MS&E 228: Heterogeneous Treatment Effects

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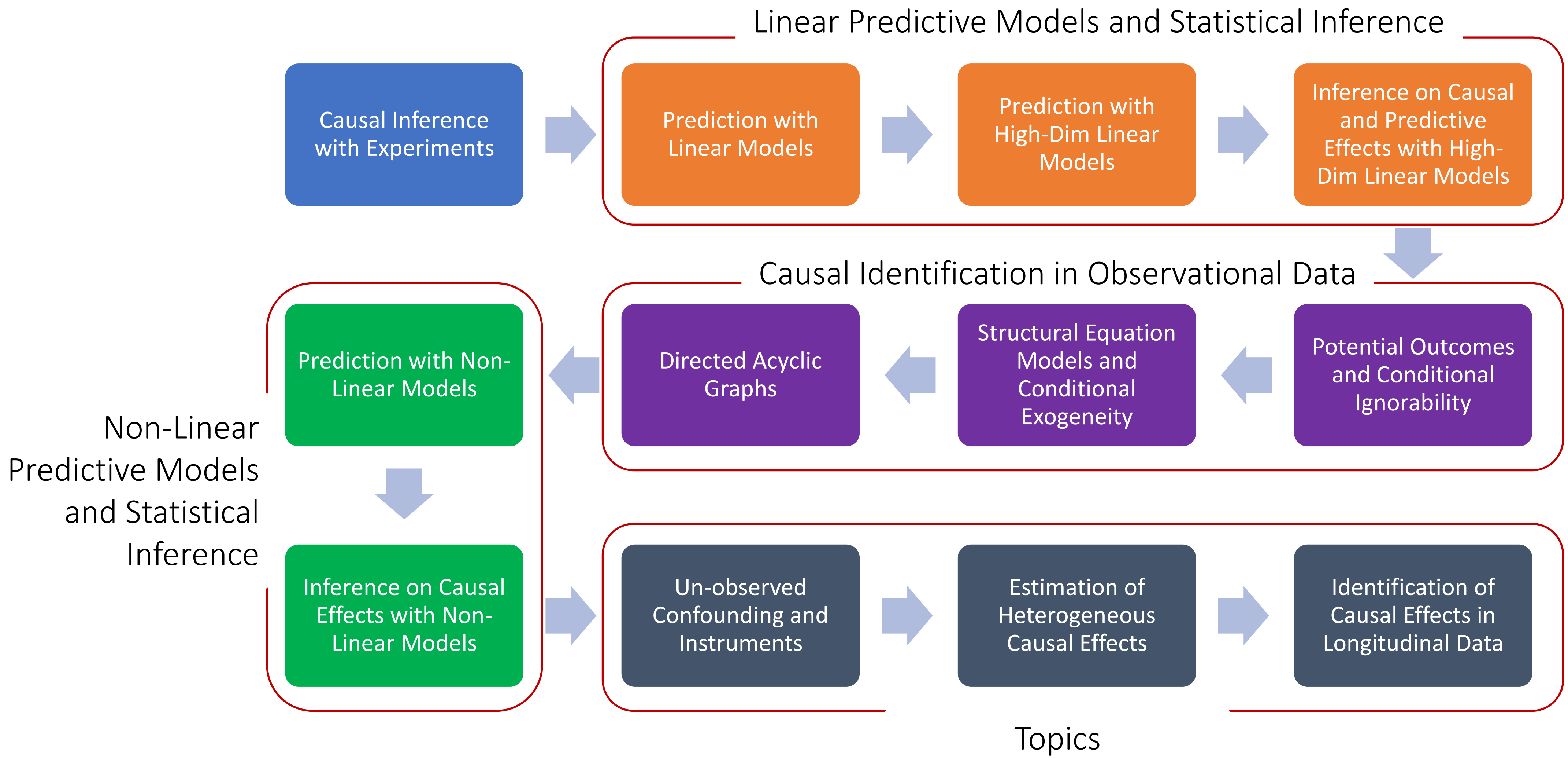
Linear Predictive Models and Statistical Inference
Causal Inference with Experiments
Prediction with Linear Models
Prediction with High-Dim Linear Models
Inference on Causal and Predictive Effects with High-Dim Linear Models
Causal Identification in Observational Data
Potential Outcomes and Conditional Ignorability
