

- Advantage: Can use full sample
- Disadvantage: Does not search for heterogeneous effects

• There is no ground truth: We never observe τ_i

- ullet There is no ground truth: We never observe au_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects

- ullet There is no ground truth: We never observe au_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects
- Require extra sample splitting

- ullet There is no ground truth: We never observe au_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects
- Require extra sample splitting
- Work well with randomized treatments.

- There is no ground truth: We never observe τ_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects
- Require extra sample splitting
- Work well with randomized treatments.
- With selection on observables, the general recommendation is propensity forests
 - Maximizes the goal of addressing confounding by ignoring heterogeneous effects when choosing splits

- There is no ground truth: We never observe τ_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects
- Require extra sample splitting
- Work well with randomized treatments.
- With selection on observables, the general recommendation is propensity forests
 - Maximizes the goal of addressing confounding by ignoring heterogeneous effects when choosing splits
 - Generalized random forests also perform well (Athey, Tibshirani, & Wager 2017)

- There is no ground truth: We never observe τ_i
- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects
- Require extra sample splitting
- Work well with randomized treatments.
- With selection on observables, the general recommendation is propensity forests
 - Maximizes the goal of addressing confounding by ignoring heterogeneous effects when choosing splits
 - Generalized random forests also perform well (Athey, Tibshirani, & Wager 2017)
 - But "the challenge in using adaptive methods... is that selection bias can be difficult to quantify" (Wager & Athey p. 24).

If treatment is not randomized

Causal trees find heterogeneous effects but cannot guarantee that confounding is addressed.

Next we focus on why high-dimensional confounding is hard

Why aren't causal trees guaranteed to address confounding?

Plan

- What does address confounding? Standardization
- Why is tree-based standardization biased? Regularization
- 3 Is there anything we can do? Chernozhukov et al.

What if $\{Y_i(0), Y_i(1)\} \not\perp W_i$ but $\{Y_i(0), Y_i(1)\} \perp W_i \mid X_i$?

What if $\{Y_i(0), Y_i(1)\} \not\perp W_i$ but $\{Y_i(0), Y_i(1)\} \perp W_i \mid X_i$?

			Potential em			
	Education	Treated	No job training	Job training	Treatment effect	
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$	
1	High school	0	0	1	1	
2	High school	0	0	1	1	
3	High school	1	0	1	1	
4	College	0	1	1	0	
5	College	1	1	1	0	
6	College	1	1	1	0	

What if $\{Y_i(0), Y_i(1)\} \not\perp W_i$ but $\{Y_i(0), Y_i(1)\} \perp W_i \mid X_i$?

			Potential employment			
	Education	Treated	No job training	Job training	Treatment effect	
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$	
1	High school	0	0	?	?	
2	High school	0	0	?	?	
3	High school	1	?	1	?	
4	College	0	1	?	?	
5	College	1	?	1	?	
6	College	1	?	1	?	

What if $\{Y_i(0), Y_i(1)\} \not\perp W_i$ but $\{Y_i(0), Y_i(1)\} \perp W_i \mid X_i$?

We need to estimate $\hat{\tau}$ within each level of X_i .

			Potential employment		
	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	0	0	?	?
3	High school	1	?	1	?
4	College	0	1	?	?
5	College	1	?	1	?
6	College	1	?	1	?

$$\begin{split} \hat{\bar{\tau}} &= \sum_{x \in \text{Support of } X} \mathbb{P}(X = x) \bigg(\bar{Y}_{i:W_i = 1, X_i = x} - \bar{Y}_{i:W_i = 0, X_i = x} \bigg) \\ &= \mathbb{P}(X_i = \text{High school}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{High school}} - \bar{Y}_{i:W_i = 0, X_i = \text{High school}} \bigg) \\ &+ \mathbb{P}(X_i = \text{College}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{College}} - \bar{Y}_{i:W_i = 0, X_i = \text{College}} \bigg) \\ &= \frac{1}{2} (1 - 0) + \frac{1}{2} (1 - 1) = 0.5 + 0 = \end{split}$$

Potential employment

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	0	0	?	?
3	High school	1	?	1	?
4	College	0	1	?	?
5	College	1	?	1	?
6	College	1	?	1	?

BART

$$\begin{split} \hat{\tau} &= \sum_{x \in \text{Support of } X} \mathbb{P}(X = x) \bigg(\bar{Y}_{i:W_i = 1, X_i = x} - \bar{Y}_{i:W_i = 0, X_i = x} \bigg) \\ &= \mathbb{P}(X_i = \text{High school}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{High school}} - \bar{Y}_{i:W_i = 0, X_i = \text{High school}} \bigg) \\ &+ \mathbb{P}(X_i = \text{College}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{College}} - \bar{Y}_{i:W_i = 0, X_i = \text{College}} \bigg) \\ &= \frac{1}{2} (1 - 0) + \frac{1}{2} (1 - 1) = 0.5 + 0 = \end{split}$$

Potential employment

ıD	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	0	0	?	?
3	High school	1	?	1	?
4	College	0	1	?	?
5	College	1	?	1	?
6	College	1	?	1	?

