Machine Learning Theory

Lecture 3: The R-Learner

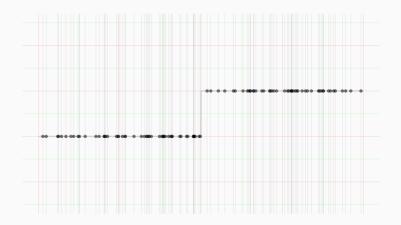
David A. Hirshberg May 24, 2024

Emory University

Least Squares Review

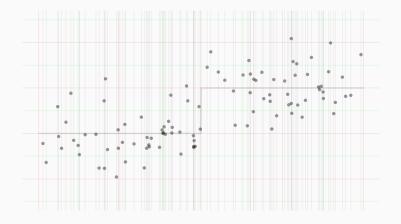


We started with a curve $\mu(x)$.



We sampled it at some points X_i .

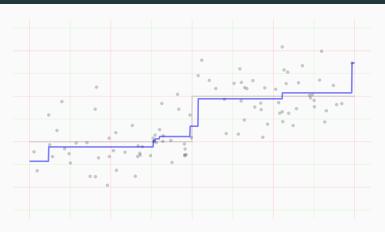
$$Y_i = \mu(X_i)$$



We added *noise* to get our observations.

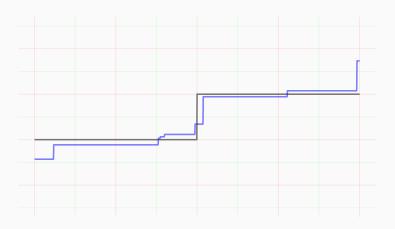
$$Y_i = \mu(X_i) + \varepsilon_i$$

,

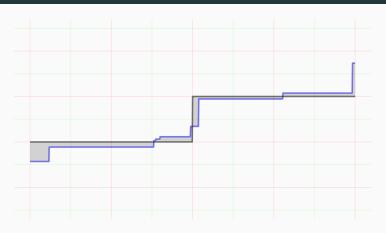


We fit a curve, e.g. an increasing one, via least squares.

$$\hat{\mu} = \mathop{\rm argmin}_{\text{increasing } m} \frac{1}{n} \sum_{i=1}^n \{ \, Y_i - m(X_i) \}^2.$$



We compared the curve we fit to the curve we started with.



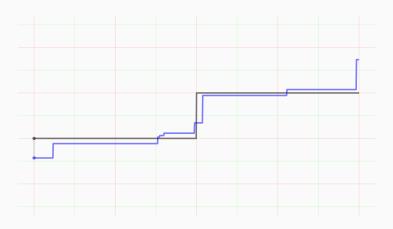
We looked at mean squared distance over the whole interval.

$$\mathrm{PMSE} = \int_0^1 \{\mu(x) - \hat{\mu}(x)\}^2 dx$$



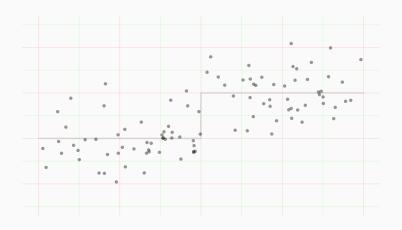
And at mean squared distance over the sample.

$$\text{SMSE} = \frac{1}{n} \sum_{i=1}^{n} \{ \mu(X_i) - \hat{\mu}(X_i) \}^2$$



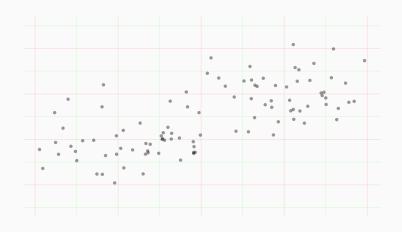
And at squared distance at the left endpoint x=0.

$${\rm MSE}_0 = \{\mu(0) - \hat{\mu}(0)\}^2$$



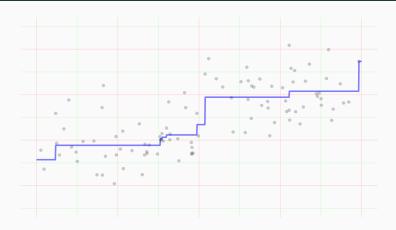
We could do all of this because we were using fake data. We knew the curve μ that we'd sampled.

