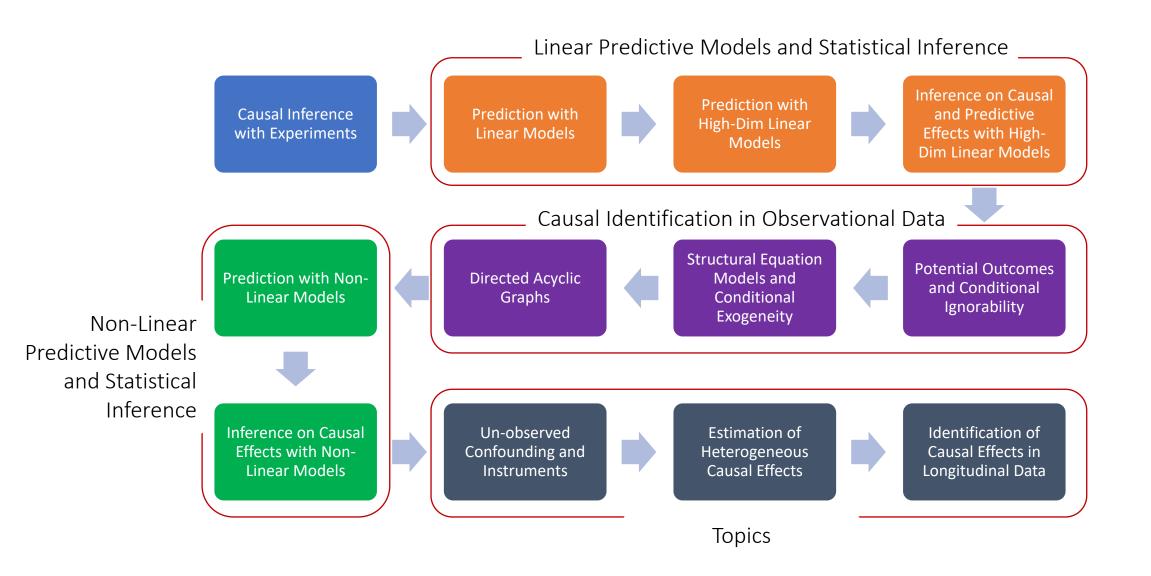
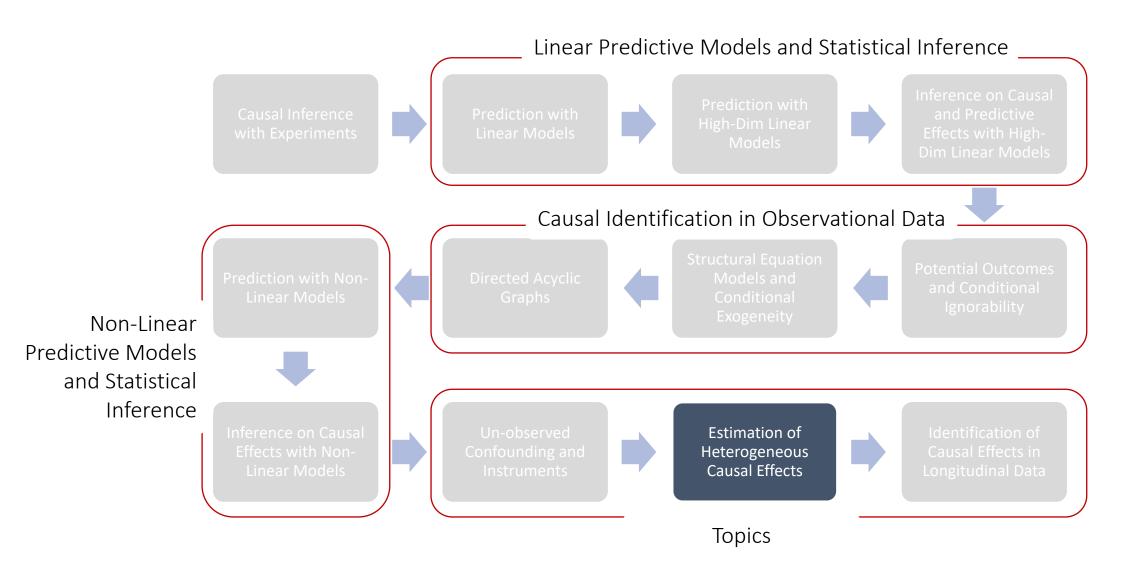
# MS&E 228: Unobserved Confounding and Instruments

