EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

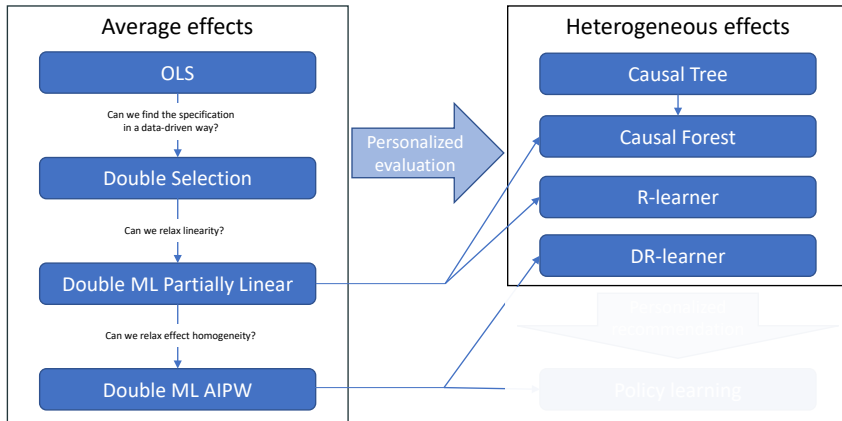# Causal Machine Learning

Heterogeneous effects: validation and description

Michael Knaus

WiSe 25/26

We learned how to predict heterogeneous effects applying concepts developed for average effect estimation

Plan of this morning

What to do with all these predicted effects?

1. How to validate estimated CATEs?

2. Best Linear Predictor

3. Sorted Group Average Treatment Effect

4. Rank-Weighted Average Treatment Effect

5. Unifying framework

6. How to describe/understand CATEs?

Too much information

After applying Causal *insert here your favorite supervised ML* or *insert here your favorite letter (combination)*-learner, we end up with (at least) N flexibly estimated CATEs
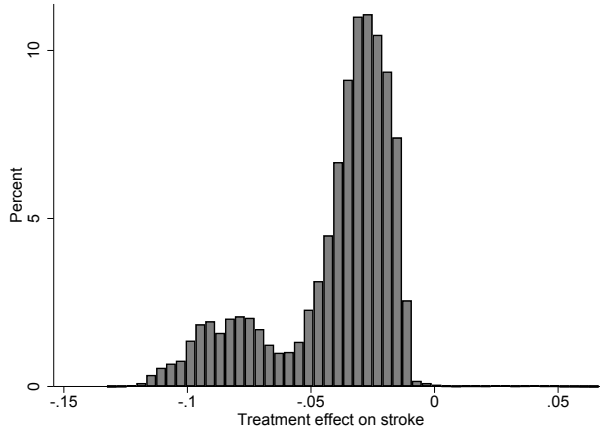
These can be useful for decision making, but how to communicate them in papers/reports or to decision makers?

Nobody can digest a table with N effects

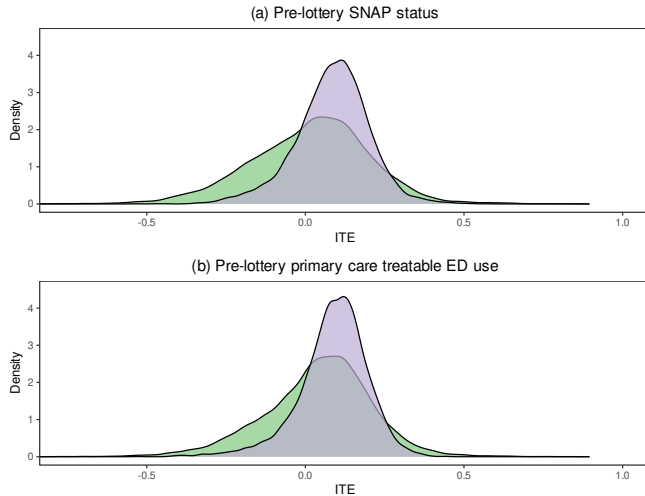The first step is usually to plot the distribution

Many different ways...

