

# **Fisher-Schultz Lecture: Generic machine learning inference on heterogeneous treatment effects in randomized experiments, with an application to immunization in India**

**Victor Chernozhukov et al. (2025), Econometrica (forthcoming).**

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# Introduction

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# Motivation

- When conducting RCT (Randomized Controlled Trials), researchers and policy makers are often curious about not only ATE but also HTE (Heterogeneous Treatment Effects).
- In such cases, ML methods are good for estimating CATE but inconsistent in most cases especially high-dimension ( $d > \log N$ )
- Also, we have a difficulty of getting uniformly valid inference.
- Lasso-based methods are not a magic bullet in that regularization bias and untestable assumption occurs.
- Consider the conditional unconfoundedness setting such that  $D \perp\!\!\!\perp (Y(1), Y(0)) | Z$  and the propensity score  $p(Z) = P[D = 1 | Z] \in (0, 1)$  is known.

## Proposed estimator

- Let  $(M, A)$  denote a random partition of  $\{1, \dots, N\}$ .
- Stage 1 : From the auxiliary sample  $A$ , we obtain ML estimators of BCA and CATE  $z \mapsto B(z)$  and  $z \mapsto S(z)$ .
  - These estimators are (of course) biased and noisy. (but it is okay !)
- Stage 2 : From the main sample  $M$ , we focus on the **feature** of CATE.
  - Best Linear Predictor (BLP) of the CATE
  - Sorted Group Average Treatment Effects (GATES) : average of CATE in group
  - Classification Analysis (CLAN) : compare the most and least affected group

## **Main identification results and estimation strategies**

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## BLP (Best Linear Predictor)

- Firstly, we obtain the estimator  $S(Z)$  for CATE  $s_0(Z)$  by some ML method using the auxiliary samples  $\mathcal{A}$ .
- BLP is defined as the projection of  $s_0(Z)$  on the linear span of 1 and  $S(Z)$  in  $L^2(P)$ .

$$\text{BLP}[s_0(Z)|S(Z)] = \arg \min_{f(Z) \in \text{Span}(1, S(Z))} \mathbb{E}[(s_0(Z) - f(Z))^2]$$

- This equals to the solution of  $\arg \min_{b_1, b_2} \mathbb{E}[(s_0(Z) - b_1 - b_2 S(Z))^2]$ .

$$\rightarrow \beta_1 = \mathbb{E}[s_0(Z)], \beta_2 = \frac{\text{Cov}(s_0(Z), S(Z))}{\text{Var}(S(Z))}$$

## First strategy : Weighted Residual BLP

- Consider the regression model with the moment condition as follows.

$$Y = \alpha' X_1 + \beta_1(D - p(Z)) + \beta_2(D - p(Z))(S(Z) - \mathbb{E}[S(Z)]) + \epsilon, \mathbb{E}[w(Z)\epsilon X] = 0$$

$$\text{where } w(Z) = \frac{1}{p(Z)(1 - p(Z))}, X = (X_1, X_2),$$

$$X_1 = (1, B(Z)), X_2 = (D - p(Z), (D - p(Z))(S(Z) - \mathbb{E}[S(Z)]))).$$

### Theorem 1

- Consider  $z \mapsto S(z)$  and  $z \mapsto B(z)$  as fixed maps. (known function)
- Assume that  $Y$  and  $X$  have finite second moments,  $\mathbb{E}[X X']$  is full rank, and  $\text{Var}(S(Z)) > 0$ .
- Then,  $(\beta_1, \beta_2)' = \arg \min_{b_1, b_2} \mathbb{E}[(s_0(Z) - b_1 - b_2 S(Z))^2]$  (Identified)

## Second strategy : Horvitz-Thompson BLP

- Horvitz-Thompson transformed response  $YH$  such that  $H = \frac{D - p(Z)}{p(Z)(1 - p(Z))}$  provides an unbiased signal about CATE :  $\mathbb{E}[YH|Z] = s_0(Z)$

$$YH = \mu' X_1 H + \beta_1 + \beta_2(S(Z) - \mathbb{E}[S(Z)]) + \epsilon, \quad \mathbb{E}[\epsilon\tilde{X}] = 0$$