Working with real data is different



What we start with is the data. We don't see any underlying curve μ .

Working with real data is different



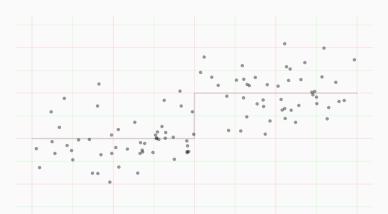
We can, of course, still fit a curve. But what are we supposed to compare it to? What curve are we trying to estimate?

What least squares estimates

The error we minimize, in large samples, approximates its expectation.

$$\frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m(X_i) \}^2 \to \mathbb{E} \{ Y_i - m(X_i) \}^2$$

So what we might hope for is to estimate the curve μ minimizing that. That's the conditional mean $\mu(x) = \mathrm{E}[Y_i \mid X_i = x]$. It's the curve giving the mean value of Y_i at every value of X_i .



Let's see what happens when we break Y_i into $\mu(X_i)$ and what's left over. What's left over plays the role of our noise ε_i . What do we know about it?

$$Y_i = \mu(X_i) + \varepsilon_i$$
 where ?

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 where $\mathrm{E}[\varepsilon_i \mid X_i] = 0$.

Now let's use this to break down what we're minimizing.

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$$E\{Y_i - m(X_i)\}^2 = E\{\varepsilon_i + \mu(X_i) - m(X_i)\}^2$$

= $E \varepsilon_i^2 + 2 E \varepsilon_i \{\mu(X_i) - m(X_i)\} + E\{\mu(X_i) - m(X_i)\}^2$

Why does this tell us the minimizer is μ ?

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Why does this tell us the minimizer is μ ?

As we vary m, it's ...

- · a constant
- · plus zero
- \cdot plus a positive term that's zero only if $m=\mu$

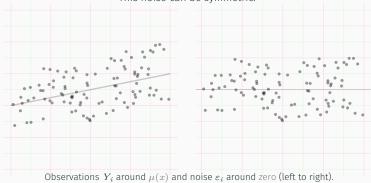
Signal and Noise in Least Squares Regression

If everything goes right, we'll approximate the conditional mean.

$$\mu(x) = \mathrm{E}[Y_i \mid X_i = x]$$

That's the signal we're trying to recover. The noise it hides in has mean zero at each X_i .

This noise can be symmetric.



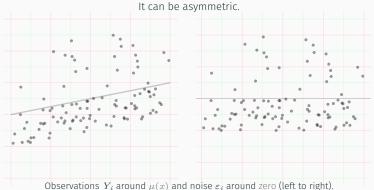
$$Y_i = X_i + \varepsilon_i$$
 where $\varepsilon_i \sim \mathsf{Uniform}(-1,1)$

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$$Y_i = X_i + \varepsilon_i$$
 where $\varepsilon_i \sim \begin{cases} \mathsf{Uniform}(0,2) & \text{with probability } 1/3 \\ \mathsf{Uniform}(-1,0) & \text{with probability } 2/3 \end{cases}$

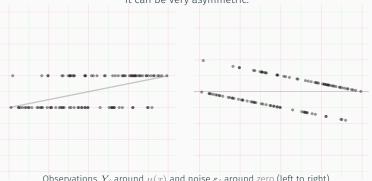
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It can be very asymmetric.



Observations Y_i around $\mu(x)$ and noise ε_i around zero (left to right).

$$Y_i = X_i + \varepsilon_i$$
 where $\varepsilon_i \sim \begin{cases} 1 - \mu(X_i) & \text{with probability } \mu(X_i) \\ -\mu(X_i) & \text{with probability } 1 - \mu(X_i) \end{cases}$



We'll have to do something else.