$$\begin{split} \hat{\bar{\tau}} &= \sum_{x \in \text{Support of } X} \mathbb{P}(X = x) \bigg(\bar{Y}_{i:W_i = 1, X_i = x} - \bar{Y}_{i:W_i = 0, X_i = x} \bigg) \\ &= \mathbb{P}(X_i = \text{High school}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{High school}} - \bar{Y}_{i:W_i = 0, X_i = \text{High school}} \bigg) \\ &+ \mathbb{P}(X_i = \text{College}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{College}} - \bar{Y}_{i:W_i = 0, X_i = \text{College}} \bigg) \\ &= \frac{1}{2} (1 - 0) + \frac{1}{2} (1 - 1) = 0.5 + 0 = \end{split}$$

Potential employment

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	W_i	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
1	High school	0	0	?	?
2	High school	0	0	?	?
3	High school	1	?	1	?
4	College	0	1	?	?
5	College	1	?	1	?
6	College	1	?	1	?

$$\begin{split} \hat{\tau} &= \sum_{x \in \text{Support of } X} \mathbb{P}(X = x) \bigg(\bar{Y}_{i:W_i = 1, X_i = x} - \bar{Y}_{i:W_i = 0, X_i = x} \bigg) \\ &= \mathbb{P}(X_i = \text{High school}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{High school}} - \bar{Y}_{i:W_i = 0, X_i = \text{High school}} \bigg) \\ &+ \mathbb{P}(X_i = \text{College}) \bigg(\bar{Y}_{i:W_i = 1, X_i = \text{College}} - \bar{Y}_{i:W_i = 0, X_i = \text{College}} \bigg) \\ &= \frac{1}{2} (1 - 0) + \frac{1}{2} (1 - 1) = 0.5 + 0 = 0.5 \end{split}$$

Potential employment

	ID	Education X_i	Treated W_i	No job training $Y_i(0)$	Job training $Y_i(1)$	Treatment effect $\tau_i = Y_i(1) - Y_i(0)$
ĺ	1	High school	0	0	?	?
	2	High school	0	0	?	?
	3	High school	1	?	1	?
	4	College	0	1	?	?
	5	College	1	?	1	?
	6	College	1	?	1	?

But when there are many cells of the covariates X_i ,

nonparametric standardization is impossible!

Why is tree-based standardization biased? Regularization

With no regularization, a tree would grow until each leaf was completely homogenous in X_i .

But this tree would be very noisy! We prune our trees so that leaves contain more observations.

- Treatment effects are more precisely estimated
- But treatment effects are biased if there is confounding within leaves

BART

Is there anything we can do? Chernozhukov et al.

Outcome equation Treatment assignment
$$Y = D\theta_0 + g_0(X) + U$$
 $D = m_0(X) + V$

One might be tempted to estimate $\hat{g}_0(X)$ by machine learning and then state:

$$\hat{\theta}_0 = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i (Y_i - \hat{g}_0(X_i))}{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i^2}$$

Is there anything we can do? Chernozhukov et al.

Algorithm

Outcome equation Treatment assignment
$$Y = D\theta_0 + g_0(X) + U$$
 $D = m_0(X) + V$

One might be tempted to estimate $\hat{g}_0(X)$ by machine learning and then state:

$$\hat{\theta}_0 = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i(Y_i - \hat{g}_0(X_i))}{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i^2}$$

This will be biased because the estimator \hat{g}_0 is regularized.

$$b = rac{1}{\mathbb{E}(D_i^2)} rac{1}{\sqrt{n}} \sum_{i \in \mathcal{I}} \overbrace{\left(m_0(X_i)(g_0(X_i) - \hat{g}_0(X_i)
ight)}^{ ext{Does not have mean 0}} + o_P(1)$$

Is there anything we can do? Chernozhukov et al.

Outcome equation Treatment assignment
$$Y = D\theta_0 + g_0(X) + U$$
 $D = m_0(X) + V$

One might be tempted to estimate $\hat{g}_0(X)$ by machine learning and then state:

$$\hat{\theta}_0 = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i(Y_i - \hat{g}_0(X_i))}{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i^2}$$

This will be biased because the estimator \hat{g}_0 is regularized.

$$b=rac{1}{\mathbb{E}(D_i^2)}rac{1}{\sqrt{n}}\sum_{i\in\mathcal{I}} \overbrace{\left(m_0(X_i)(g_0(X_i)-\hat{g}_0(X_i)
ight)}^{ ext{Does not have mean 0}} +o_P(1)$$

Key: D_i is centered at $m_0(X) \neq 0$. We should recenter D_i .

Is there anything we can do? Chernozhukov et al.

