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Feature Selection for Discovering Distributional Treatment Effect Modifiers

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Motivation: *Elucidate why treatment effects are different*

Many existing methods use a complex ML model to accurately estimate heterogeneous treatment effects across individuals. However, they offer no answer to the following question:

Different individuals have different treatment effects. ***Why?***

We answer this question by solving the feature selection problem:

Input: Observations of features $\boldsymbol{X}$, treatment A, and outcome Y

X_1	...	X_d	A	Y	Y^1	Y^0	Y^1-Y^0
Male		15 y.o.	0	82	?	82	?
Male		80 y.o.	0	174	?	174	?
Female		64 y.o.	1	135	135	?	?
Female		32 y.o.	1	110	110	?	?

Output: Features related to *treatment effect heterogeneity*

X_2 $p = 0.002$ X_5 $p = 0.019$ X_9 $p = 0.035$

Our Contributions

1. **Novel feature importance measure**
2. **Its computationally efficient estimator**
3. **Selection algorithm that controls Type I error**

Traditional mean-based approaches

Using the CATE conditioned on a single feature (i.e., the average treatment effect across individuals with identical attribute $X_m = x$):

$$T_m(x) := \mathbb{E}[Y^1 - Y^0 \mid X_m = x]$$
$$= \mathbb{E}[Y^1 \mid X_m = x] - \mathbb{E}[Y^0 \mid X_m = x], \quad (1)$$

the existing methods (e.g., [1]) seek *treatment effect modifiers*:

Definition 1 (Rothman et al. [2008]). *Feature X_m is said to be a treatment effect modifier if there are at least two values of X_m, x_m and $x_m^\star$ ($x_m \neq x_m^\star$), such that CATE T_m in (1) takes different values, i.e., $T_m(x_m) \neq T_m(x_m^\star)$.*

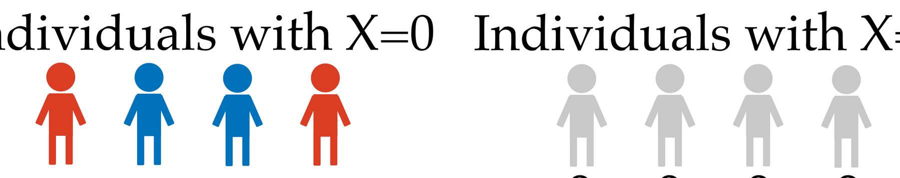
Weakness: ***Mean-based methods may overlook important features***

Example:

Y^0 \ Y^1	-1	0	1	Total
$P(Y^0, Y^1 \mid X = 0)$				
-1	0	0	0	0
0	**0.5**	0	**0.5**	**1.0**
1	0	0	0	0
Total	**0.5**	0	**0.5**	**1.0**

Y^0 \ Y^1	-1	0	1	Total
$P(Y^0, Y^1 \mid X = 1)$				
-1	0	0	0	0
0	0	**1.0**	0	**1.0**
1	0	0	0	0
Total	0	**1.0**	0	**1.0**

Individuals with X=0   Individuals with X=1



	Individuals with X=0		Individuals with X=1	
$Y^1 - Y^0$:	-1 $+1$ $+1$ -1		0 0 0 0	
$\mathbb{E}[Y^1 - Y^0 \mid X]$:	0	=	0	**Identical means**
$\mathrm{Var}[Y^1 - Y^0 \mid X]$:	1	≠	0	**Different variances**

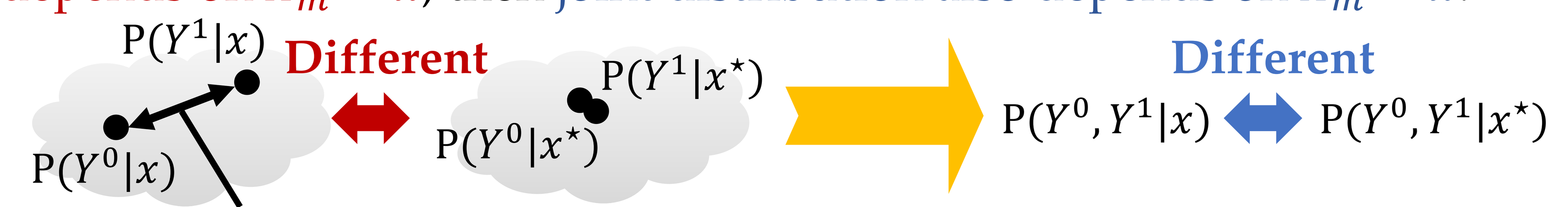
How can we detect *distributional heterogeneity*?