There are many things to estimate and many ways to estimate them. This week, we'll estimate *personalized treatment effects* using the *R-Learner*.

Personalized Treatment Effects

Context. Who did the NSW Job Training Program increase income for?

- The NSW program was implemented in the mid-1970s.
- It provided work experience and counseling for a period of 9-18 months.
- · It enrolled people who tended to have difficulty with employment, e.g.,
 - · People who'd been convicted of crimes
 - · People who'd been addicted to drugs
 - · People who'd not completed high school
- These participants were randomly assigned to the control or treatment groups.
- · Both groups were interviewed, only the treated were given these short-term jobs.
- · We want know who the treatment helps.

Specifics

- · We're looking at income in 1978, after the program ended.
- · We're interested in the impact of treatment on this.
- And we want to estimate the average effect of this treatment among participants with a given 1974 income.

Identification

Due to randomization, this is conceptually simple.

- We want to compare each participant to an imaginary version of themself—one that got a different treatment—then average over folks with the same 1974 income.
- But given randomization, this is equivalent to a real comparison.
- If there's no difference, on average, between participants with identical 1974 incomes, we can swap in a real participant for our imaginary one.
- That's the case when all participants with the same '74 income receive treatment vs. control with the same probability.

What we want is to compare two conditional means.

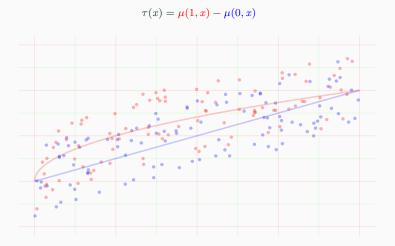
 $\tau(x) = E[Y_i(1) \mid X_i = x] - E[Y_i(0) \mid X_i = x]$

 $x=0, X_i=x]$ participant vs one w/ same '74 income x=0, x=0

participant vs imaginary version of self

- $\mu(1, x)$, the mean for treated participants with 1974 income x
- $\mu(0, x)$, the mean for untreated participants with 1974 income x

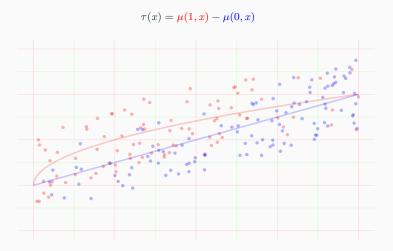
)



In this fake data, all participants receive treatment with probability 1/2.



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In this fake data, participants with lower '74 incomes receive treatment more often than those with higher '74 incomes.



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Naive Approach

We estimate the conditional mean for each treatment group, then subtract.

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

Here we've fit increasing curves to each group via least squares.

$$\hat{\mu}(w,\cdot) = \mathop{\rm argmin}_{\text{increasing } m} \ \sum_{i: W_i = w} \{\, Y_i - m(X_i) \}^2 \quad \text{ for } \quad w \in \{0,1\}.$$

What we don't like about it

- · We have to estimate two treatment-specific conditional means.
- If we don't estimate one well, we tend to get a bad treatment effect estimate.
- It's hard to encode assumptions about the treatment effect itself in our model for these conditional means.
 - e.g. constancy, $\tau(x) = \tau$.
 - e.g. approximate constancy, $\rho_{TV}(\tau) \approx 0$.
 - e.g. decreasingness, $\tau'(x) \leq 0$.

Let's try to fix that.