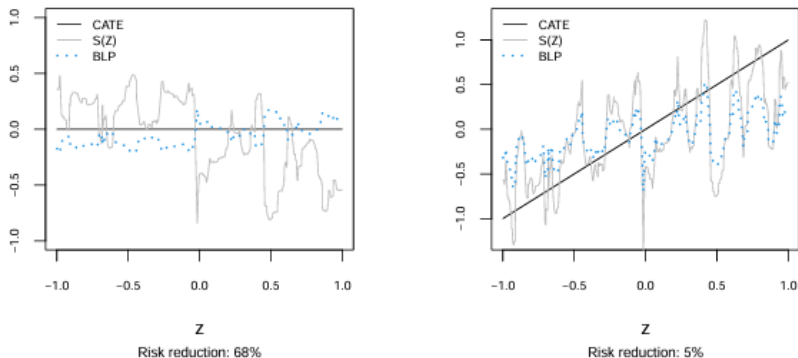
$$\text{where } X_1 = (1, B(Z), p(Z)S(Z))' \quad \tilde{X} = (X_1' H, 1, S(Z) - \mathbb{E}[S(Z)])$$

### Theorem 2

- Consider  $z \mapsto S(z)$  and  $z \mapsto B(z)$  as fixed maps. (known function)
- Assume that  $Y$  has finite second moments,  $\mathbb{E}[\tilde{X}\tilde{X}']$  is finite and full rank, and  $\text{Var}(S(Z)) > 0$ .
- Then,  $(\beta_1, \beta_2)' = \arg \min_{b_1, b_2} \mathbb{E}[(s_0(Z) - b_1 - b_2 S(Z))^2]$  (Identified)



FIGURE 1. BLP Using ML Proxy vs the ML Proxy



NOTES: The CATE is plotted with the solid black line; the proxy predictor  $S(Z)$ , produced by Random Forest, is plotted with the solid grey (light) line; and the BLP is plotted with the dotted blue line. The left panel corresponds to the no heterogeneity example,  $s_0(z) = 0$  and the right panel to the strong heterogeneity example,  $s_0(z) = z$ . In both panels, the BLP is less noisy than the ML proxy reducing the RMSE by 68% and 5%.

## GATES (sorted Group Average Treatment Effects)

- Firstly, we build the groups by the estimated value  $S(Z)$  of  $s_0(Z)$ .

$$G_k = \{S(Z) \in I_k\}, k = 1, \dots, K, I_k = [l_{k-1}, l_k) : \text{disjoint}$$

- The estimand "GATES" is defined as  $\mathbb{E}[s_0(Z)|G_k]$  for  $k = 1, \dots, K$ .
  - WR GATES

$$Y = \alpha' X_1 + \sum_{k=1}^K \gamma_k (D - p(Z)) \mathbf{1}_{G_k} + \nu, \mathbb{E}[w(Z) \nu W] = 0$$

$$\text{where } W = (X_1, W_2')', W_2 = \{(D - p(Z)) \mathbf{1}_{G_k}\}_{k=1}^K.$$

- HT GATES

$$YH = \mu_0' X_1 H + \sum_{k=1}^K \gamma_k \mathbf{1}_{G_k} + \nu, \mathbb{E}[\nu \tilde{W}] = 0$$

$$\text{where } \tilde{W} = (X_1' H, \tilde{W}_2')', \tilde{W}_2 = \{\mathbf{1}_{G_k}\}_{k=1}^K$$

## Theorem 3

- Consider  $z \mapsto S(z)$  and  $z \mapsto B(z)$  as fixed maps. (known function)
- Assume that  $Y$  has finite second moments and both  $\mathbb{E}[WW']$  and  $\mathbb{E}[\tilde{W}\tilde{W}']$  are finite and full rank.
- Then,  $\gamma = \{\gamma_k\}_{k=1}^K$  defined in two different ways are equivalent and identified.

$$\gamma_k = \mathbb{E}[s_0(Z)|G_k]$$

## CLAN (Classification Analysis)

- When BLP and GATES reveal substantial heterogeneity, it is interesting to know **the properties of the subpopulations** that are most and least affected.
  - We focus on the "least affected group"  $G_1$  and "most affected group"  $G_K$ .
- Let  $g(Y, Z)$  be a vector of characteristics of an observational unit. The estimands are

$$\delta_1 = \mathbb{E}[g(Y, Z)|G_1] \quad \text{and} \quad \delta_K = \mathbb{E}[g(Y, Z)|G_K]$$

- These parameters are identified with no assumption because they are just average of observed variables.
- We compare  $\delta_1$  and  $\delta_K$  to detect (single out) the covariates which causes the heterogeneity.
  - We can extend the comparison of not only averages but also variances or distributions.