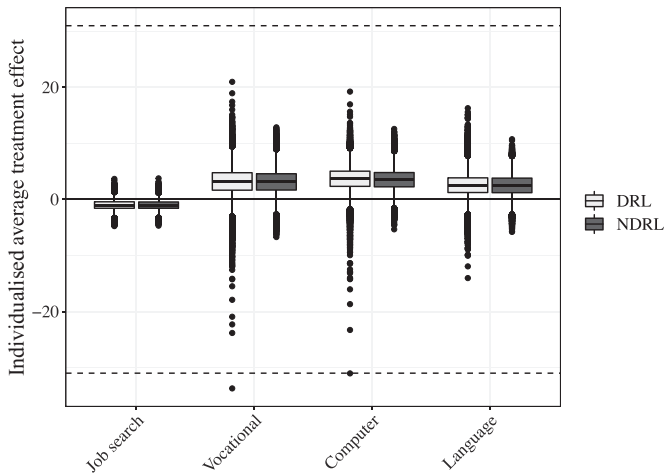Figure 4: Distribution of Treatment Effects Across VHA Patients

Source: Abaluck et al. (2020)

As density plots

(a) Pre-lottery SNAP status

(b) Pre-lottery primary care treatable ED use

Source: Denteh & Liebert, 2022

5

Source: Knaus (2022)

Okay, these are nice pictures and there seems to be heterogeneity

But what are we really looking at 🤔

In the next steps we learn how to …

1. … test whether we found systematic effect heterogeneity or just noise
2. … explore what drives the heterogeneous effects

How to validate estimated CATEs?

A challenging task

Challenges:

- Due to the missing counterfactual, we can not benchmark our predicted effect against the true effect $\Rightarrow$ no classic out-of-sample testing possible (unique to causal ML)
- Statistical inference for flexibly estimated CATEs is not available or at least challenging (shared with supervised ML)

A paradigm shift: It is statistically nearly hopeless and practically not very useful to test/validate each individual effect estimate

Instead the methods we will discuss today aim for low dimensional key features of the estimated heterogeneous effects

Today we will learn about three such new target parameters:

- Best Linear Predictor (BLP) of Chernozhukov et al. (2025)
- High-vs.-low Sorted Group Average Treatment Effect (GATES) (Chernozhukov et al., 2025)
- Rank-Weighted Average Treatment Effect (RATE) of Yadlowsky et al. (2024)

They will allow us to test the joint hypothesis that

(i) there is effect heterogeneity and
(ii) the applied learner is able to detect it at least partially

Best Linear Predictor

Chernozhukov et al. (2025) propose to look at the BEST LINEAR PREDICTOR (BLP) which is defined as the solution of the hypothetical regression of the true CATE on the demeaned predicted CATE:

Definition BLP

$$(\beta_1, \beta_2) = \underset{b_1, b_2}{\arg\min}\, \mathbb{E}\{[\tau(X) - b_1 - b_2 \underbrace{(\hat{\tau}(X) - \mathbb{E}[\hat{\tau}(X)])}_{\text{demeaned prediction}}]^2\}$$

where

- $\beta_1 = \mathbb{E}[\tau(X)] = ATE$ because of the demeaning
- $\beta_2 = \frac{Cov[\tau(X), \hat{\tau}(X)]}{Var[\hat{\tau}(X)]}$

Best Linear Predictor - interpretation

$\beta_2 = \frac{Cov[\tau(X), \hat{\tau}(X)]}{Var[\tau(X)]} = 1$ if $\hat{\tau}(X) = \tau(X)$ (what we would like to see)

$\beta_2 = 0$ if $Cov[\tau(X), \hat{\tau}(X)] = 0$ this can have two reasons

1. $\tau(X)$ is constant (no heterogeneity to detect)
2. $\tau(X)$ is not constant but the estimator is not capable of finding it (bad estimator and/or not enough observations)

Therefore, testing $H_0 : \beta_2 = 0$ is a joint test of

(i) existence of heterogeneity and

(ii) the estimators capability to find it

Best Linear Predictor - strategy A

Chernozhukov, Demirer, Duflo & Fernández-Val (2025) show that the BLP parameters are identified in RCTs (known propensity score $e(X)$)

Strategy A: Weighted residual BLP

$$(\beta_1, \beta_2) = \arg\min_{b_1, b_2} \mathbb{E}\{\omega(X)[Y - b_1(W - e(X)) - b_2(W - e(X))(\hat{\tau}(X) - \mathbb{E}[\hat{\tau}(X)]) - a\tilde{X}]^2\}$$

where $\omega(X) = [e(X)(1 - e(X))]^{-1}$

$\tilde{X}$ is not required for identification, but contains optional functions of X to reduce estimation noise, e.g $[1, \hat{m}(0, X), e(X), e(X)\hat{\tau}(X)]$

