Algorithm

Sample split

500

Causal forests

A tutorial in high-dimensional causal inference

Ian Lundberg

General Exam Frontiers of Causal Inference 12 October 2017



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

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

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Causal inference: A missing data problem

	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

Causal inference: A missing data problem

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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

$$ar{ au} = ar{Y}_{i:W_i=1}(1) - ar{Y}_{i:W_i=0}(0) \ = 1 - 0.5 \ = 0.5$$

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Causal inference: A missing data problem

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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	?	?	
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Potential employment

Causal inference: A missing data problem

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3	College	0	1	?	?
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Potential employment

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

$$\hat{ar{ au}} = ar{Y}_{i:W_i=1} - ar{Y}_{i:W_i=0}$$

= 1 - 0.5
= 0.5

Causal inference: A missing data problem

		Education	Treated	No job training	Job training	Treatment effect
I	D	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 $\tau_i = f(X_i)$? $\hat{\tau}_{\text{High school}} = \bar{Y}_{i:W_i=1,X_i=\text{High school}}$ $\hat{\tau}_{\text{College}} = \bar{Y}_{i:W_i=1,X_i=\text{College}}$ $-\bar{Y}_{i:W_i=0,X_i=\text{High school}}$ $-\bar{Y}_{i:W_i=0,X_i=\text{College}}$ = 1 - 0.5 = 1 - 1 = 0.5 = 0

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Causal inference: A missing data problem

			Potential en	ipioyment		
	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	?	?	
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Potential employment

What if there are dozens of X variables?

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Causal inference: A missing data problem

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1	High school	0	0	?	?	
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3	College	0	1	?	?	
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Potential employment

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

Causal inference: A missing data problem

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1	High school	0	0	?	?	
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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

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Start with a simpler prediction question.

Which subgroups of X have very different average outcomes?

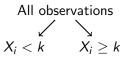
$$\mathsf{MSE}_0 = \frac{1}{n} \sum (Y_i - \bar{Y})^2$$

All observations

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

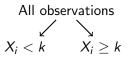
$$MSE_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i | \Pi_1)})^2$$



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

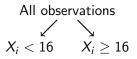
$$\mathsf{MSE}_1 = \frac{1}{n} \sum (Y_i - \bar{Y}_{j:x_j \in \ell(x_i | \Pi_1)})^2$$



Choose k to minimize MSE₁

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

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

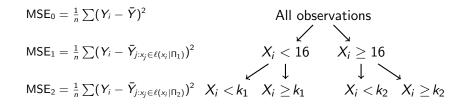


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Sac

Prediction: One tree

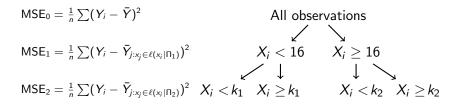


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Dac

Prediction: One tree



Choose k_1 or k_2 to minimize MSE₂

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Prediction: One tree

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

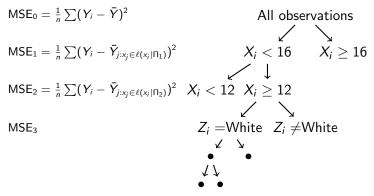
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Prediction: One tree

$$\begin{split} \mathsf{MSE}_{0} &= \frac{1}{n} \sum (Y_{i} - \bar{Y})^{2} & \mathsf{All \ observations} \\ \mathsf{MSE}_{1} &= \frac{1}{n} \sum (Y_{i} - \bar{Y}_{j:x_{j} \in \ell(x_{i} \mid \Pi_{1})})^{2} & X_{i} < 16 & X_{i} \geq 16 \\ \mathsf{MSE}_{2} &= \frac{1}{n} \sum (Y_{i} - \bar{Y}_{j:x_{j} \in \ell(x_{i} \mid \Pi_{2})})^{2} & X_{i} < 12 & X_{i} \geq 12 \\ \mathsf{MSE}_{3} & Z_{i} = \mathsf{White} & Z_{i} \neq \mathsf{White} \end{split}$$

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Could continue until all leaves had only one observation.

Unbiased but uselessly high variance!

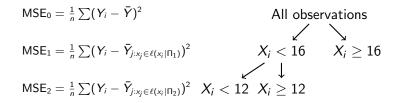
Instead, regularize: keep only splits that improve MSE by more than c.