Proposed method

Our Goal: Detect features whose values affect the **functionals** of joint distribution $P(Y^0, Y^1 \mid X_m = x)$ (e.g., treatment effect variance)

1. Detecting *distributional* treatment effect modifiers

Idea: If the discrepancy between $P(Y^0 \mid X_m = x)$ and $P(Y^1 \mid X_m = x)$ depends on $X_m = x$, then joint distribution also depends on $X_m = x$.



Measured by kernel MMD [2]: $D_m^2(x) := \mathrm{MMD}^2(P(Y^0 \mid X_m = x), P(Y^1 \mid X_m = x))$

$$= \mathbb{E}_{Y^0, Y^{0\prime} \mid X_m = X_m' = x}[k_Y(Y^0, Y^{0\prime})] + \mathbb{E}_{Y^1, Y^{1\prime} \mid X_m = X_m' = x}[k_Y(Y^1, Y^{1\prime})] - 2\,\mathbb{E}_{Y^0, Y^1 \mid X_m = x}[k_Y(Y^0, Y^1)]$$

To detect the MMD value variation, we formulate feature importance measure as the variance of squared MMD:

$$I_m := \mathrm{Var}[D_m^2(X_m)].$$

2. Estimating importance measure with IPW and RFFs

Using *inverse probability weighting* (IPW), **we reformulate $D_m^2(x)$ as**

$$\mathrm{WCMMD}^2_{X_m = x}$$
$$:= \mathbb{E}_{A, A', \boldsymbol{X}_{-m}, \boldsymbol{X}'_{-m}, Y, Y' \mid X_m = X_m' = x}[w^0(A, \boldsymbol{X}) w^0(A', \boldsymbol{X}') k_Y(Y, Y')]$$
$$+ \mathbb{E}_{A, A', \boldsymbol{X}_{-m}, \boldsymbol{X}'_{-m}, Y, Y' \mid X_m = X_m' = x}[w^1(A, \boldsymbol{X}) w^1(A', \boldsymbol{X}') k_Y(Y, Y')]$$
$$-2\,\mathbb{E}_{A, A', \boldsymbol{X}_{-m}, \boldsymbol{X}'_{-m}, Y, Y' \mid X_m = X_m' = x}[w^0(A, \boldsymbol{X}) w^1(A', \boldsymbol{X}') k_Y(Y, Y')].$$

$$w^0(A, \boldsymbol{X}) = \frac{\mathbf{I}(A = 0)}{1 - \mathrm{e}(\boldsymbol{X})} \quad w^1(A, \boldsymbol{X}) = \frac{\mathbf{I}(A = 1)}{\mathrm{e}(\boldsymbol{X})} \quad \mathrm{e}(\boldsymbol{X}) := \mathrm{P}(A = 1 \mid \boldsymbol{X})$$

Empirical estimator: $\widehat{D}_m^2(x) := \sum_{i=1}^n \sum_{j=1}^n \left(\omega_i^{0,x}\omega_j^{0,x} + \omega_i^{1,x}\omega_j^{1,x}\right) k_Y(y_i, y_j) - 2\sum_{i=1}^n \sum_{j=1}^n \omega_i^{0,x}\omega_j^{1,x} k_Y(y_i, y_j)$

If X_m is discrete, $\omega_i^{a,x} = \frac{\mathbf{I}(x_{m,i} = x)}{\sum_{l=1}^n \mathbf{I}(x_{m,l} = x)} w^a(a_i, \boldsymbol{x}_i)$; otherwise, $\omega_i^{a,x} = \frac{\frac{1}{h_{X_m}} k_{X_m}(x_{m,i}, x)}{\sum_{l=1}^n \frac{1}{h_{X_m}} k_{X_m}(x_{m,l}, x)} w^a(a_i, \boldsymbol{x}_i)$

