Experimental Evaluation of Individualized Treatment Rules

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Econometrics Seminar
University of California, Irvine
June 7, 2021

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Overview

- Individualized treatment rules (ITRs)
  - designed to increase efficiency of policies or treatments
  - personalized medicine, micro-targeting in business/politics
- Existing literature:
  1. development of optimal ITRs
  2. estimation of heterogeneous treatment effects
  3. extensive use of machine learning (ML) algorithms
- Goal: use a randomized experiment to *evaluate generic ITRs*
- Avoid assuming the "nice properties" of ML algorithms
  1. Neyman's repeated sampling framework
     - randomized treatment assignment, random sampling
     - no modeling assumption or asymptotic approximation
     - extend analysis to cross-validation regime
  2. Evaluation measures
     - shortcomings of existing metrics
     - incorporating a budget constraint
     - overall evaluation metric for general ITRs
  3. Extension to estimation of heterogeneous effects

Evaluation without a Budget Constraint

- Setup
  - Binary treatment: $T_i \in \{0, 1\}$
  - Pre-treatment covariates: $\mathbf{X} \in \mathcal{X}$
  - No interference: $Y_i(T_1 = t_1, T_2 = t_2, \ldots, T_n = t_n) = Y_i(T_i = t_i)$
  - Random sampling of units:

$$(Y_i(1), Y_i(0), \mathbf{X}_i) \overset{\text{i.i.d.}}{\sim} \mathcal{P}$$

  - Completely randomized treatment assignment:

$$\Pr(T_i = 1 \mid Y_i(1), Y_i(0), \mathbf{X}_i) = \frac{n_1}{n} \quad \text{where} \quad n_1 = \sum_{i=1}^{n} T_i$$

- Fixed (for now) ITR:

$$f : \mathcal{X} \longrightarrow \{0, 1\}$$

  - based on any ML algorithm or even a heuristic rule
  - sample splitting for experimental data, separate observational data

Neyman's Inference for the Standard Metric

- Standard metric (Population Average "Value" or PAV):

$$\lambda_f \;=\; \mathbb{E}\{Y_i(f(\mathbf{X}_i))\}$$

- A natural estimator:

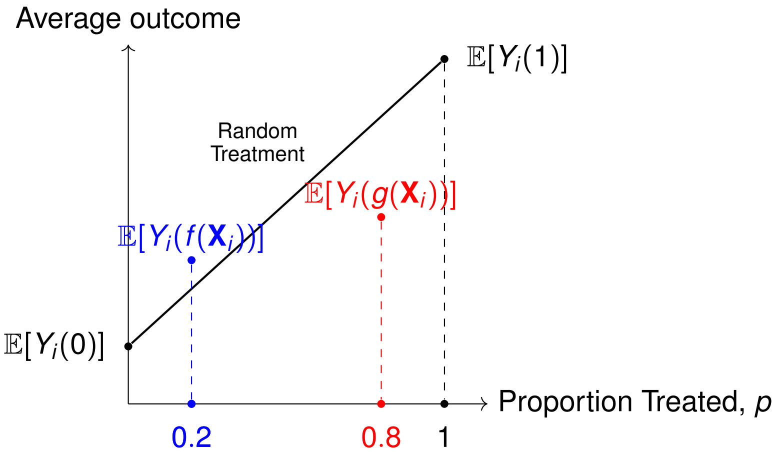
$$\hat{\lambda}_f(\mathcal{Z}) \;=\; \frac{1}{n_1}\sum_{i=1}^{n} Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)(1-f(\mathbf{X}_i)),$$

  where $\mathcal{Z} = \{\mathbf{X}_i, T_i, Y_i\}_{i=1}^n$
- Unbiasedness: $\mathbb{E}\{\hat{\lambda}_f(\mathcal{Z})\} = \lambda_f$
- Variance:

$$\mathbb{V}\{\hat{\lambda}_f(\mathcal{Z})\} \;=\; \frac{\mathbb{E}(S_{f1}^2)}{n_1} + \frac{\mathbb{E}(S_{f0}^2)}{n_0},$$