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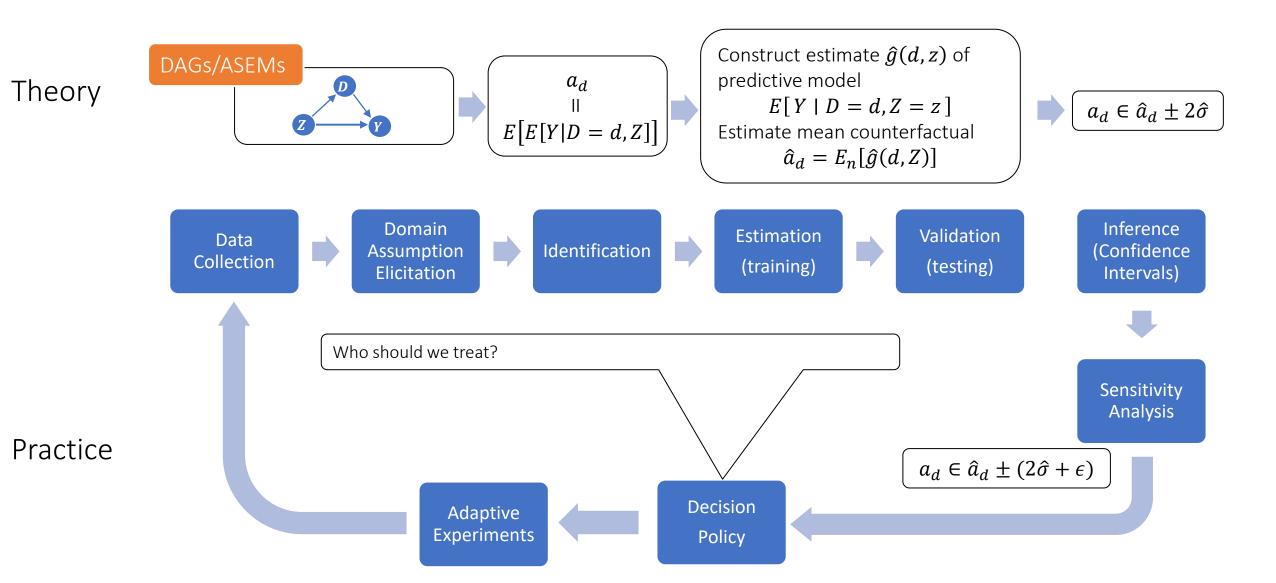




### Goals for Today

- Meta-Learners for Heterogeneous Treatment Effects
- Neural Network Approaches for Heterogeneous Effects
- Out-of-sample validation and testing

#### Causal Inference Pipeline



#### Personalized (Refined) Policies

- To understand who to treat, we need to learn how effect varies
- Conditional Average Treatment Effect

$$\theta(x) = E[Y(1) - Y(0) | X = x]$$

- Allows us to understand differences (heterogeneities) in the response to treatment for different parts of the population
- We can deploy more refined "personalized" policies
- For every person that comes, we observe an X = x and decide treat if  $\theta(x) > 0$  else don't treat

#### The intrinsic hardness of CATE

- Estimating CATE at least as hard as estimating the best prediction rule
- Inherently harder than estimating an "average"
- So far for our target causal quantities we wanted fast estimation rates and confidence intervals
- We were only ok with "decent" estimation rates for the auxiliary (nuisance) predictive models that entered our analysis

We might want to relax our goals...

# Different Approaches to Relaxing our Goals

- Goal 1: Maybe estimate a simpler projection (e.g. analogue of BLP)
- Goal 2: Confidence intervals for predictions of this simple projection
- Goal 3: Simultaneous confidence bands for predictions of this simple projection
- Goal 4: Estimation error rate for the true CATE
- Goal 5: Confidence intervals for the prediction of a CATE model
- Goal 6: Simultaneous confidence bands for joint predictions of CArmodel

Policy Learning

?? (only classical non-parametric statistic results on confidence bands of non-parametric functions)

- Goal 7: Go after optimal simple treatment policies; give me a policy with value close to the best
- Goal 8: Inference on value of candidate treatment policies
- Goal 9: Inference on value of optimal policy

• Goal 10: Identify responder or heterogeneous sub-groups; policies with statistical significance;