We express our treatment-specific conditional means in terms of a few other things.

$$\begin{split} \mu(W_i,X_i) &= \beta(X_i) + \{W_i - \pi(X_i)\}\tau(X_i) & \text{where} \\ \beta(X_i) &= \mathrm{E}[Y_i \mid X_i] & \text{is the (nonspecific) conditional mean,} \\ \pi(X_i) &= P(W_i = 1 \mid X_i), & \text{is the conditional treatment probability,} \\ \tau(X_i) &= \mathrm{E}[Y_i \mid W_i = 1, X_i] - \mathrm{E}[Y_i \mid W_i = 0, X_i] & \text{is the conditional treatment effect.} \end{split}$$

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Derivation. We start with a characterization of $\beta(X_i)$ as a marginal of $\mu(W_i, X_i)$.

Then we plug it in.

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$$\begin{split} &\beta(X_i) + \{W_i - \pi(X_i)\}\tau(X_i) \\ &= \mu(1, X_i)\pi(X_i) + \mu(0, X_i)\{1 - \pi(X_i)\} + \{W_i - \pi(X_i)\}\{\mu(1, X_i) - \mu(0, X_i)\} \\ &= \mu(1, X_i)\{\pi(X_i) + W_i - \pi(X_i)\} + \mu(X_i, 0)[\{1 - \pi(X_i)\} - \{W_i - \pi(X_i)\}] \\ &= \mu(1, X_i)W_i + \mu(0, X_i)(1 - W_i) = \mu(X_i, W_i). \end{split}$$

The R-Learner idea

$$\begin{split} \mu(W_i,X_i) &= \beta(X_i) + \{W_i - \pi(X_i)\}\tau(X_i) & \text{where} \\ \beta(X_i) &= \mathrm{E}[Y_i \mid X_i] & \text{is the (nonspecific) conditional mean,} \\ \pi(X_i) &= P(W_i = 1 \mid X_i), & \text{is the conditional treatment probability,} \\ \tau(X_i) &= \mathrm{E}[Y_i \mid W_i = 1, X_i] - \mathrm{E}[Y_i \mid W_i = 0, X_i] & \text{is the conditional treatment effect.} \end{split}$$

If we knew the nuisance functions β and π , we could estimate τ using a special model.

$$\hat{\tau} = \underset{t \in \mathcal{M}_{\tau}}{\operatorname{argmin}} \ \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m_t(W_i, X_i) \}^2 \ \text{ where } \ m_t(w, x) = \beta(x) + [w - \pi(x)] t(x).$$

This is a weighted least squares estimate of τ based on a Y_i^{τ} .

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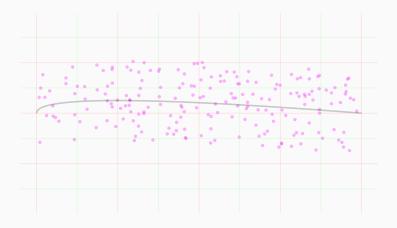
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$$\begin{split} Y_i - m_t(W_i, X_i) &= [\beta(X_i) + \{W_i - \pi(X_i)\}\tau(X_i) + \varepsilon_i] - [\beta(X_i) + \{W_i - \pi(X_i)\}t(X_i)] \\ &= \{W_i - \pi(X_i)\}\{\tau(X_i) - t(X_i)\} + \varepsilon_i \\ &= \{W_i - \pi(X_i)\}\{\tau(X_i) + \varepsilon_i^{\mathsf{T}} - t(X_i)\} \quad \text{where} \quad \varepsilon_i^{\mathsf{T}} = \frac{\varepsilon_i}{W_i - \pi(X_i)}. \end{split}$$

so what we'd minimize is weighted squared error for predicting $Y_i^{ au}$.

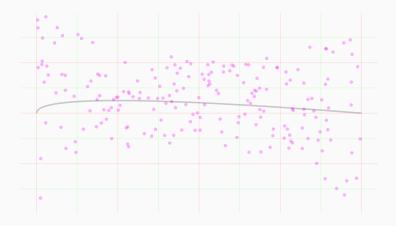
$$\hat{\tau} = \underset{t \in \mathcal{M}_{-}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \{W_i - \pi(X_i)\}^2 \{Y_i^{\tau} - t(X_i)\}^2 \quad \text{where} \quad Y_i^{\tau} = \tau(X_i) + \varepsilon_i^{\tau}.$$

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Pseudo-outcomes Y_i^{τ} when all participants receive treatment with probability 1/2.