Structural Equation Models and Conditional Exogeneity
Directed Acyclic Graphs
Non-Linear Predictive Models and Statistical Inference
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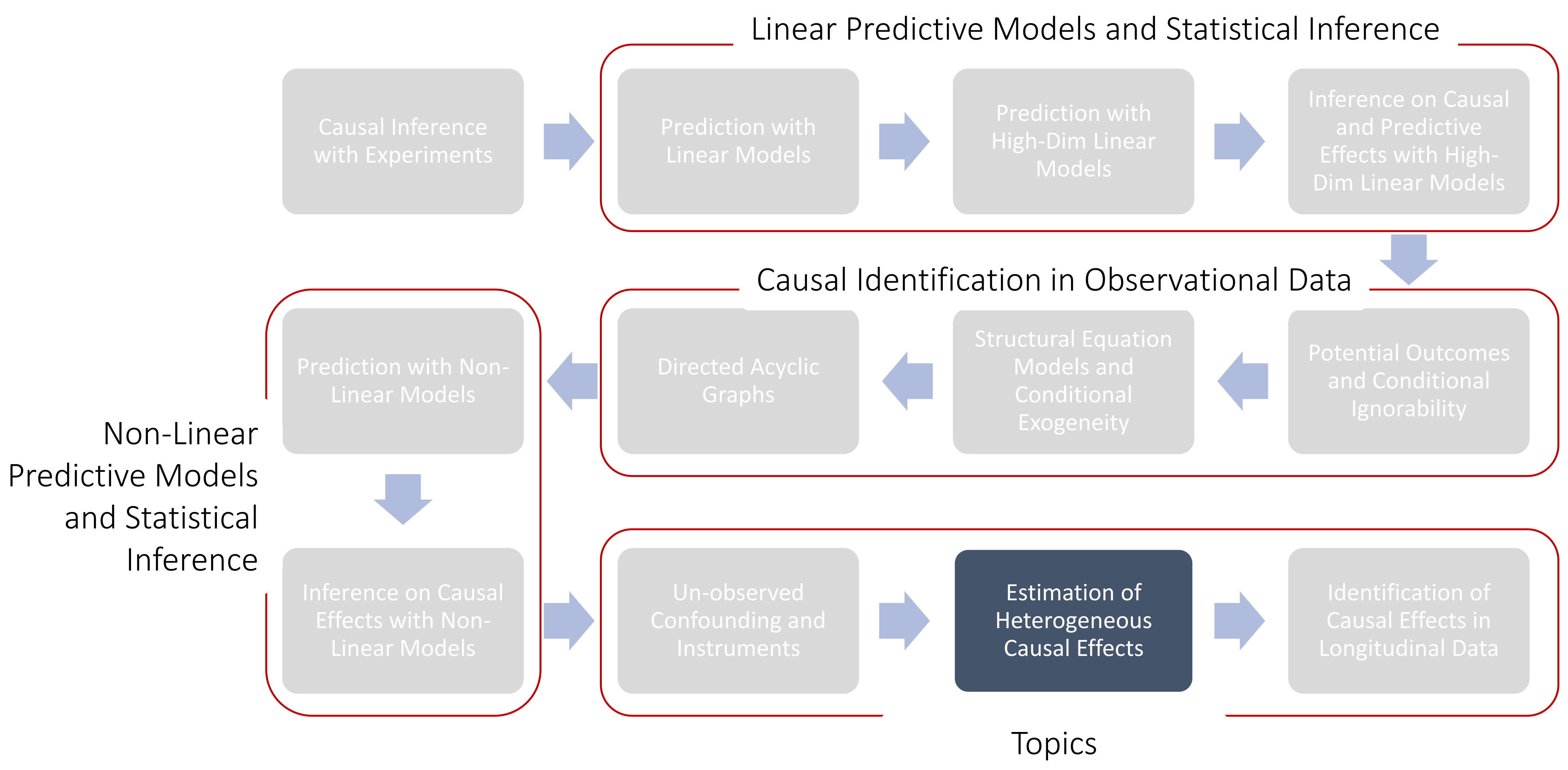
Un-observed Confounding and Instruments
Estimation of Heterogeneous Causal Effects
Identification of Causal Effects in Longitudinal Data
Topics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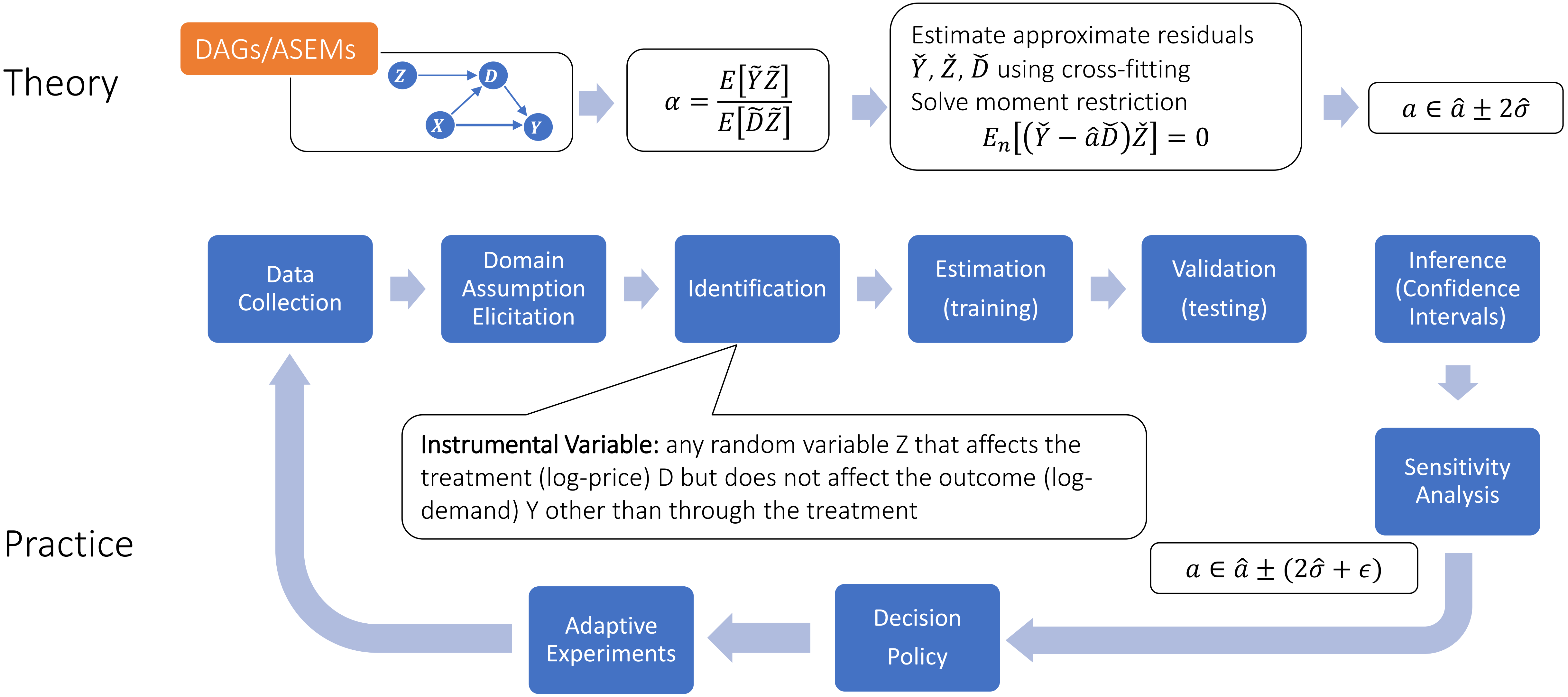
Goals for Today