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Prediction: One tree

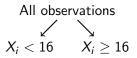
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Could continue until all leaves had only one observation. Unbiased but uselessly high variance! Instead, regularize: keep only splits that improve MSE by more than *c*.



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Prediction: One tree

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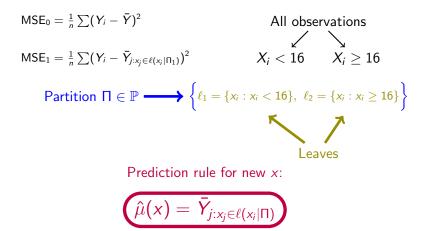
$$MSE_{1} = \frac{1}{n} \sum (Y_{i} - \bar{Y}_{j:x_{j} \in \ell(x_{i} \mid \Pi_{1})})^{2}$$

$$X_{i} < 16$$

$$X_{i} \geq 16$$

$$Partition \Pi \in \mathbb{P} \longrightarrow \left\{ \ell_{1} = \{x_{i} : x_{i} < 16\}, \ \ell_{2} = \{x_{i} : x_{i} \geq 16\} \right\}$$

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

Causal tree: What's different?

 ${\ensuremath{\textcircled{}}}$ We do not observe the ground truth



Causal tree: What's different?

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

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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.

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We want to search for true heterogeneity, not noise.

Sample splitting

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

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

Sample splitting

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

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

Honest criterion: Maximize

$$Q^{H}(\pi) \equiv -\mathbb{E}_{S^{\text{te}}, S^{\text{tr}}}\left[\mathsf{MSE}_{\mu}(S^{\text{te}}, \overset{\bullet}{S^{\text{est}}}, \pi(S^{\text{tr}}))\right]$$

where $\pi : \mathbb{R}^{p+1} \to \mathbb{P}$ is a function that takes a training sample $S^{tr} \in \mathbb{R}^{p+1}$ 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 $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

Goal: Estimate expected MSE using only the training sample.

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

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Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

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

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

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) \right)^{2} - Y_{i}^{2} \right]$$

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

$$-\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[2 \left(Y_{i} - \mu(X_{i} \mid \Pi) \right) \left(\mu(X_{i} \mid \Pi) - \hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) \right) \right]$$

Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

Expected mean squared error for a partition Π

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

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

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

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

$$-\mathbb{E}_{S^{\text{te}},S^{\text{est}}}\left[2\left(Y_{i}-\mu(X_{i}\mid \Pi)\right)\left(\mu(X_{i}\mid \Pi)-\hat{\mu}(X_{i}\mid S^{\text{est}},\Pi)\right)\right]$$

Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

Expected mean squared error for a partition $\boldsymbol{\Pi}$

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

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

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

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

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

$$-\mathbb{E}_{S^{\text{te}},S^{\text{est}}}\left[2\left(Y_{i}-\mu(X_{i}\mid \Pi)\right)\left(\mu(X_{i}\mid \Pi)-\hat{\mu}(X_{i}\mid S^{\text{est}},\Pi)\right)\right]$$

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

Sample split

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

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

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

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

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

$$-\mathbb{E}_{S^{\text{te}},S^{\text{est}}}\left[2\left(Y_{i}-\mu(X_{i}\mid \Pi)\right)\left(\mu(X_{i}\mid \Pi)-\hat{\mu}(X_{i}\mid S^{\text{est}},\Pi)\right)\right]$$

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Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

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

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

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) \right)^{2} - Y_{i}^{2} \right]$$

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

$$-\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[2 \left(Y_{i} - \mu(X_{i} \mid \Pi) \right) \left(\mu(X_{i} \mid \Pi) - \hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) \right) \right]$$

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Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

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

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) + \mu(X_{i} \mid \Pi) - \hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) \right)^{2} - Y_{i}^{2} \right]$$
First term²

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) \right)^{2} - Y_{i}^{2} \right]$$
Second term²

$$-\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(\mu(X_{i} \mid \Pi) - \hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) \right)^{2} \right]$$
2(First term)(Second term)
$$-\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[2 \left(Y_{i} - \mu(X_{i} \mid \Pi) \right) \left(\mu(X_{i} \mid \Pi) - \hat{\mu}(X_{i} \mid S^{\text{est}}, \Pi) \right) \right]$$