Linear Doubly Robust Learner

Meta-learner approaches: S-Learner, T-Learner, X-Learner, R-Learner, DR-Learner Neural Network approaches: TARNet, CFR Random Forest approaches: BART

Modified (honest) ML methods: Generalized Random Forest, Orthogonal Random Forest, Sub-sampled Nearest Neighbor Regression

Doubly Robust Policy

**Evaluation** 

Doubly Robust Policy Learning

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# Meta-Learning Approaches for CATE

### Meta-Learning Idea

• We assume conditional ignorability:  $Y(1), Y(0) \perp \!\!\! \perp D \mid Z$ 

• We want to estimate the CATE:  $E[Y(1) - Y(0) \mid X], X \subseteq Z$ 

• If we can frame CATE as a conditional expectation function, then we can deploy any ML approach for solving the corresponding Best Prediction problem

# Single Learner (S-Learner)

$$\theta(X) = E[g(1,Z) - g(0,Z) \mid X], \qquad g(D,Z) = E[Y|D,Z]$$

#### Meta-Algorithm:

- Run ML regression predicting Y from D,Z to learn g (preferably in a cross-fitting manner, i.e. fit on half the data and predict on the other half and vice versa)
- Run ML regression predicting g(1,Z)-g(0,Z) from X

# Two Learner (T-Learner)

$$\theta(X) = E[g(1,Z) - g(0,Z) \mid X], \qquad g(D,Z) = E[Y|D,Z]$$

#### Meta-Algorithm:

- Run ML regression predicting Y from Z on subset of data for which D=0 to learn  $g(0,\cdot)$  (preferably in a cross-fitting manner)
- Run ML regression predicting Y from Z on subset of data for which D=1 to learn  $g(1,\cdot)$  (preferably in a cross-fitting manner)
- Run an ML regression predicting g(1,Z)-g(0,Z) from X

### Doubly Robust Learner (DR-Learner)

$$\theta(X) = E[Y_{DR}(g,p) \mid X], \qquad Y_{DR}(g,p) \coloneqq g(1,Z) - g(0,Z) + H(D,Z) \left(Y - g(D,Z)\right)$$

$$H(D,Z) = \frac{D}{p(Z)} - \frac{1 - D}{1 - p(Z)}, \qquad g(D,Z) \coloneqq E[Y|D,Z], \qquad p(Z) \coloneqq \Pr(D = 1|Z)$$

#### Meta-Algorithm:

- Run ML regression to estimate  $g(1, \cdot)$  and  $g(0, \cdot)$  (either S or T Learner); preferably T-Learner and in cross-fitting manner
- Run ML classification to estimate  $\Pr(D=1|Z)$  and calculate H(D,Z); preferably in cross-fitting manner
- Run ML regression predicting g(1,Z) g(0,Z) + H(D,Z)(Y g(D,X)) from X

#### Cross Learner (X-Learner)

$$\tau(Z) = \tau_1(Z) \coloneqq E[Y - E[Y \mid D = 0, Z] \mid D = 1, Z]$$

$$\tau(Z) = \tau_0(Z) \coloneqq E[E[Y \mid D = 1, Z] - Y \mid D = 0, Z]$$

For the **control group** I observe  $Y(0) \equiv Y(D) = Y$  I can impute a counterfactual outcome  $\hat{Y}(1)$ , by fitting a response model  $\hat{g}_1(Z) \approx E[Y|D=1,Z]$  from the control group and predict on the treated  $\hat{Y}(1) = \hat{g}_1(Z)$   $Y(1) - Y(0) \mid Z \qquad \qquad \hat{g}_1(Z) - Y \mid D=0,Z$ 

For the **treated group** I observe  $Y(1) \equiv Y(D) = Y$  I can impute a counterfactual outcome  $\hat{Y}(0)$ , by fitting a response model  $\hat{g}_0(Z) \approx E[Y|D=0,Z]$  from the control group and predict on the treated  $\hat{Y}(0) = \hat{g}_0(Z)$   $Y(1) - Y(0) \mid Z \qquad \qquad Y - \hat{g}_0(Z) \mid D=1,Z$ 