- Heterogeneous Treatment Effects
- Statement of the problem
- A basic solution

Causal Inference Pipeline



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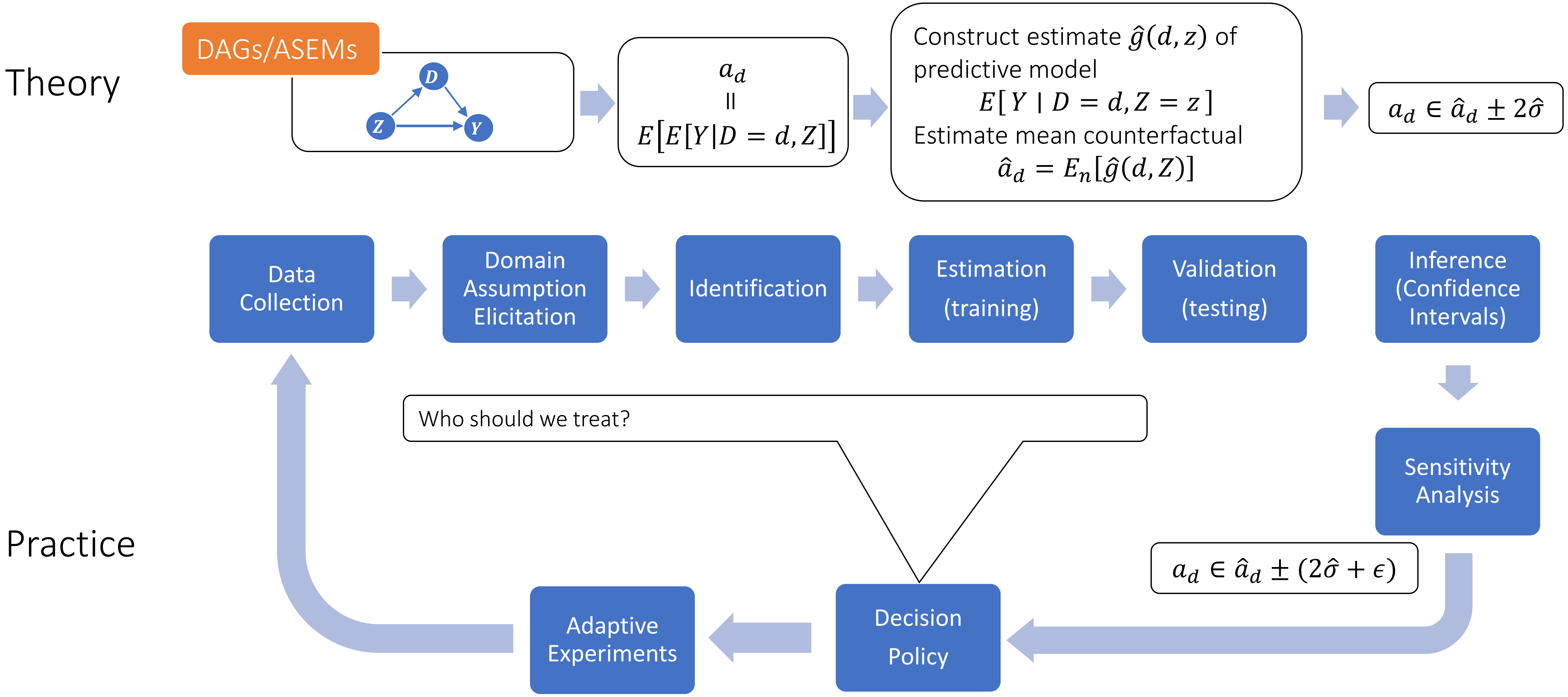

Conditional Average Treatment Effects (CATE)

aka Heterogeneous Treatment Effects

Problem with Average Treatment Effect

- So far, we mostly focused on understanding average treatment effects

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

- This quantity is not informative of who to treat
- At best we can use it to make a uniform decision for the population

$$\text{treat everyone if } \theta > 0 \text{ and don't treat otherwise}$$

- Such uniform policies can lead to severe adverse effects
- Such uniform analyses can lead us to miss on “responder subgroups”

Personalized (Refined) Policies

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

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

- 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 $\mathrm{X} = x$ and decide

$$\text{treat if } \theta(x) > 0 \text{ else don't treat}$$

The intrinsic hardness of CATE

- The CATE quantity is not just a parameter
- It is a whole function…
- Learning such conditional expectation functions is inherently harder than learning parameters
- For instance: we might never have seen in our data other samples with the exact same x
- Such quantities are known as statistically “irregular” quantities
- We have seen such quantities when were solving the best prediction rule $E[Y|X]$

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 CATE model

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

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

Policy Learning

- 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;

Doubly Robust Policy Evaluation

Doubly Robust Policy Learning

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Doubly Robust Policy Evaluation

Doubly Robust Policy Learning

Best Linear Projection of CATE

Identification by Conditioning

- Under conditional ignorability

$$Y(1), Y(0) \perp\!\!\!\perp D \mid Z$$

- CATE can be identified by conditioning

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

- If we want a CATE on some subset of variables X

$$\theta(X) = E[\,\alpha(Z) \mid X\,] = E[\pi(Z) \mid X]$$

Identification with Propensity Scores

- Under conditional ignorability

$$Y(1), Y(0) \perp\!\!\!\perp D \mid Z$$

- CATE can be identified by propensity scores

$$\alpha(Z) \coloneqq E[Y(1) - Y(0)|Z] = E[Y\, H(D,Z)|Z] = \pi(Z)$$

$$H(D,Z) = \frac{D}{\Pr(D=1|Z)} - \frac{1-D}{1-\Pr(D=1|Z)}$$

- If we want a CATE on some subset of variables X

$$\theta(X) = E[\,\alpha(Z) \mid X\,] = E[\pi(Z) \mid X]$$

Doubly Robust Identification

- Under conditional ignorability
$$Y(1), Y(0) \perp\!\!\!\perp D \mid Z$$
- CATE can be identified by combination of conditioning and propensity scores
$$a(Z) \coloneqq E\big[\, g(1, Z) - g(0, Z) + H(D, Z)\,\big(Y - g(D, Z)\big) \mid Z \,\big] = \pi(Z)$$

$$H(D, Z) = \frac{D}{p(Z)} - \frac{1 - D}{1 - p(Z)}$$

$$g(D, Z) \coloneqq E[Y|D, Z], \qquad p(Z) \coloneqq \Pr(D = 1|Z)$$

- If we want a CATE on some subset of variables X
$$\theta(X) = E[\pi(Z) \mid X] = E\big[\, g(1, Z) - g(0, Z) + H(D, Z)\,\big(Y - g(D, Z)\big) \mid X \,\big]$$

From Identification to Estimation

- If we knew the propensity or regression, we have a random variable
$$Y_{DR}(g,p) \coloneqq g(1,Z) - g(0,Z) + H(D,Z)\left(Y - g(D,Z)\right)$$

- Such that what we are looking for is the CEF
$$\theta(X) \coloneqq E[Y_{DR}(g,p)|X]$$

- In the non-linear prediction section, we saw that this is the solution to the Best Prediction rule problem!