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E(A) =

Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

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

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

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) \right)^{2} - Y_{i}^{2} \right]$$

$$E(A) = 0 \text{ by assumption}$$

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

$$Cov(A, B) = 0 \text{ because } Y_{i} \text{ is from}$$

$$a \text{ sample independent of } S^{\text{est}}$$

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

a sample

Analytic estimator for $\text{EMSE}_{\mu}(\Pi)$ (p. 7356)

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

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

$$= -\mathbb{E}_{S^{\text{te}}, S^{\text{est}}} \left[\left(Y_{i} - \mu(X_{i} \mid \Pi) \right)^{2} - Y_{i}^{2} \right]$$

$$E(A) = 0 \text{ by assumption}$$

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

$$= 0$$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{pmatrix} -\mathbb{E}_{X_{i},S^{\text{est}}}\left[(\hat{\mu}(X_{i} \mid S^{\text{est}},\Pi) - \mu(X_{i} \mid \Pi))^{2}\right] \\ \text{They have } \hat{\mu}^{2} \text{ here but I think they are wrong} \\ \text{I think} \qquad \downarrow \\ = \mathbb{E}_{X_{i}}\left[\mu^{2}(X_{i} \mid \Pi)\right] - \mathbb{E}_{S^{\text{est}},X_{i}}\left[\mathbb{V}(\hat{\mu}(X_{i} \mid S^{\text{est}},\Pi))\right] \end{pmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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Algorithm

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Sample split

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

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

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

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

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

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

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

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

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

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

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

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

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

Intro

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

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

Algorithm

Sample split

Honest inference for treatment effects

Note: We still assume randomized treatment assignment

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Honest inference for treatment effects

Population-average potential outcomes within leaves:

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

Honest inference for treatment effects

Population-average potential outcomes within leaves:

$$\mu(w, x \mid \Pi) \equiv \mathbb{E} \begin{bmatrix} Y_i(w) \mid X_i \in \ell(x \mid \Pi) \end{bmatrix}$$
Potential outcome for
treatment w
(heterogeneous by X_i)
Averaged over controls
X_i in the leaf

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BART

Honest inference for treatment effects

Population-average potential outcomes within leaves:

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

Average causal effect:

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

Honest inference for treatment effects

Population-average potential outcomes within leaves:

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Average effect evaluated at (potentially moderating)
covariate value x

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Population-average potential outcomes within leaves:

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

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

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Population-average potential outcomes within leaves:

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

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

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BART

Population-average potential outcomes within leaves:

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

Average causal effect:

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

Compact notation

Estimate:

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

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Estimate:

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

MSE for treatment effects:

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

Estimate:

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

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.

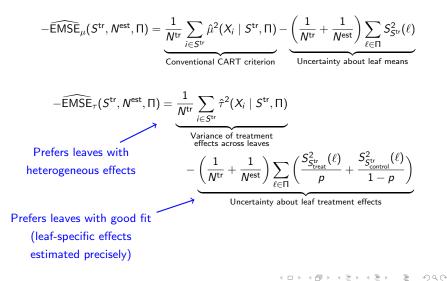
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$$\widehat{\mathsf{EMSE}}_{\mu}(S^{\mathrm{tr}}, N^{\mathrm{est}}, \Pi) = \underbrace{\frac{1}{N^{\mathrm{tr}}} \sum_{i \in S^{\mathrm{tr}}} \hat{\mu}^{2}(X_{i} \mid S^{\mathrm{tr}}, \Pi)}_{\text{Conventional CART criterion}} - \underbrace{\left(\frac{1}{N^{\mathrm{tr}}} + \frac{1}{N^{\mathrm{est}}}\right) \sum_{\ell \in \Pi} S_{S^{\mathrm{tr}}}^{2}(\ell)}_{\text{Uncertainty about leaf means}}$$
$$-\widehat{\mathsf{EMSE}}_{\tau}(S^{\mathrm{tr}}, N^{\mathrm{est}}, \Pi) = \underbrace{\frac{1}{N^{\mathrm{tr}}} \sum_{i \in S^{\mathrm{tr}}} \hat{\tau}^{2}(X_{i} \mid S^{\mathrm{tr}}, \Pi)}_{\text{Variance of treatment effects across leaves}} - \underbrace{\left(\frac{1}{N^{\mathrm{tr}}} + \frac{1}{N^{\mathrm{est}}}\right) \sum_{\ell \in \Pi} \left(\frac{S_{S^{\mathrm{tr}}_{\mathrm{treat}}}^{2}(\ell)}{p} + \frac{S_{S^{\mathrm{tr}}_{\mathrm{control}}}^{2}(\ell)}{1-p}\right)}$$