To reduce the computation time, **we approximate k_Y** with RFFs [3]:

$$k_Y(y_i, y_j) \approx \widetilde{k}_Y(y_i, y_j) = \langle \boldsymbol{z}(y_i), \boldsymbol{z}(y_j) \rangle_{\mathbb{R}^r}, \quad \boldsymbol{z}(y) = \begin{bmatrix} \sqrt{2}\cos(\lambda_1 y + \zeta_1) \\ \vdots \\ \sqrt{2}\cos(\lambda_r y + \zeta_r) \end{bmatrix}$$

which yields

$$\widetilde{D}_m^2(x) := \langle \widetilde{\mu}_{Y^0|x}, \widetilde{\mu}_{Y^0|x} \rangle_{\mathbb{R}^r} + \langle \widetilde{\mu}_{Y^1|x}, \widetilde{\mu}_{Y^1|x} \rangle_{\mathbb{R}^r} - 2\langle \widetilde{\mu}_{Y^0|x}, \widetilde{\mu}_{Y^1|x} \rangle_{\mathbb{R}^r}.$$

$$\widetilde{\mu}_{Y^0|x} = \sum_{i=1}^n \omega_i^{0,x} \boldsymbol{z}(y_i) \quad \widetilde{\mu}_{Y^1|x} = \sum_{i=1}^n \omega_i^{1,x} \boldsymbol{z}(y_i)$$

Estimated feature importance:

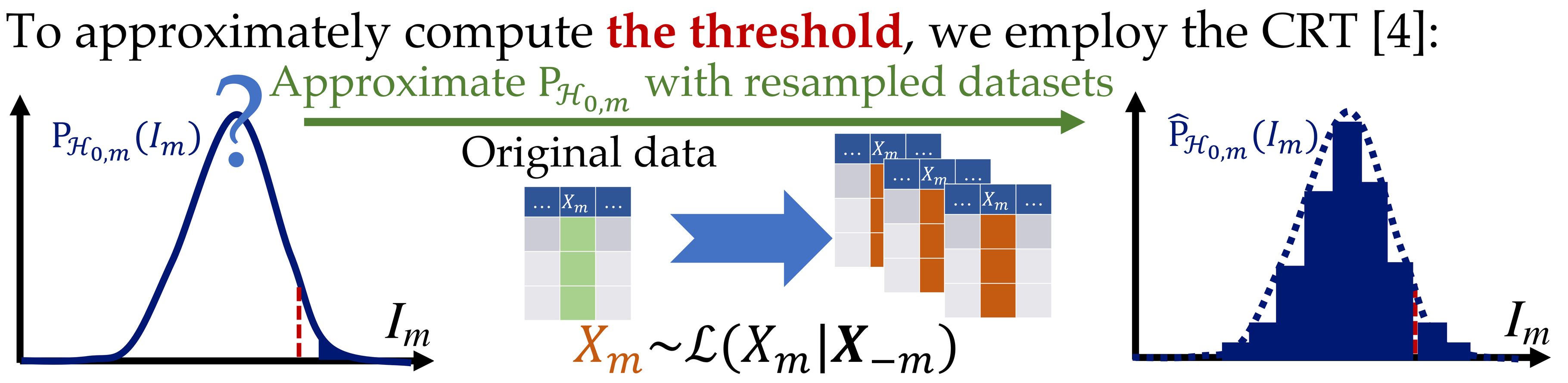
$$\widetilde{I}_m = \frac{1}{n-1} \sum_{\iota=1}^n \left(\widetilde{D}_m^2(x_{m,\iota}) - \frac{1}{n} \sum_{\varsigma=1}^n \widetilde{D}_m^2(x_{m,\varsigma}) \right)^2$$

3. Multiple tests with conditional randomization test (CRT)

We select features by performing multiple hypothesis tests:

$$\mathcal{H}_{0,m}: I_m = 0 \quad \text{and} \quad \mathcal{H}_{1,m}: I_m > 0. \quad (m=1, \ldots, d)$$