## **”Variational” estimation and inference methods**

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- Let  $\theta$  denote a generic target parameter such as BLP  $\beta_2$  or GATE  $\gamma_k$ .
- There are two principal sources of sampling uncertainty.
  - **Estimation uncertainty** regarding the parameter  $\theta$ , conditional on the data subpopulations
  - Uncertainty or "variation" **induced by the data splitting**
- Actually, estimation uncertainty is a standard topic, so, as usual, we can solve this problem by the **Gaussian approximation** to construct a confidence interval.
- On the other hands, data-splitting uncertainty is a novel topic, which is solved by taking a **median** of any estimators in permuated splitting.

## Estimation uncertainty in single split

- Consider a sample split  $\{(a, m)\}$  of  $\{1, \dots, N\}$  with  $|a| = N - n, |m| = n$ .
- All estimators  $\theta_a$  satisfies the sufficient conditions for being approximately Gaussian, conditionally on  $Data_a$ .

$$P\left(\frac{\hat{\theta}_a - \theta_a}{\hat{\sigma}_a} < z | Data_a\right) \rightarrow \Phi(z) \text{ for } z \in \mathbb{R}, \text{ as } N \text{ and } n \rightarrow \infty$$

- Therefore, the confidence interval represents

$$[L_a, U_a] = [\hat{\theta}_a \pm \Phi^{-1}(1 - \frac{\alpha}{2})\hat{\sigma}_a]$$

- We have straightforward inference conditional on a single data split.

## Splitting uncertainty in multiple splits

- For each data split  $\{(a, m)\}$  such that  $a \in \mathcal{A}$ , we obtain estimators  $\{\hat{\theta}_a | a \in \mathcal{A}\}$ .
  - Then, we take the median of it :  $\hat{\theta} = M[\hat{\theta}_a | Data]$
  - Also, the  $\beta$ -quantile confidence interval is

$$[L, U] \text{ where } L = Q_\beta(L_a | Data), U = Q_{1-\beta}(U_a | Data)$$

- Median and  $\beta$ -quantile achieves the **concentration** property.

$$\mathbb{E}[|\hat{\theta} - \theta_0|] \leq \mathbb{E}[|\hat{\theta}_a - \theta_0|] \text{ for any } \hat{\theta}_a$$

$$\max\{\mathbb{E}[|U - \theta_0|], \mathbb{E}[|L - \theta_0|]\} \leq \max\{\mathbb{E}[|U_a - \theta_0|], \mathbb{E}[|L_a - \theta_0|]\} \text{ for any } U_a, L_a$$

$$|U - L| \leq \sup_{a \in \mathcal{A}} |U_a - L_a|$$

- By taking the median or quantile, we have a kind of robustness.



# **Causal machines that learn CATE better**

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# Causal learners for Stage 1

- In Stage 1, using the auxiliary sample  $A$ , we estimate
    - BCA (Baseline Conditional Average) :  $b_0(Z) = \mathbb{E}[Y(0)|Z]$
    - CATE (Conditional Average Treatment Effect) :  $s_0(Z) = \mathbb{E}[Y(1) - Y(0)|Z]$
- solve **either** of Weighted Residual (WR) learner or Horvitz-Thompson (HT) learner.

$$(B, S) \in \arg \min_{b \in \mathcal{B}, s \in \mathcal{S}} \sum_{i \in A} \frac{1}{p(Z_i)(1 - p(Z_i))} \{Y_i - b(Z_i) - (D_i - p(Z_i))s(Z_i)\}^2$$

$$(B, S) \in \arg \min_{b \in \mathcal{B}, s \in \mathcal{S}} \sum_{i \in A} \left\{ \frac{D_i - p(Z_i)}{p(Z_i)(1 - p(Z_i))} (Y_i - b(Z_i)) - s(Z_i) \right\}^2$$

where  $\mathcal{B}$  and  $\mathcal{S}$  are functional parameter spaces

- 以後は簡単のため,  $w(Z) = \frac{1}{p(Z)(1 - p(Z))}$ ,  $H = \frac{D - p(Z)}{p(Z)(1 - p(Z))}$  と表記する.