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Pseudo-outcomes Y_i^{τ} when participants with lower '74 incomes receive treatment more often than those with higher '74 incomes.

The real R-Learner

$$\hat{\tau}_{\star} = \underset{t \in \mathcal{M}_{\tau}}{\operatorname{argmin}} \, \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m_t(W_i, X_i) \}^2 \quad \text{where} \quad m_t(w, x) = \beta(x) + [w - \pi(x)] t(x)$$

- · This is what we've been talking about doing.
- But we can't really do it because we don't know the nuisance function β .
- That's why it's a nuisance. We need to know it, even if we're not interested in it.
- To actually use the R-Learner, we'll have to substitute an estimate.

$$\hat{\tau} = \underset{t \in \mathcal{M}_{\tau}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m_t(W_i, X_i) \}^2 \quad \text{where} \quad m_t(w, x) = \hat{\beta}(x) + [w - \pi(x)] t(x)$$

$$\text{and} \quad \hat{\beta} = \underset{b \in \mathcal{M}_{\tau}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - b(X_i) \}^2$$

The real R-Learner as least squares

$$\hat{\tau} = \operatorname*{argmin}_{t \in \mathcal{M}_{\tau}} \frac{1}{n} \sum_{i=1}^{n} \{ \, Y_i - m_t(\,W_i, X_i) \}^2 \quad \text{ where } \quad m_t(w, x) = \hat{\beta}(x) + [w - \pi(x)] t(x)$$

This is another weighted least squares estimate of au.

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This is another weighted least squares estimate of τ .

$$\begin{split} Y_i - m_t(W_i, X_i) &= [\beta(X_i) + \{W_i - \pi(X_i)\}\tau(X_i) + \varepsilon_i] - \left[\hat{\beta}(X_i) + \{W_i - \pi(X_i)\}t(X_i)\right] \\ &= \{W_i - \pi(X_i)\}\{\tau(X_i) - t(X_i)\} + \{\beta(X_i) - \hat{\beta}(X_i)\} + \varepsilon_i \\ &= \{W_i - \pi(X_i)\}\{\tau(X_i) + \varepsilon_i^{\mathsf{T}} + \delta_i - t(X_i)\} \quad \text{where} \quad \delta_i = \frac{\beta(X_i) - \hat{\beta}(X_i)}{W_i - \pi(X_i)} \end{split}$$

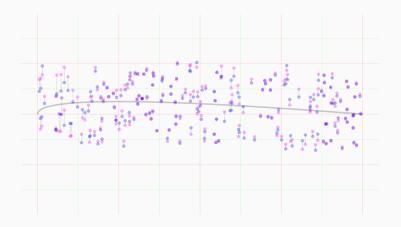
we're minimizing weighted squared error for predicting a corrupted

$$\hat{\tau} = \operatorname*{argmin}_{t \in \mathcal{M}_{\tau}} \frac{1}{n} \sum_{i=1}^{n} \{W_i - \pi(X_i)\}^2 \{Y_i^{\tau} + \delta_i - t(X_i)\}^2 \quad \text{where} \quad Y_i^{\tau} = \tau(X_i) + \varepsilon_i^{\tau}.$$

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The corrupted s

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When all participants receive treatment with probability 1/2.

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When participants with lower '74 incomes receive treatment more often than those with higher '74 incomes. Noiser at the edges.