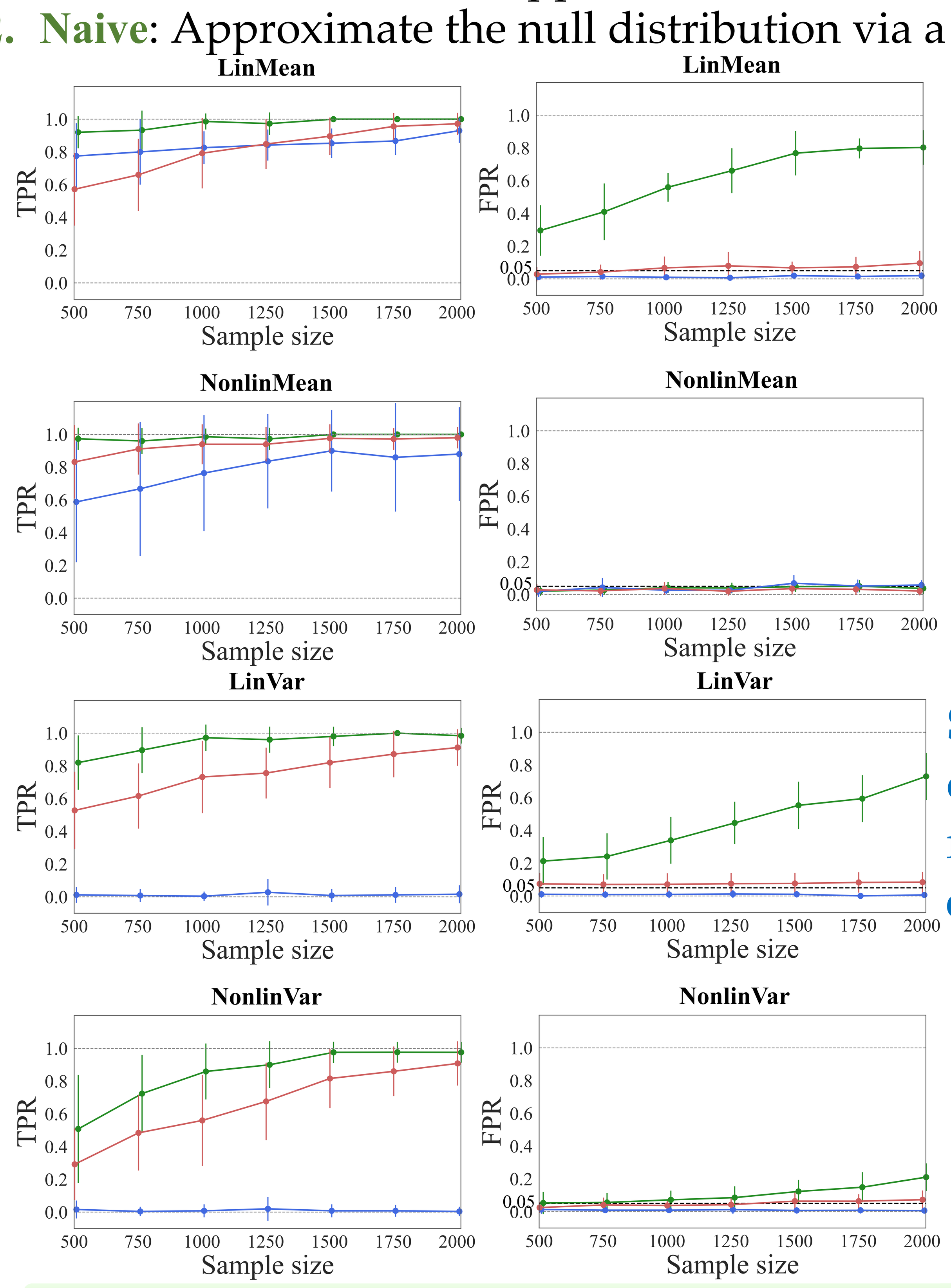
To approximately compute **the threshold**, we employ the CRT [4]:



Experimental results

Synthetic data We compare our method with the two baselines:

1. **SI-EM** [1]: Mean-based approach
2. **Naive**: Approximate the null distribution via a naive bootstrap



Naive cannot control the FPR to $\alpha = 0.05$

SI-EM cannot detect the features related to treatment effect variance

Proposed achieves high TPR while controlling FPR

Real-world data We use health record dataset (from NHANES)

Treatment A: obesity **Outcome Y**: low-grade systemic inflammation

Features $\boldsymbol{X}$: e.g., age, gender, race, past medical history (e.g., asthma, stroke)

Feature	Adjusted p-value
Age	0.0075 ± 0.0305
Gender	0.0046 ± 0.0269
Number of cigarettes smoked	0.0 ± 0.0

Not detected by SI-EM

[1] Qingyuan Zhao, Dylan S. Small, and Ashkan Ertefaie. "**Selective inference for effect modification via the lasso**". Journal of Royal Statistical Society: Series B (Statistical Methodology), 84(2):382–413, 2022.

[2] Arthur Gretton, Karsten M. Borgwardt, Malte J Rasch, Bernhard Schölkopf, and Alexander Smola. "**A kernel two-sample test**". JMLR, 13(1):723–773, 2012.

[3] Ali Rahimi and Benjamin Recht. "**Random features for large-scale kernel machines**". In NeurIPS, volume 3, page 5, 2007.

[4] Emmanuel Candes, Yingying Fan, Lucas Janson, and Jinchi Lv. "**Panning for gold: 'Model-X'knockoffs for high dimensional controlled variable selection**". Journal of Royal Statistical Society: Series B (Statistical Methodology), 80 (3):551–577, 2018.