Blast from the Past: Best Prediction Rule

- Given n samples $(Z_1, Y_1), \dots, (Z_n, Y_n)$ drawn iid from a distribution D
- Want an estimate $\hat{g}$ that approximates the Best Prediction

$$g \coloneqq \operatorname*{argmin}_{\tilde{g}} E\left[\left(Y\ - \tilde{g}(Z)\right)^2\right]$$

- Best Prediction rule is Conditional Expectation Function (CEF)

$$g(Z) = E[Y|Z]$$

- We want our estimate $\tilde{g}$ to be close to g in RMSE

$$\|\hat{g} - g\| = \sqrt{E_Z\left(\hat{g}(S) - g(Z)\right)^2} \to 0, \qquad \text{as } n \to \infty$$

Blast from the Past: Linear CEF

- If CEF is assumed linear with respect to known engineered features
$$E[\,Y \mid Z\,] = \beta' \psi(Z)$$

- Then the Best Prediction rule (CEF) coincides with the Best Linear Prediction rule (BLP)

- We can use OLS if $\psi(Z)$ is low-dimensional (p≪n) or the multitude of approaches we learned if $\psi(Z)$ is high-dimensional (Lasso, ElasticNet, Ridge, Lava)

From Identification to Estimation

- If we knew the propensity or regression, we have a random variable
$$Y_{DR}(g,p) \coloneqq g(1,Z) - g(0,Z) - H(D,Z)\left(Y - g(D,Z)\right)$$
- Such that what we are looking for is the CEF
$$\theta(X) \coloneqq E[Y_{DR}(g,p)|X]$$
- We can reduce CATE estimation to a Best Prediction rule problem!
$$\theta \coloneqq \underset{g}{\operatorname{argmin}} E\left[\left(Y_{DR}(g,p) - g(X)\right)^2\right]$$
- ML techniques can be used to solve this problem and provide RMSE rates
$$\sqrt{E\left[\left(\theta(X) - \hat{\theta}(X)\right)^2\right]} \approx 0$$

Doubly Robust Learning

[Foster, Syrgkanis, '19 Orthogonal Statistical Learning]

- Split your data in half
  - Train ML model $\hat{g}$ for $g_0(D,Z) \triangleq E[Y|D,Z]$ on the first, predict on the second and calculate regression estimate of each potential outcome

$$\tilde{Y}_i^{(d)} = \hat{g}(d, Z_i)$$

  and vice versa

  - Train ML classification model $\hat{p}_d$ for $p_d(Z) \triangleq Pr[D = d\ |Z]$ on the first, predict on the second, calculate propensity $\hat{p}_{d,i} = \Pr[D = d|Z_i]$ and vice versa
- Calculate doubly robust values:

$$\tilde{Y}_{i,DR}^{(d)} = \tilde{Y}_i^{(d)} + \frac{\left(Y_i - \tilde{Y}_i^{(D_i)}\right) 1\{D_i = d\}}{\hat{p}_{d,i}}$$

- Any ML algorithm to solve the regression:

$$\tilde{Y}_{i,DR}^{(1)} - \tilde{Y}_{i,DR}^{(0)} \quad \sim \quad X$$

Blast from the Past: Best Linear Prediction (BLP) Problem

- The BLP minimizes the MSE

$$\min_{b \in \mathbb{R}^p} E\left[\left(Y - b'\psi(X)\right)^2\right]$$

- Since by the variance decomposition

$$E\left[\left(Y - b'\psi(X)\right)^2\right] = E\left[(Y - E[Y|X])^2\right] + E\left[\left(E[Y|X] - b'\psi(X)\right)^2\right]$$

- First part does not depend on b. The BLP minimizes

$$\min_{b \in \mathbb{R}^p} E\left[\left(E[Y|X] - b'\psi(X)\right)^2\right]$$

- The BLP is the **best linear approximation of the CEF**

From Identification to Estimation

- If we knew the propensity or regression, we have a random variable
$$Y_{DR}(g,p) \coloneqq g(1,Z) - g(0,Z) + H(D,Z)\left(Y - g(D,Z)\right)$$
- Such that what we are looking for is the CEF
$$\theta(X) \coloneqq E[Y_{DR}(g,p)|X]$$
- Estimate best linear approximation to the CATE via the BLP problem:
$$\beta \coloneqq \underset{b}{\operatorname{argmin}}\, E\left[\left(Y_{DR}(g,p) - b'\psi(X)\right)^2\right]$$

$$\theta_{BLP}(X) = \beta'\psi(X)$$

Normal Equations

- Equivalently, the solution to the normal equations

$$E\left[\left(Y_{DR}(g,p) - \beta'\psi(X)\right)\psi(X)\right] = 0$$

- Falls into the moment equation framework with nuisance components
- Nuisance components are g, p and target parameter is β
- Moment is Neyman orthogonal with respect to g, p (why?)
- Local insensitivity (orthogonality) holds even conditional on X

$$\lim_{\epsilon \to 0} \frac{E\left[\, Y_{DR}\left(g + \epsilon\, \nu_g, p + \epsilon\, \nu_p\right) \mid X \,\right] - E[\, Y_{DR}(g,p) \mid X \,]}{\epsilon} = 0$$

Asymptotic Normality

- *For conciseness, define* $\hat{Y} = Y_{DR}(\hat{g}, \hat{p})$ and $\Psi = \psi(X)$

$$E_n\left[\left(\hat{Y} - \hat{\beta}'\Psi\right)\Psi\right] = 0 \Leftrightarrow \hat{\beta} = E_n[\Psi\Psi']^{-1}E_n\left[\Psi\hat{Y}\right]$$

- *Assume* that $E[\Psi\Psi'] \succcurlyeq 0$

- *Assume* $\hat{g}, \hat{p}$ estimated on separate sample (or cross-fitting), are consistent and:

$$\sqrt{n} \cdot \mathrm{RMSE}(\hat{g}) \cdot \mathrm{RMSE}(\hat{p}) \rightarrow_p 0$$

- *Assume* random variables Y, D, Ψ have bounded fourth moments

$$\sqrt{n}(\hat{\beta} - \beta_0) \rightarrow_d N(0, V),$$

Estimate asymptotically normal

$$\hat{V} = E_n[\Psi\Psi']^{-1}E_n\left[\left(\hat{Y} - \hat{\beta}'\Psi\right)^2\Psi\Psi'\right]E_n[\Psi\Psi']^{-1}$$

"Sandwich" estimate of variance
(HC0 in OLS packages)