Uncertainty about leaf treatment effects

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Adapt EMSE_{μ} to estimate EMSE_{τ}



Algorithm

Sample split

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Four partitioning estimators

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1. Causal trees

Split by

$$-\widehat{\mathsf{EMSE}}_{\tau}(S^{\mathrm{tr}}, N^{\mathrm{est}}, \Pi) = \underbrace{\frac{1}{N^{\mathrm{tr}}} \sum_{i \in S^{\mathrm{tr}}} \hat{\tau}^{2}(X_{i} \mid S^{\mathrm{tr}}, \Pi)}_{Variance of treatment}}$$
Prefers leaves with good fit (leaf-specific effects estimated precisely)
$$-\underbrace{\left(\frac{1}{N^{\mathrm{tr}}} + \frac{1}{N^{\mathrm{est}}}\right) \sum_{\ell \in \Pi} \left(\frac{S_{\mathsf{Streat}}^{2}(\ell)}{p} + \frac{S_{\mathsf{Streat}}^{2}(\ell)}{1-p}\right)}_{Uncertainty about leaf treatment effects}$$

- Benefit: Prioritizes heterogeneity (τ̂ varies a lot) and fit (within-leaf precision)
- Drawback: Cannot be done with off-the-shelf CART methods

2. Transformed outcome trees

Transform the outcome

$$Y_i^* = Y_i \frac{W_i - p}{p(1 - p)} \to \mathbb{E}(Y_i^* \mid X_i = x) = \tau(x)$$

$$\begin{split} \mathbb{E}(Y_{i}^{*}) &= \mathbb{E}\left[Y_{i}\frac{W_{i}-p}{p(1-p)}\right] \\ &= \mathbb{E}\left[Y_{i}\frac{W_{i}}{p(1-p)}\right] - \mathbb{E}\left[Y_{i}\frac{p}{p(1-p)}\right] \\ &= \mathbb{E}\left[Y_{i}(1)\frac{W_{i}}{p(1-p)}\right] - \mathbb{E}\left[\left(Y_{i}(1)W_{i}+Y_{i}(0)(1-W_{i})\right)\frac{p}{p(1-p)}\right] \\ &= Y_{i}(1)\frac{1}{p(1-p)}\mathbb{E}[W_{i}] - Y_{i}(1)\frac{p}{p(1-p)}\mathbb{E}[W_{i}] - Y_{i}(0)\frac{p}{p(1-p)}\mathbb{E}[1-W_{i}] \\ &= Y_{i}(1)\frac{1-p}{p(1-p)}\mathbb{E}[W_{i}] - Y_{i}(0)\frac{p}{p(1-p)}\mathbb{E}[1-W_{i}] \\ &= Y_{i}(1)\frac{p(1-p)}{p(1-p)} - Y_{i}(0)\frac{p(1-p)}{p(1-p)} \\ &= Y_{i}(1)-Y_{i}(0) = \tau_{i} \end{split}$$

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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 W
 → p (by chance), then sample average within leaf is a poor estimator of *î*.

3. Fit-based trees

Replace

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

with the fit-based split rule

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

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 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.

From trees to forests: Double-sample trees

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

- Draw a sample of size s
- 2 Split into an \mathcal{I} and \mathcal{J} sample.
- 3 Grow a tree on the $\mathcal J$ sample
- (4) Estimate leaf-specific $\hat{\tau}_{\ell}$ 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.

- 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 $\hat{\tau}_\ell$ on each leaf

Repeat many times.