# Oracle properties of the population objective functions

## Theorem 4

- Suppose  $Y, b(Z), s(Z), w(Z) \in L^2$  (2 乗可積分).
- Then, the expectation of the loss functions can be decomposed

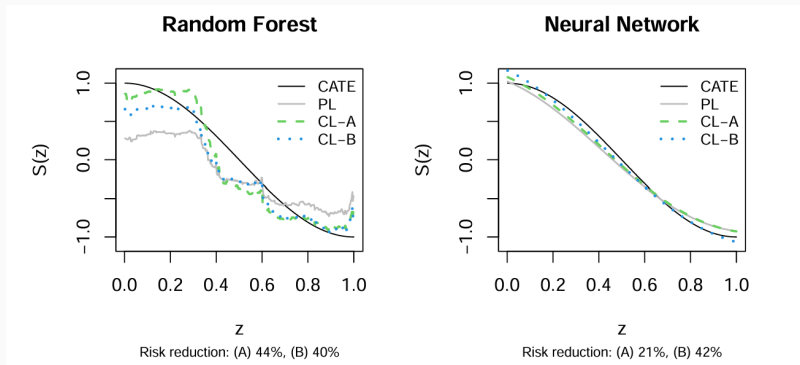
$$\mathbb{E}[w(Z)\{Y - b(Z) - (D - p(Z))s(Z)\}^2] = \mathbb{E}[(s_0(Z) - s(Z))^2] + C_{ib}$$

$$\mathbb{E}[(H(Y - b(Z) - s(Z)))^2] = \mathbb{E}[(s_0(Z) - s(Z))^2] + C_{2b}$$

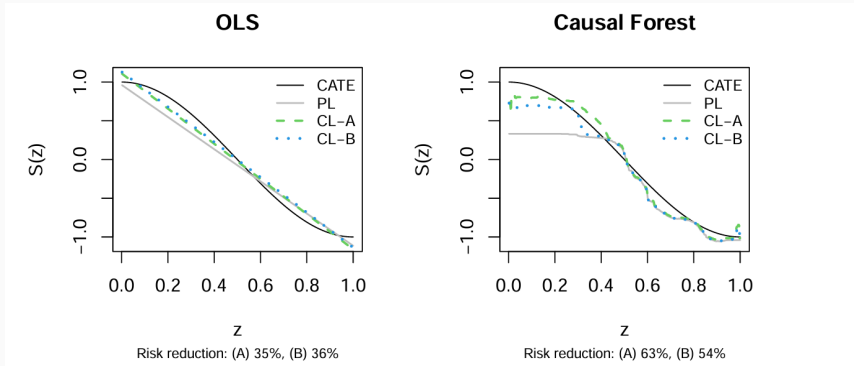
where

$$C_{1b} = \mathbb{E}[w(Z)(\tilde{b}_0(Z) - b(Z))^2] + C_1, C_{1b} = \mathbb{E}[w(Z)(\bar{b}_0(Z) - b(Z))^2] + C_2$$

- This theorem shows that the minimizers provide the best approximation for  $s_0(Z)$  in the sense of mean-squared error in the class  $\mathcal{S}$ .
- Moreover, this occurs even though we do not know  $s_0(Z)$ . (oracle!)



- We compare the CATE learners derived from
  - the standard predictive Random Forest (RF) and Neural Network (NN)
  - Causal Learners (CL) from RF and NN that solve the objective function
- We find that the causal learners (CL) are better approximating the CATE function.



- We can improve the standard predictive OLS by the causal OLS that solves the objective function.
- Also, improve the causal forest by a causal boosting step that solves the objective function.

## Implementation Details

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## Inference algorithm

1. Split the sample into the main sample  $M$  and the auxiliary sample  $A$ .
2. Using  $A$ , train each (optional) ML method and output prediction  $B$  (BCA) and  $S$  (CATE) for  $M$ .
3. Estimate BLP, GATES and CLAN using  $M$ .
4. If the winning ML methods were not chosen, we chose the best-of-fit in median-aggregated estimator  $\hat{\theta}$ . (e.g. cross-validation)
5. Compute and report quantile-aggregated point-estimate, p-values, and confidence intervals.

## **Final marks**

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- We focus the estimation of HTE, which is usually biased and inconsistent.
- Thus, we use ML method for proxying CATE, then, feature just best linear predictor, which is easy to interpret.
- This agnostic approach enables us to be valid in high-dimension, not to make strong assumption, and to avoid over-fitting.
- For sample splitting, we take a median for robustness.

## References

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## References

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