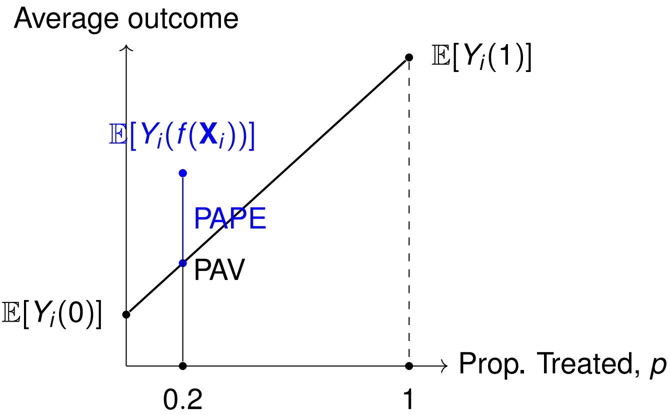
  where $S_{ft}^2 = \sum_{i=1}^n (Y_{fi}(t) - \overline{Y_f(t)})^2/(n-1)$,
  $Y_{fi}(t) = \mathbf{1}\{f(\mathbf{X}_i) = t\}Y_i(t)$, and $\overline{Y_f(t)} = \sum_{i=1}^n Y_{fi}(t)/n$ for $t = \{0,1\}$

A Problem of Comparing ITRs Using the PAV



- $\lambda_f < \lambda_g$: but g is performing worse than the random (i.e., non-individualized) treatment rule whereas f is not
- Need to account for the proportion treated

Accounting for the Proportion of Treated Units



- Population Average Prescriptive Effect (PAPE):

$$\tau_f = \mathbb{E}\{Y_i(f(\mathbf{X}_i)) - p_f Y_i(1) - (1 - p_f) Y_i(0)\}$$

where $p_f = \Pr(f(\mathbf{X}_i) = 1)$ is the proportion treated under f

Estimating the Population Average Prescriptive Effect

- An unbiased estimator of PAPE τ_f:

$$\hat{\tau}_f(\mathcal{Z}) = \frac{n}{n-1}\Bigg[\underbrace{\frac{1}{n_1}\sum_{i=1}^{n} Y_i T_i f(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)(1-f(\mathbf{X}_i))}_{\text{PAV of ITR}}$$

$$- \underbrace{\frac{\hat{p}_f}{n_1}\sum_{i=1}^{n} Y_i T_i - \frac{1-\hat{p}_f}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)}_{\text{PAV of random treatment rule with the same treated proportion}}\Bigg]$$

where $\hat{p}_f = \sum_{i=1}^{n} f(\mathbf{X}_i)/n$

- We also derive its variance, and propose its consistent estimator
- Not invariant to additive transformation: $Y_i + c$
- Solution: centering $\mathbb{E}(Y_i(1) + Y_i(0)) = 0 \rightsquigarrow$ minimum variance

Estimating and Evaluating ITRs via Cross-Validation

- Estimate and evaluate an ITR using the same experimental data
- How should we account for both estimation uncertainty and evaluation uncertainty under the Neyman's framework?
- Setup:
  - Learning algorithm
    $$F : \mathcal{Z} \longrightarrow \mathcal{F}.$$
  - K-fold cross-validation: $\mathcal{Z} = \{\mathcal{Z}_1, \mathcal{Z}_2, \ldots, \mathcal{Z}_K\}$
    $$\hat{f}_{-k} = F(\mathcal{Z}_1, \mathcal{Z}_2, \ldots, \mathcal{Z}_{k-1}, \mathcal{Z}_{k+1}, \ldots, \mathcal{Z}_K)$$
  - Evaluation metric estimators:
    $$\hat{\lambda}_F = \frac{1}{K}\sum_{k=1}^{K} \hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k), \quad \hat{\tau}_F = \frac{1}{K}\sum_{k=1}^{K} \hat{\tau}_{\hat{f}_{-k}}(\mathcal{Z}_k)$$
- Uncertainty over both evaluation data and all random sets of training data (of a fixed size) as well as treatment assignment

Causal Estimands

- Population Average Value (PAV)
  - Generalized ITR averaging over the random sampling of training data $\mathcal{Z}^{tr}$

$$\bar{f}_F(\mathbf{x}) \;=\; \mathbb{E}\{\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{x}) \mid \mathbf{X}_i = \mathbf{x}\} \;=\; \Pr(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{x}) = 1 \mid \mathbf{X}_i = \mathbf{x})$$