Advantages of forests:

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

Wager & Athey 2017

Why *propensity* forests:

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

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Summary of causal trees and forests

• There is no ground truth: We never observe τ_i

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- Causal trees search for leaves with
 - heterogeneous effects across leaves
 - precisely-estimated leaf effects

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- 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

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Why aren't causal trees guaranteed to address confounding?

Plan

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

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What works: Nonparametric standardization

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

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			Potential em	ployment		
	Education	Treated	No job training	Job training	Treatment effect	
ID	X_i	Wi	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$	
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	
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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 .

	Education	Treated	No job training	Job training	Treatment effect
ID	X_i	Wi	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$
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Potential employment

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

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	Education	Treated	No job training	Job training	Treatment effect	
ID	X_i	Wi	$Y_i(0)$	$Y_i(1)$	$\tau_i = Y_i(1) - Y_i(0)$	
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	Xi High school High school High school College College	XiWiHigh school0High school0High school1College0College1	X_i W_i $Y_i(0)$ High school00High school00High school1?College01College1?	X_i W_i $Y_i(0)$ $Y_i(1)$ High school00?High school00?High school1?1College01?College1?1

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ID	Education <i>X</i> i	Treated <i>W</i> i	No job training <i>Y_i</i> (0)	Job training $Y_i(1)$	Treatment effect $ au_i = Y_i(1) - Y_i(0)$
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6	College	1	?	1	?

What works: Nonparametric standardization

But when there are many cells of the covariates X_i ,

nonparametric standardization is impossible!

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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

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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:

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

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

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

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

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Is there anything we can do? Chernozhukov et al.

$$\underbrace{Y = D\theta_0 + g_0(X) + U}^{\text{Outcome equation}} \qquad \underbrace{Treatment assignment}_{D = m_0(X) + V}$$

- $\texttt{1} \quad \texttt{Split the sample into } \mathcal{I} \text{ and } \mathcal{J}$
- 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)

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

Stimate 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

$$\hat{\mathcal{D}}_{0} = \frac{\frac{1}{n} \sum_{i \in \mathcal{I}} \hat{\mathcal{V}}_{i}(Y_{i} - \hat{g}_{0}(X_{i}))}{\frac{1}{n} \sum_{i \in \mathcal{I}} \hat{\mathcal{V}}_{i}D_{i}}$$

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

$$\sqrt{n}(\hat{ heta}_0- heta_0)=a^*+b^*+c^*$$

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

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

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

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

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

$$\sqrt{n}(\hat{ heta}_0- heta_0)=a^*+b^*+c^*$$

Regularization bias:

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

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

Bounded above by

Rate of convergence of
$$\hat{m}_0 \rightarrow m$$
 $\hat{g}_0 \rightarrow g$ Rate of convergence of $\hat{g}_0 \rightarrow g$

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

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

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

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

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

$$\begin{split} Y &= \sum_{j=1}^{m} g_j(x \mid T_j, M_j) + \epsilon \\ &\epsilon \sim N(0, \sigma^2) \\ T_j \text{ prior} \\ P(\underbrace{D_j = d}_{\text{Tree depth}}) &= \alpha (1 + d)^{-\beta} \\ \text{Split variable} \sim \text{Uniform}(\text{Available variables}) \\ \text{Split value} \sim \text{Uniform}(\text{Available split values}) \\ \mu_{ij} \mid T_j \text{ prior} \\ \underbrace{\mu_{ij}}_{\mu_{ij}} &\sim N\left(\underline{\mu_m, \sigma_{\mu}^2}\right) \end{split}$$

Free *i* leaf *j*
Chosen so that
high probability of

$$E(Y|x) \in (y_{\min}, y_{\max})$$

 σ prior

 $\sigma \sim rac{
u \lambda}{\chi^2_{
u}}$ (inverse chi-square)

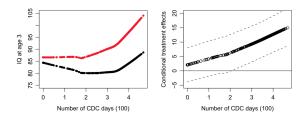
They recommend $\{\alpha = .95, \beta = 2\} \rightarrow 97\%$ of prior probability is on 4 or fewer terminal nodes.

Chipman, George, & McCulloch 2010

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
- ④ Difference to estimate $\hat{\tau}_i$
- ⑤ Plot effects



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

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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.