See Appendix A of the paper for a detailed derivation

Chernozhukov et al. (2025) show that the BLP parameters are identified in RCTs (known propensity score $e(X)$)

Strategy B: Horvitz-Thompson BLP

$$(\beta_1, \beta_2) = \underset{b_1, b_2}{\arg\min} \, \mathbb{E}\{[HY - b_1 - b_2(\hat{\tau}(X) - \mathbb{E}[\hat{\tau}(X)]) - aH\tilde{X}]^2\}$$

where $H = \frac{W - e(X)}{e(X)(1 - e(X))}$ are the familiar IPW weights

$\tilde{X}$ is not required for identification, but may be used to reduce estimation noise

Note that HY serves as a pseudo-outcome

See Appendix A of the paper for a detailed derivation

1. Split your sample in training and test set
2. Learn a model for $\tau(X)$ in the training sample
3. Predict $\hat{\tau}(X)$ in the test sample
4. Run the regression of strategy A and/or B in the test sample
5. Test $H_0 : \beta_2 = 0$ as usual

This will give you the BLP of one specific training/test split

Chernozhukov et al. (2025) also show how to aggregate results from repeated splits but we will focus for simplicity on the single split case

Chernozhukov et al. (2025) evaluate the effect of an intervention in Indian villages analyzing the effect of a bundle of immunization incentives (W) on "Number of children who completed the immunization schedule" (Y)

TABLE 3. BLP of Immunization Incentives Using Causal Proxies

	Elastic Net		Neural Network	
ATE (β_1)	HET (β_2)	ATE (β_1)	HET (β_2)
2.814	1.047	2.441	0.899
(1.087,4.506)	(0.826,1.262)	(0.846,3.979)	(0.685,1.107)
[0.004]	[0.000]	[0.004]	[0.000]

Notes: Medians over 250 splits. Median Confidence Intervals ($\alpha = .05$) in parenthesis. P-values for the hypothesis that the parameter is equal to zero against the two-sided alternative in brackets.

From BLP to rank-based methods

The BLP is the idealized regression of the true CATE on the estimated CATE

Rejecting $H_0 : \beta_2 = 0$ implies that truth and estimation correlate significantly

Another way to investigate whether the estimated CATEs are any good is to

1. rank observations in the test set according to their estimated CATE
2. and test whether the effects for those with higher ranks show greater effects out-of-sample

We expect that effects differ significantly in case we detected systematic heterogeneity

Sorted Group Average Treatment Effect

Chernozhukov et al. (2025) propose to look at the SORTED GROUP AVERAGE TREATMENT EFFECTS (GATES) which are defined as:
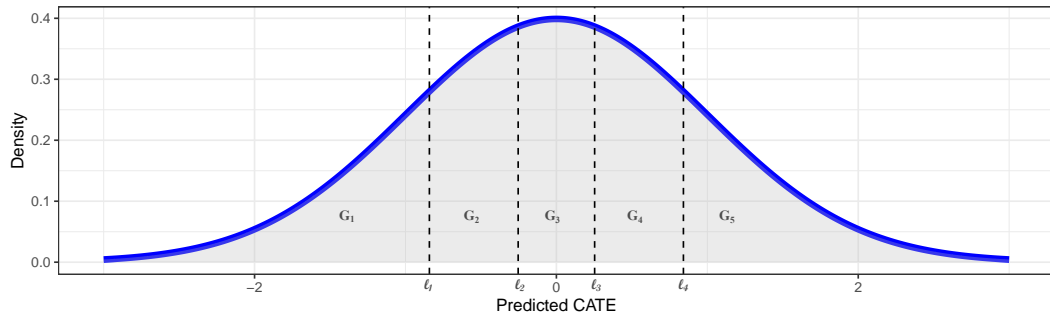
Definition GATES

$$\gamma_k = \mathbb{E}[\tau(X) \mid G_k], \ k = 1, ..., K$$

where $G_k = \{\hat{\tau}(X) \in I_k\}$ with $I_k = [l_{k-1}, l_k)$ and $-\infty = l_0 < l_1 < ... < l_K = \infty$

In words: We slice the distribution of $\hat{\tau}(X)$ into K parts and are interested in the average effect of individuals within each slice

γ_k is then the mean of the true CATEs in the group G_k formed by the predicted CATEs