  - Estimand

$$\lambda_F \;=\; \mathbb{E}\left\{\bar{f}_F(\mathbf{X}_i)Y_i(1) + (1 - \bar{f}_F(\mathbf{X}_i))Y_i(0)\right\}$$

- Population Average Prescriptive Effect (PAPE)
  - Proportion treated

$$p_F \;=\; \mathbb{E}\{\bar{f}_F(\mathbf{X}_i)\}.$$

  - Estimand

$$\tau_F \;=\; \mathbb{E}\{\lambda_F - p_F Y_i(1) - (1 - p_F)Y_i(0)\}.$$

Inference under Cross-Validation

- Under Neyman's framework, the cross-validation estimators are unbiased, i.e., $\mathbb{E}(\hat{\lambda}_F) = \lambda_F$ and $\mathbb{E}(\hat{\tau}_F) = \tau_F$
- The variance of the PAV estimator

$$\mathbb{V}(\hat{\lambda}_F) = \underbrace{\frac{\mathbb{E}(S_{\hat{f}1}^2)}{m_1} + \frac{\mathbb{E}(S_{\hat{f}0}^2)}{m_0}}_{\text{evaluation uncertainty}} + \underbrace{\mathbb{E}\left\{\mathrm{Cov}(\hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_i), \hat{f}_{\mathcal{Z}^{tr}}(\mathbf{X}_j) \mid \mathbf{X}_i, \mathbf{X}_j)\tau_i\tau_j\right\}}_{\text{estimation uncertainty}} - \underbrace{\frac{K-1}{K}\mathbb{E}(S_F^2)}_{\substack{\textit{efficiency gain due} \\ \textit{to cross-validation}}}$$

for $i \neq j$ where m_t is the size of the training set with $T_i = t$, $\tau_i = Y_i(1) - Y_i(0)$, $S_F^2 = \sum_{k=1}^K \left\{\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k) - \overline{\hat{\lambda}_{\hat{f}_{-k}}(\mathcal{Z}_k)}\right\}^2 / (K-1)$

- Analogous results for the PAPE τ_F

Evaluation with a Budget Constraint

- Policy makers often face a binding budget constraint p
- Scoring rule:

$$s : \mathcal{X} \longrightarrow \mathcal{S} \quad \text{where} \quad \mathcal{S} \subset \mathbb{R}$$

- Example: CATE $s(\mathbf{x}) = \mathbb{E}(Y_i(1) - Y_i(0) \mid \mathbf{X}_i = \mathbf{x})$
- (Fixed) ITR with a budget constraint:

$$f(\mathbf{X}_i, c) \ = \ \mathbf{1}\{s(\mathbf{X}_i) > c\},$$

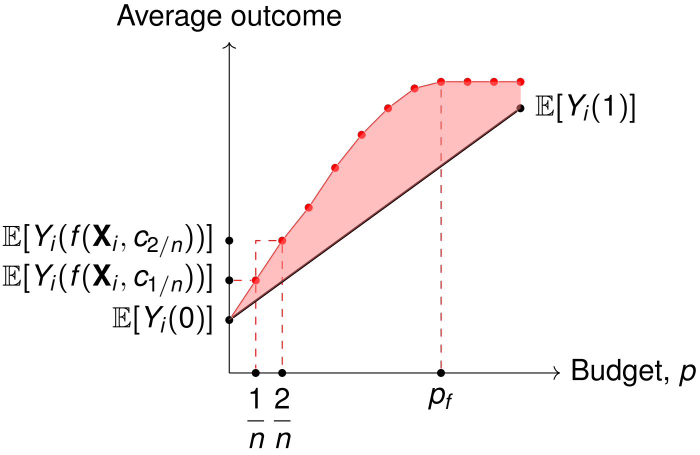
where $c_p(f) \ = \ \inf\{c \in \mathbb{R} : \Pr(f(\mathbf{X}_i, c) = 1) \leq p\}$

- PAPE under a budget constraint

$$\tau_{fp} \ = \ \mathbb{E}\{Y_i(f(\mathbf{X}_i, c_p(f))) - pY_i(1) - (1-p)Y_i(0)\}.$$