### Cross Learner (X-Learner)

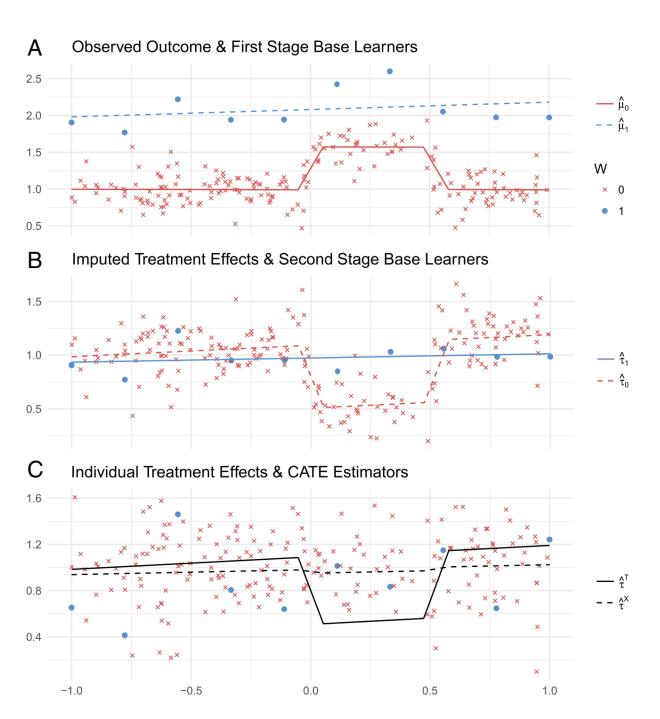
$$\hat{\tau}_1(Z) \coloneqq E[Y - \hat{g}_0(Z) \mid D = 1, Z]$$

$$\hat{\tau}_0(Z) \coloneqq E[\,\hat{g}_1(Z) - Y \mid D = 0, Z\,]$$

- Which one should we use?
- If for some Z most training data received D=1, then model  $\hat{g}_1$  will be a better predictor than  $\hat{g}_0$ ; we should go with  $\hat{\tau}_0$
- If for some Z most training data received D=0, then model  $\hat{g}_0$  will be a better predictor than  $\hat{g}_1$ ; we should go with  $\hat{\tau}_1$

$$\hat{\tau}(Z) = \Pr(D = 1|Z) \,\hat{\tau}_0(Z) + (1 - \Pr(D = 1|Z)) \,\hat{\tau}_1(Z)$$

#### X-Learner Kunzel et al, 2019



# Cross Learner (X-Learner) Meta Algorithm

- ullet Train ML regression  $\widehat{g}_0$  by predicting Y from Z among control samples
- Construct variables  $T_i^1 \coloneqq Y \hat{g}_0(Z)$  for all treated samples
- Train ML regression  $\hat{ au}_1$  by predicting  $T_i^1$  from Z among treated samples
- ullet Train ML regression  $\widehat{g}_1$  by predicting Y from Z among treated samples
- Construct variables  $T_i^0 \coloneqq \hat{g}_1(Z) Y$  for all control samples
- ullet Train ML regression  $\hat{ au}_0$  by predicting  $T_i^0$  from Z among control samples
- ullet Train ML classifier to construct  $\hat{p}(Z)$  predicting probability D=1 given Z
- ullet Train final ML regression model predicting from X the variable

$$\hat{\tau}(Z) = \hat{p}(Z) \hat{\tau}_0(Z) + (1 - \hat{p}(Z)) \hat{\tau}_1(Z)$$

### Residual Learner (R-Learner)

Since we have that:

$$\tau(Z) = E[Y|D = 1, Z] - E[Y|D = 0, Z]$$

• We can write:

$$E[Y|D,Z] = \tau(Z)D + f(Z)$$

• Equivalently:

$$Y = \tau(Z)D + f(Z) + \epsilon, \qquad E[\epsilon|D,Z] = 0$$

- If we further know that  $\tau(Z) = \theta(X)$  (effect only depends on X)  $E[Y|D,Z] = \theta(X)D + f(Z)$
- We can then write:

$$Y - E[Y|Z] = \theta(X) (D - E[D|Z]) + \epsilon$$

# Residual Learner (R-Learner)

- If we know that  $\tau(Z) = \theta(X)$  (effect only depends on X), we can write  $\tilde{Y} = \theta(X) \ \tilde{D} + \epsilon$ ,  $E[\epsilon | D, Z] = 0$
- Equivalently,  $\theta(\cdot)$  is the minimizer of the square loss:

$$E\left[\left(\widetilde{Y}-\theta(X)\widetilde{D}\right)^2\right]$$

- Predict residual outcome  $\tilde{Y}$  from residual treatment  $\tilde{D}$  and X with a model of the form  $\theta(X)\tilde{D}$
- Can also be phrased as a "weighted" square loss

$$E\left[\widetilde{D}^2\left(\widetilde{Y}/\widetilde{D}-\theta(X)\right)^2\right]$$