Asymptotic Linearity

- *For conciseness, define* $\hat{Y} = Y_{DR}(\hat{g}, \hat{p})$, $Y_0 = Y_{DR}(g_0, p_0)$ and $\Psi = \psi(X)$

$$E_n\left[\left(\hat{Y} - \hat{\beta}'\Psi\right)\Psi\right] = 0 \Leftrightarrow \hat{\beta} = E_n[\Psi\Psi']^{-1} E_n\left[\Psi\hat{Y}\right]$$

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- *Assume* $\hat{g}, \hat{p}$ estimated on separate sample (or cross-fitting), are consistent and:

$$\sqrt{n} \cdot \mathrm{RMSE}(\hat{g}) \cdot \mathrm{RMSE}(\hat{p}) \to_p 0$$

- *Assume* random variables Y, D, Ψ have bounded fourth moments

$$\sqrt{n}(\hat{\beta} - \beta_0) \approx \sqrt{n} E_n[\Phi_0],$$

Estimate asymptotically behaves as an average of a random variable Φ_0

$$\Phi_0 = E[\Psi\Psi']^{-1}\Psi\left(Y_0 - \beta_0'\Psi\right),$$

Influence function of estimate $\hat{\beta}$

$$\hat{\Phi} = E_n[\Psi\Psi']^{-1}\Psi\left(\hat{Y} - \hat{\beta}'\Psi\right)$$

Estimate of influence function

Confidence Bands

- Any CATE BLP prediction is also asymptotically linear

$$\sqrt{n}\left(\hat{\theta}_{BLP}(x) - \theta_{BLP}(x)\right) = \sqrt{n} \cdot x'\left(\hat{\beta} - \beta_0\right) \approx \sqrt{n}\, E_n[x'\Phi_0]$$

- Holds jointly for all $x \in X$ (as long as $|X|$ not growing exponential in n)

$$\max_{x \in X} \left| \sqrt{n}\left(\hat{\theta}_{BLP}(x) - \theta_{BLP}(x)\right) - \sqrt{n}\, E_n[x'\Phi_0] \right| \approx 0$$

- High-dimensional CLT theorems also imply that jointly:

$$\left\{\sqrt{n}\left(\hat{\theta}_{BLP}(x) - \theta_{BLP}(x)\right)\right\}_{x \in X} \sim_a N(0, V), \qquad V_{x_1 x_2} = x_1' E[\Phi_0 \Phi_0'] x_2$$

Confidence Bands

- Analogous to inference on many coefficients
- Now the many predictions take the role of the many coefficients
- Confidence band: construct intervals

$$CI(x) := \left[\hat{\theta}(x) \pm c\sqrt{\hat{V}_{xx}/n}\right]$$

- Such that

$$\Pr\left(\forall x\colon\ \theta(x) \in CI(x)\right) \to 1 - \alpha$$

Confidence Bands

- Confidence band: construct intervals

$$CI(x) := \left[\hat{\theta}(x) \pm c\sqrt{\frac{\hat{V}_{xx}}{n}}\right], \qquad \Pr\big(\forall x\colon\ \theta(x) \in CI(x)\big) \to 1 - \alpha$$

- Note that

$$\Pr\big(\forall x\colon\ \theta(x) \in CI(x)\big) = \Pr\left(\max_{x\in X}\left|\frac{\sqrt{n}\left(\theta(x) - \hat{\theta}(x)\right)}{\sqrt{\hat{V}_{xx}}}\right| \le c\right)$$

- By Gaussian approximation, for $D = \mathrm{diag}(V)$

$$\Pr\left(\max_{x\in X}\left|\frac{\sqrt{n}\left(\theta(x) - \hat{\theta}(x)\right)}{\sqrt{\hat{V}_{xx}}}\right| \le c\right) \approx \Pr\left(\left\|N\left(0, D^{-1/2} V D^{-1/2}\right)\right\|_{\infty} \le c\right)$$

By Gaussian approximation, choose c as the $1 - \alpha$ quantile of the maximum entry in a gaussian vector drawn with covariance $D^{-1/2} V D^{-1/2}$

$$\mathrm{D} \coloneqq \mathrm{diag(V)} = \begin{bmatrix} V_{11} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & V_{mm} \end{bmatrix}$$

For 95% confidence band, c slightly larger than 1.96

Computationally Friendlier Version: Multiplier Bootstrap

- By asymptotic linearity we know that:

$$\frac{\sqrt{n}\left(\theta(x) - \hat{\theta}(x)\right)}{\sqrt{\hat{V}_{xx}}} \approx \sqrt{n}\, E_n\left[\frac{x'\Phi_0}{\sqrt{V_{xx}}}\right]$$

- For every sample $i = 1 \dots n$, draw independent Gaussian, i.e. $\epsilon = (\epsilon_1, \dots, \epsilon_n) \sim N(0, I)$. Consider

$$Q_\epsilon(x) \coloneqq \frac{1}{\sqrt{n}} \sum_i \frac{x'\Phi_0}{\sqrt{V_{xx}}} \epsilon_i$$

- **Observation.** The vector of random variables $Q_\epsilon(x_1), \dots, Q_\epsilon\left(x_{|X|}\right)$, over the randomness of ϵ follows asymptotically the desired distribution $N\left(0, D^{-1/2} V D^{-1/2}\right)$
- Approximately the same holds for $\left(\hat{Q}(x_1), \dots, \hat{Q}\left(x_{|X|}\right)\right)$ with $\hat{Q}_\epsilon(x) \coloneqq \frac{1}{\sqrt{n}} \sum_i \frac{x'\hat{\Phi}}{\sqrt{\hat{V}_{xx}}} \epsilon_i$

- **Repeat process $\boldsymbol{B}$ times:** each repetition b draw vector $\epsilon_1^{(b)}, \dots, \epsilon_n^{(b)}$ and calculate maximum over x

$$Z^{(b)} \coloneqq \max_{x \in X} \left|\hat{Q}_{\epsilon^{(b)}}(x)\right|$$

- Set c to be the $1 - \alpha$ quantile of $Z^{(b)}$ over the B repetitions

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Doubly Robust Policy Evaluation

Doubly Robust Policy Learning

Non-Parametric Confidence Intervals

Generalized Random Forest

- We want to estimate a solution $\theta(x)$ to a conditional moment restriction
$$E[\, m(Z;\theta) \mid X = x \,] = 0$$
- 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 child 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 built 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:
$$E\left[\left(\tilde{Y} - \theta(x)\widetilde{D}\right)\widetilde{D} \mid X = x\right] = 0$$

