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

Motivation

- When conducting RCT (Randomized Controlled Trails), reseachers 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 $\{1, ..., N\}$.
- Stage 1 : From the auxilirary samlple 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 Preditor (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

BLP (Best Linear Predictor)

- Firstly, we obtain the estimator $S(Z)$ for CATE $s_0(Z)$ by some ML method using the auxilirary 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 $\arg\min_{b_1, b_2} \mathbb{E}[(s_0(Z) - b_1 - b_2 S(Z))^2]$.

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

First strategy : Weighted Residual BLP

- Consider the regresson 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, $\mathbb{E}[XX']$ 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 TH such that $H = \dfrac{D - p(Z)}{p(Z)(1 - p(Z))}$ provides an unbiased signal about CATE : $\mathbb{E}[YH|Z] = s_0(Z)$

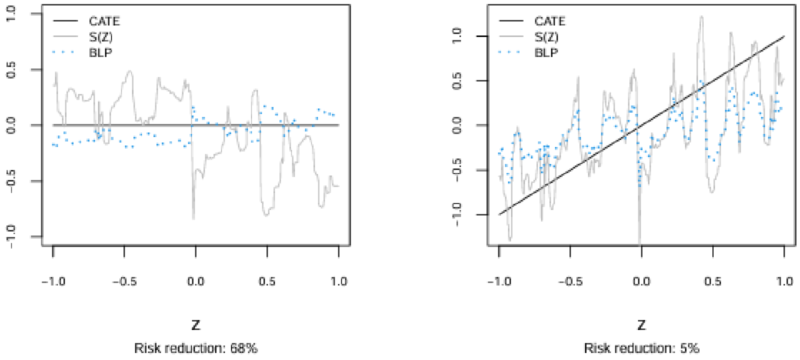
$$YH = \mu' X_1 H + \beta_1 + \beta_2(S(Z) - \mathbb{E}[S(Z)]) + \epsilon, \ \mathbb{E}[\epsilon \tilde{X}] = 0$$

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

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 $s_0(Z)$.

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

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

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

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

Identification of GATES

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 δ_1 and δ_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

Uncertainty

- Let θ denote a generic target parameter such as BLP β_2 or GATE γ_k.
- There are two principal sources of sampling uncertainty.
  - Estimation uncertainty regarding the parameter θ, 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 $\{1, ..., N\}$ with $|a| = N - n, |m| = n$.
- All estimators θ_a satisfies the sufficient conditions for being approxmately Gaussian, conditionally on $Data_a$.

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

- 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 sigle 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 β-quantile confidence interval is

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

- Median and β-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

Causal learners for Stage 1

- In Stage 1, using the auxilirary sample A, we estimate
  - BCA (Baseline Conditional Average) : $b_0(Z) = \mathbb{E}[Y(0)|Z]$
  - CATE (Conditional Average Treatment Effect) : $s_0(Z) = \mathbb{E}[Y(1) - Y(0)|Z]$

$\rightarrow$ [1]solve either of Weighted Residual (WR) learner or Horvitz-Thompson (HT) learner.

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

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

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

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

Oracle properties of the population objective functions

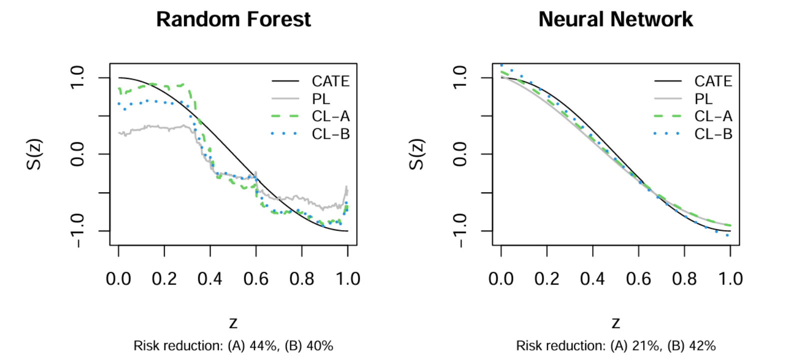
Theorem 4

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

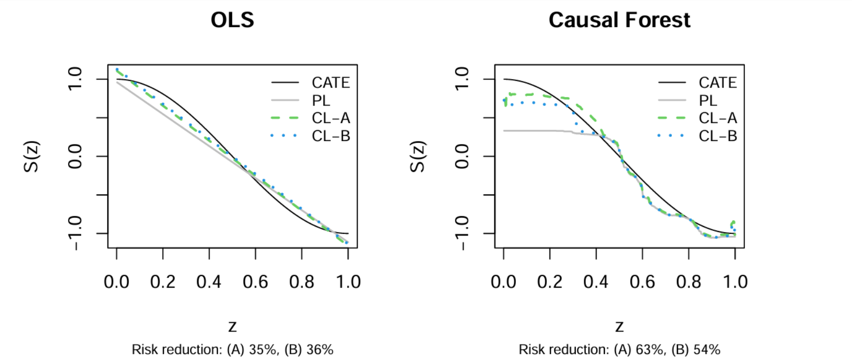
$$\mathbb{E}[w(Z)\{Y - b(Z) - (D - p(Z))s(Z)\}^2] = \mathbb{E}[(s_0(Z) - s(Z))^2] + C_{ib}$$
$$\mathbb{E}[(H(Y - b(Z) - s(Z)))^2] = \mathbb{E}[(s_0(Z) - s(Z))^2] + C_{2b}$$

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 approxmation 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 preditive 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 taht solves the objective function.
- Also, improve the causal forest by a causal boosting step that solves the objective function.

Implementation Details

Inference algorithm

1. Split the sample into the main sample M and the auxilirary 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-varidation)
5. Compute and report quantile-aggregated point-estimate, p-values, and confidence intervals.

Final marks

Summary

- 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.

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