• Predict  $\widetilde{Y}/\widetilde{D}$  from X with sample weights  $\widetilde{D}^2$ 

# Residual Learner (R-Learner) Meta Algorithm

• Train ML regression to predict Y from Z and calculate residual  $\tilde{Y} \approx Y - E[Y|Z]$  (preferably in cross-fitting manner)

• Train ML regression to predict D from Z and calculate residual  $\widetilde{D} \approx D - E[D|Z]$  (preferably in cross-fitting manner)

• Train ML regression with sample weights, to predict  $\widetilde{Y}/\widetilde{D}$  from X with sample weights  $\widetilde{D}^2$ 

# Residual Learner (R-Learner)

• When  $\theta(X) = \alpha' \phi(X)$  for some known feature map  $\phi$  then this is equivalent to learning heterogeneous effects with interactions

$$E\left[\left(\widetilde{Y}-\alpha'\phi(X)\widetilde{D}\right)^2\right]$$

ullet Equivalent to OLS with outcome  $ilde{Y}$  and regressors  $\phi(X)\widetilde{D}$ 

#### Residual Learner (R-Learner)

- If  $\tau$  does not only depend on X then  $\theta$  is a "projection"
- But it is a weighted one, it is the minimizer of the loss

$$E\left[\left(E\left[\tilde{Y}\mid Z,D\right]-\theta(X)\tilde{D}\right)^{2}\right]=E\left[\left(\tau(Z)\tilde{D}-\theta(X)\tilde{D}\right)^{2}\right]$$

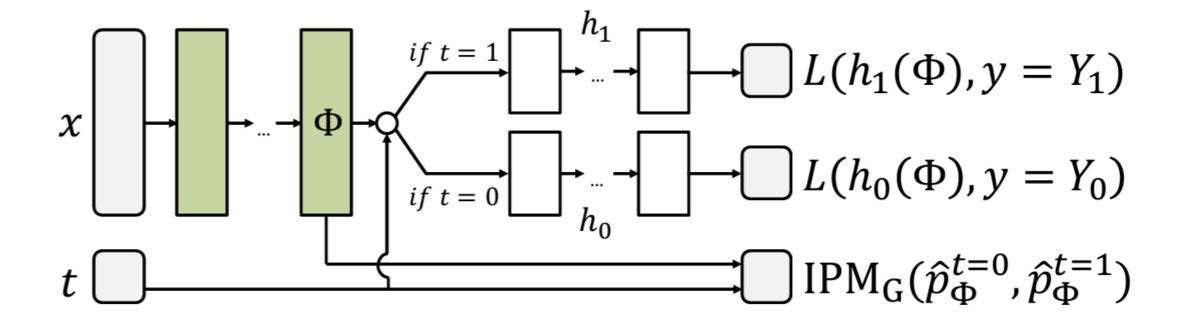
$$=E\left[\left(\tau(Z)-\theta(X)\right)^{2}E\left[\tilde{D}^{2}\mid Z\right]\right]=E\left[\left(\tau(Z)-\theta(X)\right)^{2}Var(D\mid Z)\right]$$

- ullet We put more weight on regions of Z with more randomized treatment
- If some regions of the population were assigned treatments roughly deterministically, then they are ignored in the approximation

#### Comparing Meta-Learners

- S and T-Learners are typically poor performing as they heavily depend on outcome modelling; among them the T-Learner should be preferred
- X-Learner is a better version of S and T as it incorporates propensity knowledge
- DR-Learner and R-Learner, both possess "Neyman orthogonality" properties as they carefully combine outcome and treatment assignment modelling
- The error of the final cate model is not heavily impacted by the errors in the auxiliary models (Orthogonal Statistical Learning)
- DR-Learner estimates un-weighted projection of true CATE on model space, but can be "high-variance" due to inverse propensity
- R-Learner estimates variance weighted projection but is much more stable to extreme propensities as it never divides by propensity.