Outcome equation Treatment assignment
$$\overbrace{Y = D\theta_0 + g_0(X) + U}$$

$$D = m_0(X) + V$$

- ① Split the sample into ${\mathcal I}$ and ${\mathcal J}$
- 2 Estimate $\hat{g}_0(X)$ using sample \mathcal{J}
- 3 Estimate $\hat{m}_0(X)$ using sample \mathcal{J}
- 4 Orthogonalize D on X (approximately)

$$\hat{V} = D - \hat{m}_0(X)$$

Sestimate the treatment effect

$$\hat{\theta}_0 = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i(Y_i - \hat{g}_0(X_i))}{\frac{1}{n} \sum_{i \in \mathcal{I}} D_i^2}$$

Chernozhukov et al. 2016

De-biased

$$\hat{\theta}_0 = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} \hat{V}_i(Y_i - \hat{g}_0(X_i))}{\frac{1}{n} \sum_{i \in \mathcal{I}} \hat{V}_i D_i}$$



BART

Bias remaining in de-biased estimator (Chernozhukov et al.)

$$\sqrt{n}(\hat{\theta}_0 - \theta_0) = a^* + b^* + c^*$$

Bias remaining in de-biased estimator (Chernozhukov et al.)

$$\sqrt{n}(\hat{\theta}_0 - \theta_0) = a^* + b^* + c^*$$

$$a^* = rac{1}{\mathbb{E}(V^2)} rac{1}{\sqrt{n}} \sum_{i \in \mathcal{T}} V_i U_i
ightarrow N(0, \Sigma)$$

Because a^* converges to mean 0, we don't worry about it.

Bias remaining in de-biased estimator (Chernozhukov et al.)

$$\sqrt{n}(\hat{\theta}_0 - \theta_0) = a^* + b^* + c^*$$

Regularization bias:

$$b^* = rac{1}{\mathbb{E}(V^2)} rac{1}{\sqrt{n}} \sum_{i \in \mathcal{I}} \left(\hat{m}_0(X_i) - m_0(X_i)
ight) \left(\hat{g}_0(X_i) - g_0(X_i)
ight)$$

Vanishes "under a broad range of data-generating processes."

Bounded above by



BART

Regularization + confounding

Bias remaining in de-biased estimator (Chernozhukov et al.)

Algorithm

$$\sqrt{n}(\hat{\theta}_0 - \theta_0) = a^* + b^* + c^*$$

An example of the third term in the partially linear model:

$$c^* = \frac{1}{\sqrt{n}} \sum_{i \in \mathcal{I}} V_i \bigg(\hat{g}_0(X_i) - g_0(X_i) \bigg)$$

If \hat{g}_0 is estimated on an auxiliary sample \mathcal{J} , then V_i and $\hat{g}_0(X_i)$ will be uncorrelated and $\mathbb{E}(c^*) = 0$.

BART: Bayesian Additive Regression Trees

Differs from random forests:

- Fixed number of trees
- Backfits repeatedly over the fixed number of trees
- Strong prior encourages shallow trees
- Uncertainty comes automatically from posterior samples

BART model

Intro

$$Y = \sum_{j=1}^{m} g_j(x \mid T_j, M_j) + \epsilon$$

$$\epsilon \sim N(0, \sigma^2)$$

$$T_j \text{ prior}$$

$$P(\underbrace{D_j = d}_{\text{Tree depth}}) = \alpha(1+d)^{-\beta}$$

$$\text{Split variable} \sim \text{Uniform}(\text{Available variables})$$

$$\text{Split value} \sim \text{Uniform}(\text{Available split values})$$

$$\mu_{ij} \mid T_j \text{ prior}$$

$$\mu_{ij} \sim N\left(\underbrace{\mu_m, \sigma_\mu^2}_{\text{Chosen so that high probability of }}_{E(Y|x) \in (y_{\min}, y_{\max})}\right)$$

$$\sigma \text{ prior}$$

$$\sigma \sim \frac{\nu \lambda}{\sqrt{2}} \text{ (inverse chi-square)}$$

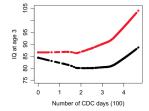
They recommend $\{\alpha = .95, \beta = 2\} \rightarrow 97\%$ of prior probability is on 4 or fewer terminal nodes.

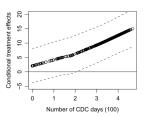
Intro

BART for causal inference

Goal: Model the response surface as a function of treatment and pre-treatment covariates

- ① Fit a flexible model for Y = f(X, W)
- ② Set W = 0 to predict $\hat{Y}_i(0)$ for all i
- 3 Set W=1 to predict $\hat{Y}_i(1)$ for all i
- ullet Difference to estimate $\hat{ au}_i$
- ⑤ Plot effects





BART: Benefits and drawbacks

Benefits

- Less researcher discretion for tuning parameters
- Automatic posterior uncertainty estimates

Drawbacks

- Not guaranteed to address confounding due to regularization
- No theoretical guarantees of centering over truth
- Splitting is based on prediction and is not explicitly optimized for causal inference within leaves

Summary

- Causal trees can detect high-dimensional covariate-based treatment effect heterogeneity
- Work well with high-order interactions
- Causal forests give theoretically valid confidence intervals
- Bayesian approaches (BART) are less theoretically verified but give easy uncertainty
- With high-dimensional confounding, all methods are biased but can be designed to be consistent.