- We derive the bias (and its finite sample bound) and variance under the Neyman's framework
- Extensions: cross-validation, diff. in PAPE between two ITRs

The Area Under Prescriptive Effect Curve (AUPEC)



- Measure of performance across different budget constraints
- We show how to do inference with and without cross-validation
- Normalized AUPEC $=$ average percentage gain using an ITR over the randomized treatment rule across a range of budget contraints

Simulations

- Atlantic Causal Inference Conference data analysis challenge
- Data generating process
  - 8 covariates from the Infant Health and Development Program (originally, 58 covariates and 4,302 observations)
  - population distribution = original empirical distribution
  - Model

$$Y_i(t) \;=\; \mu(\mathbf{X}_i) + \tau(\mathbf{X}_i)t + \sigma(\mathbf{X}_i)\epsilon_i,$$

    where $t = 0, 1$, $\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$, and

$$\begin{aligned}
\mu(\mathbf{x}) &= -\sin(\Phi(\pi(\mathbf{x}))) + x_{43}, \\
\pi(\mathbf{x}) &= 1/[1 + \exp\{3(x_1 + x_{43} + 0.3(x_{10} - 1)) - 1\}], \\
\tau(\mathbf{x}) &= \xi(x_3 x_{24} + (x_{14} - 1) - (x_{15} - 1)), \\
\sigma(\mathbf{x}) &= 0.25\sqrt{\mathbb{V}(\mu(\mathbf{x}) + \pi(\mathbf{x})\tau(\mathbf{x}))}.
\end{aligned}$$

- Two scenarios: large vs. small treatment effects $\xi \in \{2, 1/3\}$
- Sample sizes: $n \in \{100, 500, 2,000\}$

Results I: Fixed ITR

- f: Bayesian Additive Regression Tree (BART)
- No budget constraint, 20% constraint
- g: Causal Forest
- h: LASSO

		$n = 100$			$n = 500$			$n = 2000$		
Estimator	truth	cov.	bias	s.d.	cov.	bias	s.d.	cov.	bias	s.d.
Small effect										
$\hat{\tau}_f$	0.066	94.3	0.005	0.124	96.2	0.001	0.053	95.1	0.001	0.026
$\hat{\tau}_f(c_{0.2})$	0.051	93.2	−0.002	0.109	94.4	0.001	0.046	95.2	0.002	0.021
$\widehat{\Gamma}_f$	0.053	95.3	0.001	0.106	95.1	0.001	0.045	94.8	−0.001	0.024
$\widehat{\Delta}_{0.2}(f, g)$	−0.022	94.0	0.006	0.122	95.4	0.002	0.051	96.0	0.000	0.026
$\widehat{\Delta}_{0.2}(f, h)$	−0.014	93.9	−0.001	0.131	94.9	−0.000	0.060	95.3	−0.000	0.030
Large effect										
$\hat{\tau}_f$	0.430	94.7	−0.000	0.163	95.7	0.000	0.064	94.4	-0.000	0.031
$\hat{\tau}_f(c_{0.2})$	0.356	94.7	0.004	0.159	95.7	0.002	0.072	95.8	0.000	0.035
$\widehat{\Gamma}_f$	0.363	94.3	−0.005	0.130	94.9	0.003	0.058	95.7	0.000	0.029
$\widehat{\Delta}_{0.2}(f, g)$	−0.000	96.9	0.008	0.151	97.9	−0.002	0.073	98.0	−0.000	0.026
$\widehat{\Delta}_{0.2}(f, h)$	0.000	94.7	−0.004	0.140	97.7	−0.001	0.065	96.6	0.000	0.033

Results II: Estimated ITR

- 5-fold cross validation
- F: LASSO
- std. dev. for $n = 500$ is roughly half of the fixed $n = 100$ case