Neural Network CATE Learners (CFR Net) Shalit et al. 17



# Model Selection and Evaluation

#### Model Selection and Evaluation

- Each of the meta learners is defined based on a loss function.
- We can use loss function for model selection and out-of-sample performance evaluation
- To compare across any CATE learner, we can evaluate based on an "orthogonal loss", which is robust to nuisance estimation
- R-Loss: for a separate sample, calculate residuals  $\tilde{Y}$ ,  $\tilde{D}$  in a cross-fitting manner. For any candidate CATE model  $\theta$  evaluate

$$L(\theta) := E\left[\left(\widetilde{Y} - \theta(X)\widetilde{D}\right)^{2}\right]$$

• DR-Loss: for a separate sample, calculate regression model g (using T-Learner) and propensity model p. For any candidate CATE model  $\theta$  evaluate

$$L(\theta) \coloneqq E\left[\left(Y_{DR}(g, p) - \theta(X)\right)^{2}\right]$$

### Evaluation via Testing Approaches

• If CATE model  $\theta$  was good, then BLP of CATE, when using  $(1, \theta(X))$  as the feature map, should assign a lot of weight on  $\theta(X)$ 

• Run OLS regression predicting  $Y_{DR}(g,p)$  using regressors  $\left(1,\theta(X)\right)$   $E\left[\left(Y_{DR}(g,p)-\beta_0-\beta_1\theta(X)\right)^2\right]$ 

• Construct confidence intervals and test whether  $\beta_1 \neq 0$ ; then  $\theta(X)$  correlates with the true CATE! Ideally  $(\beta_0 = 0, \beta_1 = 1)$ 

#### Validation via GATEs

• For any large enough group G, we can calculate out-of-sample group average effects by simply averaging  $Y_{DR}(g,p)$ 

$$GATE(G) := E[Y(1) - Y(0)|X \in G] = E[Y_{DR}(g,p)|X \in G]$$

• If the CATE model  $\theta$  is accurate, then if we restrict to some group G then the average of  $\theta$  over this group, should match the out-of-sample group average treatment effect

$$E[\theta(X)|X \in G] \approx GATE(G)$$

• We can measure such GATE discrepancies out-of-sample

#### Validation via Calibration

- One natural definition of groups is the "percentile groups of the CATE predictions"
- For the top 25% of the CATE predictions based on the model  $\theta$ , the mean of model predictions, should match the out-of-sample GATE for that group
- Consider a set of quantiles  $q_1, \ldots, q_K$  (e.g. 0, 25, 50, 75)
- Consider the distribution D of  $\theta(X)$  over the training data X
- Let  $G_i$  be the groups defined as  $\{X : \theta(X) \in [q_i \ q_{i+1}] \ quantile \ of \ D\}$  $\tau_i \coloneqq E[\theta(X)|X \in G_i] \approx GATE(G_i) \coloneqq E[Y_{DR}(g,p)|X \in G_i]$
- Calibration score:

CalScore
$$(\theta) := \sum_{i} \Pr(G_i) |\tau_i - GATE(G_i)|$$

• Normalized calibration score:  $1 - \frac{\text{CalScore}(\theta)}{\text{CalScore}(constant \ CATE = E[Y_{DR}(g,p)])}$ 

# CalScore=0.8117 -0.20 -0.25 -0.30 -0.40 -0.45 -0.55 -0.425 -0.400 -0.375 -0.350 -0.325 -0.300 -0.275

# Testing for Heterogeneity

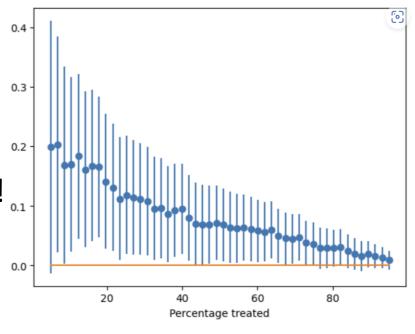
- We can easily construct joint confidence intervals for all the GATEs
- GATEs are the coefficients in the BLP of CATE using group one-hot-encoding as features  $E\left[\left(Y_{DR}(g,p)-\beta'(1\{X\in G_1\},...,1\{X\in G_K\})\right)^2\right]$
- We can use joint confidence intervals for BLP via the DR-Learner
- If there was heterogeneity, then we should have that there are GATEs whose confidence intervals are non-overlapping