Robustness



- One very interesting property of the R-Learner is that it's insensitive to $\hat{\beta}$.
 - · That is, it works well even if $\hat{\beta}$ is a pretty bad estimate.
 - Or, at least, it works almost as well as a version using β itself.
- That is, we estimate τ essentially as if we were doing weighted least squares prediction of the pseudo-outcomes.
 - The 'corruption' of the pseudo-outcomes we really predict isn't a big deal.
 - \cdot We're using our knowledge about the treatment probability $\pi(x)$ to help us.
- · Let's look at how this works for a very simple treatment effect model \mathcal{M}_{τ} .

An Exercise

Show that, in the case that we use the constant treatment effect model $\mathcal{M}_{ au}=\{t(x)=c:c\in\mathbb{R}\}$, these two versions of the R-learner differ by a term that's small relative to $1/\sqrt{n}$ as long as $\hat{n}\to m$. That is, show that

$$\sqrt{n}(\hat{\tau} - \hat{\tau}_\star) \to 0$$
 if $\hat{m} \to m$

$$\hat{\tau}_{\hat{\beta}} = \underset{t \in \mathbb{R}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m_t(W_i, X_i) \}^2 \text{ where } m_t(w, x) = \hat{\beta}(x) + [w - \pi(x)]t$$

$$\hat{\tau}_{\beta} = \underset{t \in \mathbb{R}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m_t(W_i, X_i) \}^2 \text{ where } m_t(w, x) = \beta(x) + [w - \pi(x)]t$$

You may treat \hat{m} as a non-random function. In practice, we'll split our sample in two and estimate \hat{m} and $\hat{\tau}$ on different halves, which allows us to justify this rigorously.

Hint. Solve for $\hat{\tau}$ and $\hat{\tau}_{\star}$ explicitly by setting derivatives to zero, then compare the results. When you do, pay attention to the mean and *standard deviation* of your terms.

Step 1. Solving for $\hat{\tau}$ as a function of β

$$\hat{\tau}_b = \operatorname*{argmin}_{t \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^n \{ Y_i - m_t(W_i, X_i) \}^2 \text{ where } m_t(w, x) = b(x) + [w - \pi(x)]t$$
 solves

$$0 = \frac{d}{dt} \Big|_{t=\hat{\tau}_b} \frac{1}{n} \sum_{i=1}^n \{ Y_i - b(X_i) - [W_i - \pi(X_i)]t \}^2$$

= $\frac{1}{n} \sum_{i=1}^n 2\{ Y_i - b(X_i) - [W_i - \pi(X_i)]\hat{\tau}_b \} \times - [W_i - \pi(X_i)].$

$$\frac{2}{n} \sum_{i=1}^{n} [W_i - \pi(X_i)] \{ Y_i - b(X_i) \} = \frac{2}{n} \sum_{i=1}^{n} [W_i - \pi(X_i)]^2 \hat{\tau}_b$$

Rearranging.

and therefore

$$\hat{\tau}_b = \frac{\frac{1}{n} \sum_{i=1}^n \{ W_i - \pi(X_i) \} \{ Y_i - b(X_i) \}}{\frac{1}{n} \sum_{i=1}^n \{ W_i - \pi(X_i) \}^2}$$

Comparison

$$\hat{\tau}_b = \frac{\frac{1}{n} \sum_{i=1}^n \{ W_i - \pi(X_i) \} \{ Y_i - b(X_i) \}}{\frac{1}{n} \sum_{i=1}^n \{ W_i - \pi(X_i) \}^2}$$

for $b = \hat{\beta}$ and $b = \beta$. Comparing,

$$\begin{split} \hat{\tau}_{\hat{\beta}} - \hat{\tau}_{\beta} &= \frac{\frac{1}{n} \sum_{i=1}^{n} \{W_{i} - \pi(X_{i})\} [\{Y_{i} - \hat{\beta}(X_{i})\} - \{Y_{i} - \beta(X_{i})\}]}{\frac{1}{n} \sum_{i=1}^{n} \{W_{i} - \pi(X_{i})\}^{2}} \\ &= \frac{\frac{1}{n} \sum_{i=1}^{n} \{W_{i} - \pi(X_{i})\} \{\beta(X_{i}) - \hat{\beta}(X_{i})\}}{\frac{1}{n} \sum_{i=1}^{n} \{W_{i} - \pi(X_{i})\}^{2}} \end{split}$$

What this tells us about the difference $\hat{\tau}_{\hat{\beta}} - \hat{\tau}_{\beta}$.