- (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

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Doubly Robust Policy Learning

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)

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

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

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 $g(1,Z) - g(0,Z) + H(D,Z)\big(Y - g(D,X)\big)$ 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 treatment group and predict on the control $\hat{Y}(1) = \hat{g}_1(Z)$

$$Y(1) - Y(0) \mid Z \quad \sim \quad \hat{g}_1(Z) - Y \mid D = 0, Z$$

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 $\hat{Y}(0) = \hat{g}_0(Z)$

$$Y(1) - Y(0) \mid Z \quad \sim \quad Y - \hat{g}_0(Z) \mid D = 1, Z$$

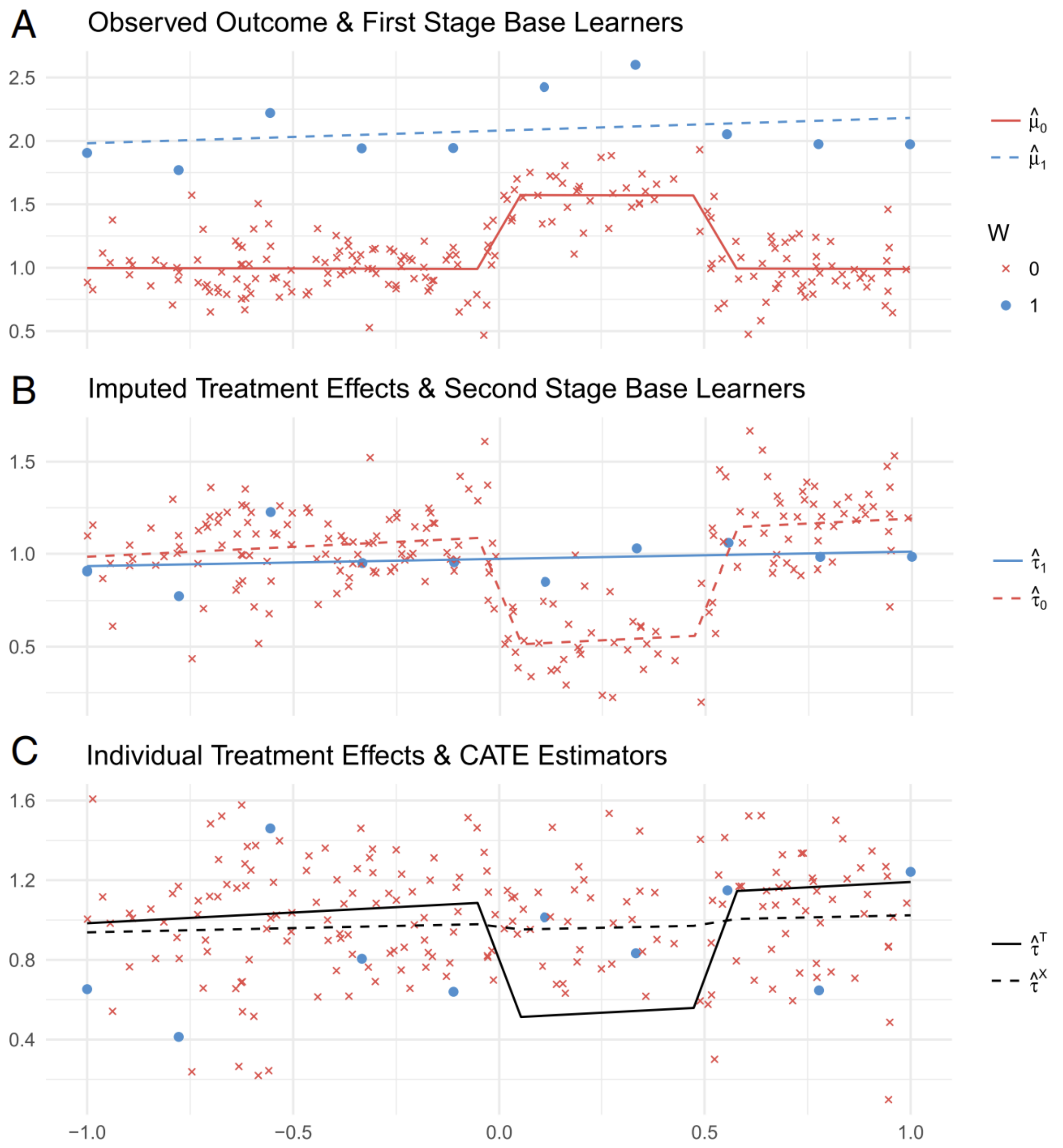
Cross Learner (X-Learner)

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

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

- 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 $\hat{\tau}_1$

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



A
Observed Outcome & First Stage Base Learners
B
Imputed Treatment Effects & Second Stage Base Learners
C
Individual Treatment Effects & CATE Estimators
W
0
1

Cross Learner (X-Learner) Meta Algorithm

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

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

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
$$\tilde{Y} = \theta(X)\,\widetilde{D} + \epsilon, \qquad E[\epsilon\,|D, Z] = 0$$
- Equivalently, $\theta(\cdot)$ is the minimizer of the square loss:
$$E\left[\left(\tilde{Y} - \theta(X)\widetilde{D}\right)^2\right]$$
- Predict residual outcome $\tilde{Y}$ from residual treatment $\widetilde{D}$ and X with a model of the form $\theta(X)\widetilde{D}$
- Can also be phrased as a "weighted" square loss
$$E\left[\widetilde{D}^2\left(\tilde{Y}/\widetilde{D} - \theta(X)\right)^2\right]$$
- Predict $\tilde{Y}/\widetilde{D}$ 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 $\tilde{Y}/\widetilde{D}$ from X with sample weights $\widetilde{D}^2$

Residual Learner (R-Learner)

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

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

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

Residual Learner (R-Learner)

- If τ does not only depend on X then θ is a "projection"
- But it is a weighted one, it is the minimizer of the loss

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

- 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.