#### Stratification Motivated Evaluation

- If we were to "prioritize" into treatment based on  $\theta$  with a target to treat around q-percent of the population then what would be the ATE of the treated group
- Consider the distribution D of  $\theta(X)$  over the training data X
- We can define the group:

$$G_q := \{X : \theta(X) \ge (1 - q) - th \ quantile \ of \ D\}$$
  
$$\tau(q) = E[Y_{DR}(g, p) \mid X \in G_q] - E[Y_{DR}(g, p)]$$

- Ideally, au(q) should be always positive and increasing!  $_{\scriptscriptstyle 0.1}$
- AUTOC pprox the area under the curve au(q)

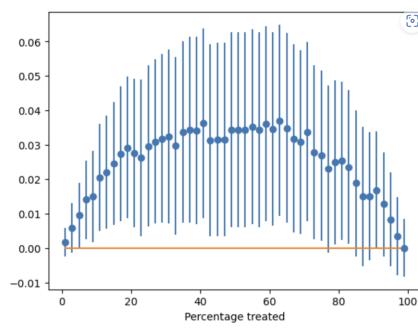


#### Stratification Motivated Evaluation

- If we were to "prioritize" into treatment based on  $\theta$  with a target to treat around q-percent of the population then what would be the policy value we would get over treating q percentage at random
- Consider the distribution D of  $\theta(X)$  over the training data X
- We can define the group:

$$G_q := \{X : \theta(X) \ge (1 - q) - th \ quantile \ of \ D\}$$
  
$$\tau(q) = q \left( E \left[ Y_{DR}(g, p) \mid X \in G_q \right] - E \left[ Y_{DR}(g, p) \right] \right)$$

- Ideally,  $\tau(q)$  should be large positive for some values!
- QINI: the area under the curve au(q)



# Policy Learning

# Candidate Policy

- What if I have a candidate policy  $\pi$  on who to treat
- The average policy effect is of the form:

$$V(\pi) = E[\pi(X)(Y(1) - Y(0))]$$

Under conditional ignorability:

$$V(\pi) = E[\pi(X)(E[Y|D=1,Z] - E[Y|D=0,Z])]$$

- We can also measure performance via the doubly robust outcome  $V(\pi) = E[\pi(X) Y_{DR}(g, p)]$
- Also falls in the Neyman orthogonal moment estimation framework  $E[\pi(X)Y_{DR}(g,p)-\theta]=0$
- We can easily construct confidence intervals

# Policy Optimization

• We can optimize over a space of policies  $\Pi$  on the samples

$$\hat{V}(\pi) = E_n[\pi(X)Y_{DR}(\hat{g}, \hat{p})]$$

• Regret:

$$\max_{\pi \in \Pi} V(\pi) - V(\hat{\pi})$$

- Regret not impacted a lot by errors in  $\hat{g}$  or  $\hat{p}$
- Performance as if true g, p were known (assuming estimation rates are  $n^{-\frac{1}{4}}$

# Non-Parametric Confidence Intervals

#### Generalized Random Forest

- We want to estimate a solution to a conditional moment restriction  $\theta(x) \coloneqq E[m(Z;\theta) \mid X = x]$
- We do so by splitting constructing a tree that at each level optimizes the heterogeneity of the values of the local solution created at the resulting children nodes
- At the end we have many trees each defining a neighborhood structure
- For every candidate x we use the trees to define a set of weights with every training point and we solve the moment equation

$$\sum_{i} w_i(x) m(Z_i; \theta) = 0$$

#### Generalized Random Forest

- If each tree is built in an honest manner (i.e. samples used in the final weighted moment equation are separate from samples used to determine splits)
- If each tree is build in a balanced manner (at least some constant fraction on each side of the split)
- If each tree is built on a sub-sample without replacement, of an appropriate size
- Then the prediction  $\theta(x)$  is asymptotically normal and we can construct confidence intervals via an appropriate bootstrap procedure

#### **GRF for CATE**

We can do this with the residual moment:

$$E[(\widetilde{Y} - \theta(x)\widetilde{D})\widetilde{D} \mid X = x] = 0$$

 (Orthogonal Random Forest) We can also do a similar approach with the doubly robust targets

$$E[Y_{DR}(g,p) - \theta(x) \mid X = x] = 0$$

We can also do this even when X is a subset of Z