- 1. It's *almost* an average of independent random variables with mean zero, as $\mathrm{E}\{W_i \pi(X_i) | X_i\} = \pi(X_i) \pi(X_i) = 0.$
- It would be if we replaced the denominator with its expectation, which the law of large numbers more or less justifies.

$$\hat{\tau}_{\hat{\beta}} - \hat{\tau}_{\beta} = \frac{\frac{1}{n} \sum_{i=1}^{n} \{W_i - \pi(X_i)\} \{\beta(X_i) - \hat{\beta}(X_i)\}}{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_i - \pi(X_i)\}^2} \times \frac{1}{Q} \quad \text{for} \quad Q = \frac{\frac{1}{n} \sum_{i=1}^{n} \{W_i - \pi(X_i)\}^2}{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_i - \pi(X_i)\}^2}$$

Making Sense of This

$$\hat{\tau}_{\hat{\beta}} - \hat{\tau}_{\beta} = \frac{\frac{1}{n} \sum_{i=1}^{n} \{W_i - \pi(X_i)\} \{\beta(X_i) - \hat{\beta}(X_i)\}}{\frac{1}{n} \sum_{i=1}^{n} E\{W_i - \pi(X_i)\}^2} \times \frac{1}{Q} \quad \text{for} \quad Q \to 1$$

If we ignore the largely irrelevant factor 1/Q (see Slutsky's Theorem), then ...

- 1. This difference is an average of independent mean-zero random variables.
- 2. So it's approximately normal with variance $1/n\times$ the average of the term variances.

What is this variance?

$$\begin{split} V &= \frac{1}{n} \times \frac{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_{i} - \pi(X_{i})\}^{2} \{\beta(X_{i}) - \hat{\beta}(X_{i})\}^{2}}{\left\{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_{i} - \pi(X_{i})\}^{2}\right\}^{2}} \\ &\leq \frac{1}{n} \times \frac{\|\beta - \hat{\beta}\|_{L_{\infty}(\mathbf{P_{n}})}^{2} \times \frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_{i} - \pi(X_{i})\}^{2}}{\left\{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_{i} - \pi(X_{i})\}^{2}\right\}^{2}} \\ &= \frac{1}{n} \times \frac{\|\beta - \hat{\beta}\|_{L_{\infty}(\mathbf{P_{n}})}^{2}}{\frac{1}{n} \sum_{i=1}^{n} \mathrm{E}\{W_{i} - \pi(X_{i})\}^{2}} \end{split}$$

The difference $\hat{\tau}_{\hat{\beta}} - \hat{\tau}_{\beta}$ (more or less, i.e. ignoring Q) has mean zero and standard deviation ...

$$\sqrt{V} = \frac{\|\beta - \hat{\beta}\|_{L_{\infty}(P_n)}}{\sqrt{n} \times \sqrt{\frac{1}{n} \sum_{i=1}^{n} E\{W_i - \pi(X_i)\}^2}}$$
$$\lesssim \frac{\|\beta - \hat{\beta}\|_{L_{\infty}(P_n)}}{\sqrt{n}}$$

If we have a consistent estimate of β , i.e. if $\|\beta - \hat{\beta}\|_{L_{\infty}(\mathbf{P_n})} \to 0$, this difference is negligible relative to the difference $\hat{\tau}_{\beta} - \tau$, which has standard deviation $\propto 1/\sqrt{n}$. In other words, our actual estimator $\hat{\tau}_{\hat{\beta}}$ and the oracle estimator $\hat{\tau}_{\beta}$ are asymptotically equivalent: they have the same asymptotic distribution.