Model Selection and Evaluation

Model Selection within Method

- Each of the meta learners is defined based on a loss function
- We can use loss function for model selection within each meta-learning approach
- For each hyper-parameter evaluate the out-of-sample loss in a cross-validation manner and choose the best hyper-parameter for the meta-learning method
- This way we have M CATE models, $\hat{\theta}_1, \dots, \hat{\theta}_M$ from each meta-learning approach

Model Selection Across Methods

- To compare across any CATE learner, we can evaluate based on a "Neyman orthogonal loss", which is robust to nuisance estimation
- **R-Loss:** for a separate sample, calculate residuals $\tilde{Y}, \widetilde{D}$ in a cross-fitting manner. For any candidate CATE model θ evaluate
$$L(\theta) \coloneqq E\left[\left(\tilde{Y} - \theta(X)\widetilde{D}\right)^2\right]$$
- **DR-Loss:** for a separate sample, calculate regression model g (using T-Learner) and propensity model p. For any candidate CATE model θ evaluate
$$L(\theta) \coloneqq E\left[\left(Y_{DR}(g,p) - \theta(X)\right)^2\right]$$
- Given M estimated CATE models $\hat{\theta}_1, \dots, \hat{\theta}_M$, evaluate the loss out-of-sample and choose the best model
$$m^* \coloneqq \operatorname*{argmin}_m L(\theta_m)$$

Ensembling and Stacking

- We can also use these losses to construct stacked ensembles of a set of CATE models $\left(\hat{\theta}_1, \dots, \hat{\theta}_M\right)$:

$$\hat{\theta}_w(X) = \sum_{m=1}^{M} w_m \hat{\theta}_m(X)$$

- **Stacking with R-Loss:** (penalized) linear regression predicting $\tilde{Y}$ with regressors $\theta_1(X)\widetilde{D}, \dots, \theta_M(X)\widetilde{D}$

$$\min_w E_n\left[\left(\tilde{Y} - \sum_{m=1}^{M} w_m \hat{\theta}_m(X)\,\widetilde{D}\right)^2\right] + \lambda \text{Penalty}(w)$$

- **Stacking with DR-Loss:** (penalized) linear regression predicting $Y_{DR}(g, p)$ with regressors $\theta_1(X), \dots, \theta_M(X)$

$$\min_w E_n\left[\left(Y_{DR}(g, p) - \sum_{m=1}^{M} w_m \hat{\theta}_m(X)\right)^2\right] + \lambda \text{Penalty}(w)$$

Evaluation via Testing Approaches

- If CATE model $\hat{\theta}$ was good, then out-of-sample BLP of CATE, when using $\left(1, \hat{\theta}(X)\right)$ as feature map, should assign a lot of weight on $\hat{\theta}(X)$
- Run OLS regression predicting $Y_{DR}(g, p)$ using regressors $\left(1, \hat{\theta}(X)\right)$

$$E\left[\left(Y_{DR}(g, p) - \beta_0 - \beta_1 \hat{\theta}(X)\right)^2\right]$$

- Construct confidence intervals and test whether $\beta_1 \neq 0$; then $\theta(X)$ correlates with the true CATE! Ideally $(\beta_0 = 0, \beta_1 = 1)$
- The parameter β_1 is identifying the quantity (in the population limit):

$$\beta_1 := \frac{Cov\left(Y(1) - Y(0), \hat{\theta}(X)\right)}{Var\left(\hat{\theta}(X)\right)}$$

Validation via GATEs

- For any large enough group G, we can calculate out-of-sample group average effects by simply averaging $Y_{DR}(g, p)$
$$GATE(G) \coloneqq E[Y(1) - Y(0) | X \in G] = E[Y_{DR}(g, p) | X \in G]$$

- If the CATE model $\hat{\theta}$ is accurate, then if we restrict to some group G then the average of $\hat{\theta}$ over this group, should match the out-of-sample group average treatment effect
$$E\left[\hat{\theta}(X) \middle| X \in G\right] \approx GATE(G)$$

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

Validation via Calibration

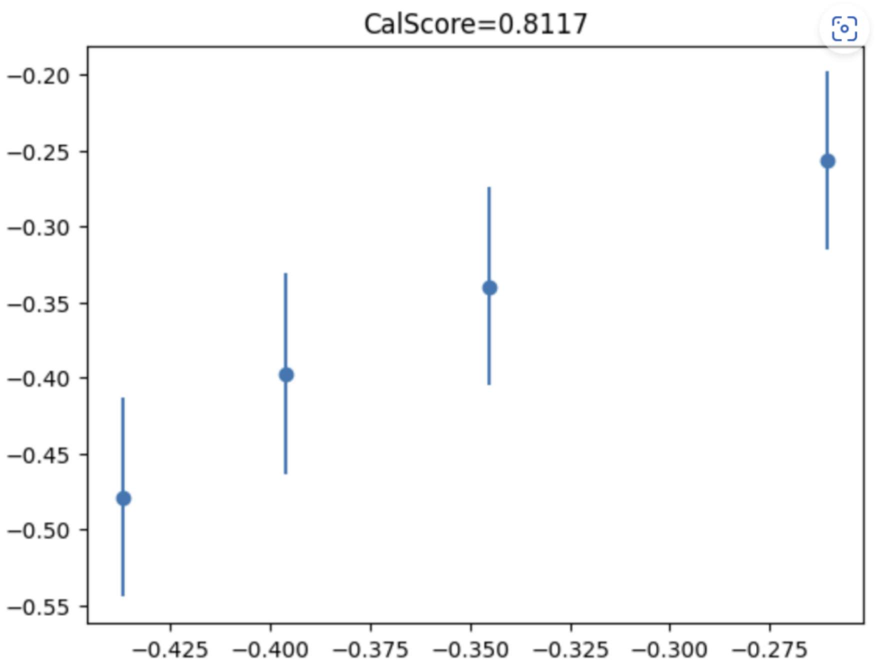
- One natural definition of groups is the "percentile groups of the CATE predictions"
- For the top 25% of the CATE predictions based on the model θ, the mean of model predictions, should match the out-of-sample GATE for that group
- Consider a set of quantiles $q_1, .., q_K$ (e.g. 0, 25, 50, 75)
- Consider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

$$\tau_i \coloneqq E\left[\hat{\theta}(X) \middle| X \in G_i\right] \approx GATE(G_i) \coloneqq E[Y_{DR}(g, p) | X \in G_i]$$

- Calibration score:

$$\mathrm{CalScore}(\theta) \coloneqq \sum_i \Pr(G_i) \cdot |\tau_i - GATE(G_i)|$$

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



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

$$E\left[\left(Y_{DR}(g,p) - \beta'(1\{X \in G_1\}, \dots, 1\{X \in G_K\})\right)^2\right]$$