	$n = 100$			$n = 500$			$n = 2000$		
Estimator	cov.	bias	s.d.	cov.	bias	s.d.	cov.	bias	s.d.
Small effect									
$\hat{\lambda}_F$	96.4	0.001	0.216	96.7	0.002	0.100	97.2	0.002	0.046
$\hat{\tau}_F$	94.6	-0.002	0.130	95.5	-0.002	0.052	94.4	-0.000	0.027
$\hat{\tau}_F(c_{0.2})$	95.4	-0.003	0.120	95.4	-0.002	0.043	96.8	0.001	0.029
$\widehat{\Gamma}_F$	98.2	0.002	0.117	96.8	-0.001	0.048	95.9	0.001	0.001
Large effect									
$\hat{\lambda}_H$	96.9	-0.007	0.261	96.5	-0.003	0.125	97.3	0.001	0.062
$\hat{\tau}_F$	93.6	-0.000	0.171	93.0	0.000	0.093	95.3	0.001	0.041
$\hat{\tau}_F(c_{0.2})$	94.8	-0.002	0.170	96.2	-0.005	0.075	95.8	0.001	0.037
$\widehat{\Gamma}_F$	98.5	0.001	0.126	98.9	0.005	0.053	99.0	0.001	0.026

Application to the STAR Experiment

- Experiment involving 7,000 students across 79 schools
- Randomized treatments (kindergarden):
  1. $T_i = 1$: small class (13–17 students)
  2. $T_i = 0$: regular class (22–25)
  3. regular class with aid
- Outcome: SAT scores
- Literature on heterogeneous treatments in labor economics
- 10 covariates
  - 4 demographics: gender, race, birth month, birth year
  - 6 school characteristics: urban/rural, enrollment size, grade range, number of students on free lunch, percentage white, number of students on school buses
- Sample size: $n = 1,911$, 5-fold cross-validation
- Average Treatment Effects:
  - SAT reading: 6.78 (s.e.=1.71)
  - SAT math: 5.78 (s.e.=1.80)

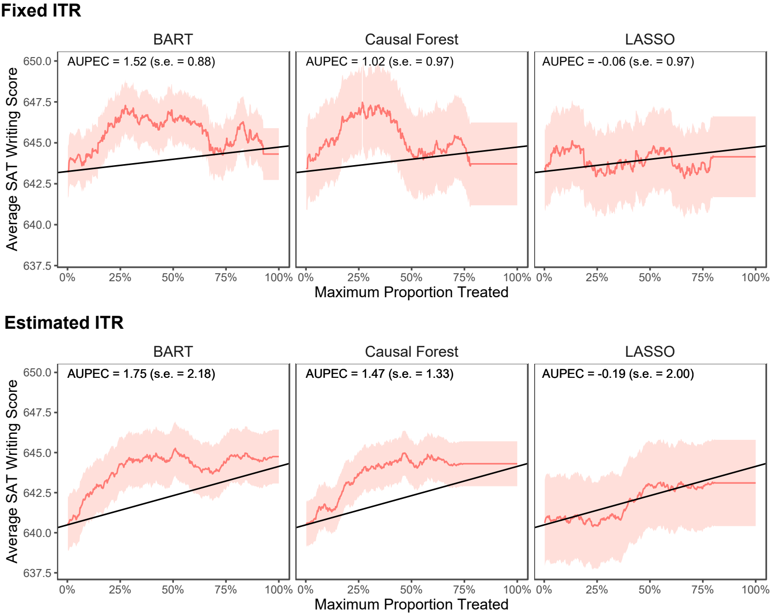
Results I: ITR Performance

	BART			Causal Forest			LASSO		
	est.	s.e.	treated	est.	s.e.	treated	est.	s.e.	treated
Fixed ITR									
No budget constraint									
Reading	0	0	100%	−0.38	1.14	84.3%	−0.41	1.10	84.4%
Math	0.52	1.09	86.7	0.09	1.18	80.3	1.73	1.25	78.7
Writing	−0.32	0.72	92.7	−0.70	1.18	78.0	−0.30	1.26	80.0
Budget constraint									
Reading	−0.89	1.30	20	0.66	1.23	20	−1.17	1.18	20
Math	0.70	1.25	20	2.57	1.29	20	1.25	1.32	20
Writing	2.60	1.17	20	2.98	1.18	20	0.28	1.19	20
Estimated ITR									
No budget constraint									
Reading	0.19	0.37	99.3%	0.31	0.77	86.6%	0.32	0.53	87.6%
Math	0.92	0.75	84.7	2.29	0.80	79.1	1.52	1.60	75.2
Writing	1.12	0.86	88.0	1.43	0.71	67.4	0.05	1.37	74.8
Budget constraint									
Reading	1.55	1.05	20	0.40	0.69	20	−0.15	1.41	20
Math	2.28	1.15	20	1.84	0.73	20	1.50	1.48	20
Writing	2.31	0.66	20	1.90	0.64	20	−0.47	1.34	20