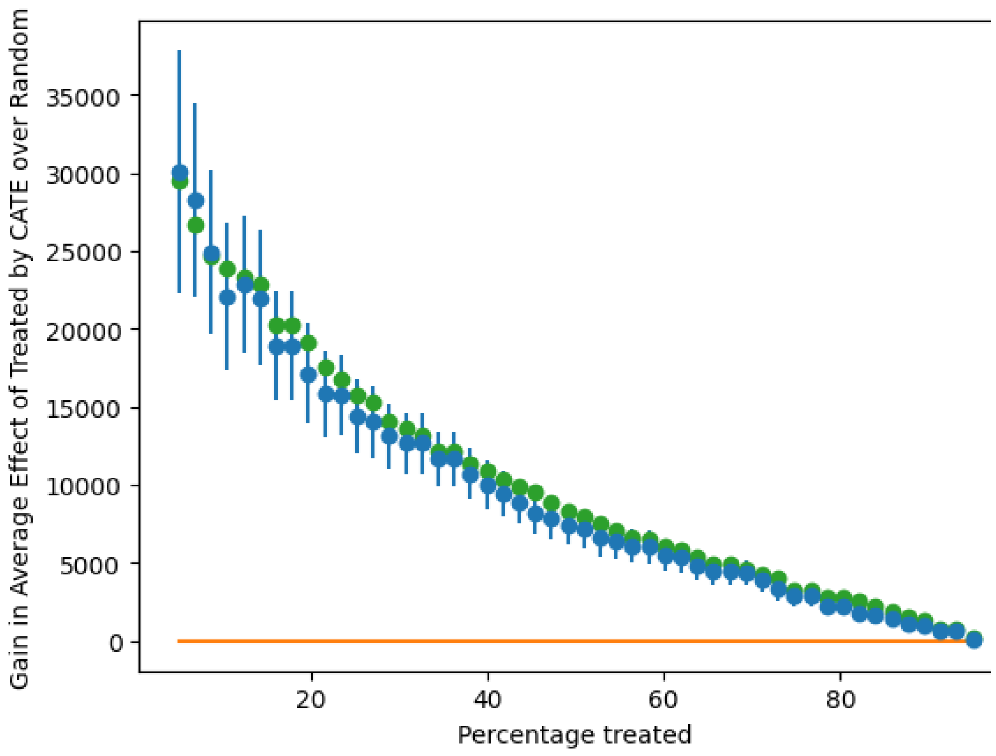
- We can use joint confidence intervals for BLP via the DR-Learner
- If there was heterogeneity, then we should have that there are GATEs whose confidence intervals are non-overlapping

Stratification Motivated Evaluation

- If we were to “prioritize” into treatment based on $\hat{\theta}$ with a target to treat around q-percent of population then what would be the GATE of the treated group
- Consider distribution D_n of $\theta(X)$ over training data X
- We can define the groups:

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

- Ideally, $\tau(q)$ should be always positive and increasing!
- AUTOC $\approx$ the area under the curve $\tau(q)$



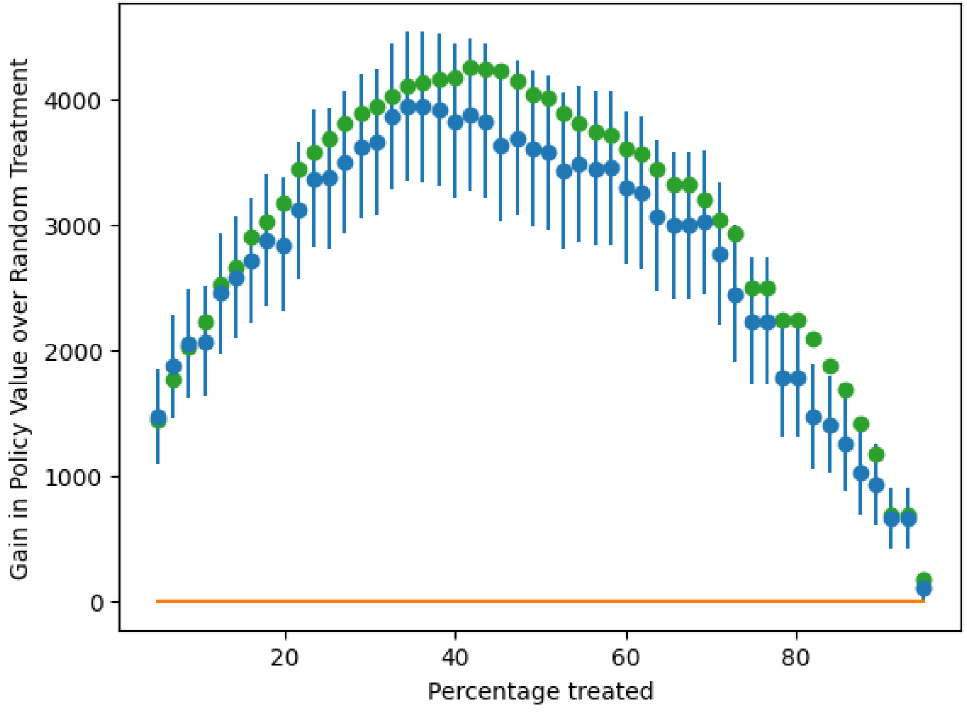
Stratification Motivated Evaluation

- If we were "prioritize" into treatment based on $\hat{\theta}$ 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 distribution D_n of $\hat{\theta}(X)$ over the training data X
- We can define the group:

$$G_q \coloneqq \{X: \hat{\theta}(X) \geq (1-q) - th\ quantile\ of\ D_n\}$$

$$\tau_Q(q) = \Pr(X \in G_q)\ (E[\,Y_{DR}(g,p) \mid X \in G_q\,] - E[Y_{DR}(g,p)])$$

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



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

Linear Doubly Robust Learner

- 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 CATE model

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

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

Policy Learning

- 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;

Doubly Robust Policy Evaluation

Doubly Robust Policy Learning

Policy Learning

Candidate Policy

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

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

- 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 Π 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 (assuming estimation rates of $n^{-\frac{1}{4}}$)
- Maximizing $V(\pi)$ can be viewed as sample-weighted classification, with labels $\mathbf{sign}\big(Y_{DR}(g, p)\big)$ and sample weights $|Y_{DR}(g, p)|$
- Any classification method can be deployed