Results II: Comparison between ML Algorithms

	Causal Forest vs. **BART**		Causal Forest vs. **LASSO**		**BART** vs. **LASSO**	
	est.	95% CI	est.	95% CI	est.	95% CI
Fixed ITR						
Math	1.55	[−0.35, 3.45]	1.83	[−0.50, 4.16]	0.28	[−2.39, 2.95]
Reading	1.86	[−0.79, 4.51]	1.31	[−1.49, 4.11]	−0.55	[−4.02, 2.92]
Writing	0.38	[−1.66, 2.42]	2.69	[−0.27, 5.65]	2.32	[−0.53, 5.15]
Estimated ITR						
Reading	−1.15	[−3.99, 1.69]	0.55	[−1.05, 2.15]	1.70	[−0.90, 4.30]
Math	−0.43	[−2.57, 3.43]	0.34	[−1.32, 2.00]	0.77	[−1.99, 3.53]
Writing	−0.41	[−1.63, 0.80]	2.37	[0.76, 3.98]	2.79	[1.32, 4.26]

Results III: AUPEC



Extension to Heterogeneous Treatment Effects

- Inference for heterogeneous treatment effects discovered via a generic ML algorithm
  - cannot assume ML algorithms converge uniformly
  - avoid computationally intensive method (e.g., repeated cross-fitting)
  - use Neyman's repeated sampling framework for inference
- Setup:
  - Conditional Average Treatment Effect (CATE):

$$\tau(\mathbf{x}) \;=\; \mathbb{E}(Y_i(1) - Y_i(0) \mid \mathbf{X}_i = \mathbf{x})$$

  - CATE estimation based on ML algorithm

$$s : \mathcal{X} \longrightarrow \mathcal{S} \subset \mathbb{R}$$

  - Sorted Group Average Treatment Effect (GATE; Chernozhukov et al. 2019)

$$\tau_k \;:=\; \mathbb{E}(Y_i(1) - Y_i(0) \mid c_{k-1}(s) \leq s(\mathbf{X}_i) < c_k(s))$$

    for $k = 1, 2, \ldots, K$ where c_k represents the cutoff between the $(k-1)$th and kth groups

GATE Estimation as ITR Evaluation

- A natural GATE estimator

$$\hat{\tau}_k \;=\; \frac{K}{n_1}\sum_{i=1}^{n} Y_i T_i \hat{f}_k(\mathbf{X}_i) - \frac{K}{n_0}\sum_{i=1}^{n} Y_i (1-T_i)\hat{f}_k(\mathbf{X}_i),$$

where $\hat{f}_k(\mathbf{X}_i) \;=\; \mathbf{1}\{s(\mathbf{X}_i) \geq \hat{c}_k(s)\} - \mathbf{1}\{s(\mathbf{X}_i) \geq \hat{c}_{k-1}(s)\}$

- Rewrite this as the PAPE:

$$\hat{\tau}_k \;=\; K\underbrace{\left\{\frac{1}{n_1}\sum_{i=1}^{n} Y_i T_i \hat{f}_k(\mathbf{X}_i) + \frac{1}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)(1-\hat{f}_k(\mathbf{X}_i))\right.}_{\text{estimated PAV}}$$
$$\left.\underbrace{-\frac{1}{n_0}\sum_{i=1}^{n} Y_i(1-T_i)}_{\text{no one gets treated}}\right\}.$$

- Our results can be extended to both sample-splitting and cross-fitting cases

Concluding Remarks

- Individualized treatment rules (ITRs) are used in many fields
- Inference about ITRs has been largely model-based
  - We show how to experimentally evaluate ITRs
  - We incorporate budget constraints
  - No modeling assumption or asymptotic approximation is required
  - Complex machine learning algorithms can be used
  - Applicable to cross-validation estimators
  - Simulations: good small sample performance
- Ongoing extensions
  - heterogeneous treatment effects using machine learning
  - dynamic ITRs
- Paper (JASA, forthcoming): **https://arxiv.org/abs/1905.05389**
- Software: **https://github.com/MichaelLLi/evalITR**