If the slices are build on the true CATE, we would observe the following monotonicity

$$\gamma_1^* \leq ... \leq \gamma_K^*$$

where the $*$ indicates that the parameter builds on the true CATE

$\Rightarrow$ We expect to see the same monotonicity if $\hat{\tau}(X)$ provides a good approximation of $\tau(X)$

Situations where $\gamma_1, ..., \gamma_K$ are similar indicate that no systematic heterogeneity was detected

Sorted Group Average Treatment Effect - identification

Similar to the BLP, the GATES are identified using two different strategies

Strategy A: Weighted residual GATES

$$(\gamma_1, ..., \gamma_K) = \arg\min_g \mathbb{E}\{\omega(X)[Y - \sum_k g_k(W - e(X))\mathbb{1}[G_k] - a\tilde{X}]^2\}$$

Strategy B: Horvitz-Thompson GATES

$$(\gamma_1, ..., \gamma_K) = \arg\min_g \mathbb{E}\{[HY - \sum_k g_k\mathbb{1}[G_k] - aH\tilde{X}]^2\}$$

Again covariates $\tilde{X}$ are not required for identification, but reduce estimation noise

See Appendix A of the paper for a detailed derivation

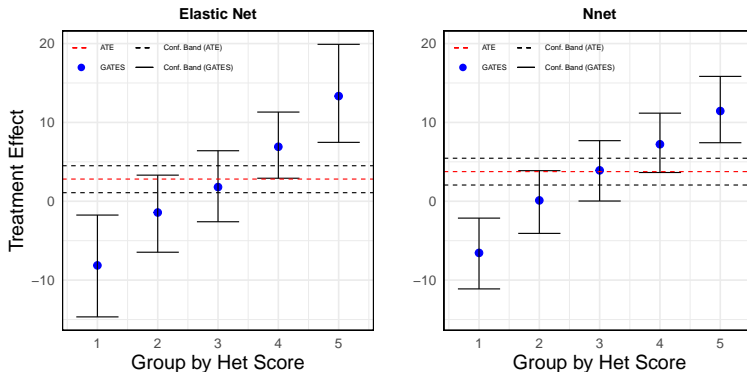## Sorted Group Average Treatment Effect - implementation

1. Split your sample in training and test set
2. Learn a model for $\tau(X)$ in the training sample
3. Predict $\hat{\tau}(X)$ in the test sample
4. Sort $\hat{\tau}(X)$ and create K slices
5. Run the regression of strategy A and/or B in the test sample
6. Test for example $H_0 : \gamma_K - \gamma_1 = 0$

This will give you the GATES of one specific training/test split

Chernozhukov et al. (2025) also show how to aggregate results from repeated splits, but we focus on single splits

Sorted Group Average Treatment Effect - example

FIGURE 5. GATES of Immunization Incentives

Notes: GATES of Immunization Incentives, based upon Causal Learners. Median point estimates and Median confidence interval ($\alpha = .05$) in parenthesis, over 250 splits.

Sorted Group Average Treatment Effect - example

TABLE 4. GATES of 20% Most and Least Affected Groups

| | Elastic Net | | | Nnet | | |
	20% Most (G_5)	20% Least (G_1)	Difference	20% Most (G_5)	20% Least (G_1)	Difference
GATE	13.230	-8.000	21.60	11.210	-6.551	18.13
$\gamma_k := \hat{\mathrm{E}}[s_0(Z) \mid G_k]$	(8.219,18.67)	(-13.41,-2.574)	(13.70,29.74)	(7.721,14.47)	(-10.37,-2.786)	(12.84,23.52)
	[0.000]	[0.009]	[0.000]	[0.000]	[0.002]	[0.000]
Control Mean	2.19	12.68	-10.56	1.19	10.32	-9.17
$:= \hat{\mathrm{E}}[b_0(Z) \mid G_k]$	(1.27,3.06)	(11.73,13.59)	(-11.84,-9.38)	(0.44,1.87)	(9.65,11.02)	(-10.17,-8.14)
	[0.00]	[0.00]	[0.00]	[0.00]	[0.00]	[0.00]

Notes: Medians over 250 splits. Median confidence interval ($\alpha = .05$) in parenthesis. P-values for
the hypothesis that the parameter is equal to zero against the two-sided alternative in brackets.

Rank-Weighted Average Treatment Effect

Yadlowsky et al. (2024) define the RANK-WEIGHTED AVERAGE TREATMENT EFFECT (RATE) induced by the estimated CATEs as follows:

$$\theta_\alpha(\hat{\tau}) := \int_0^1 \alpha(u) TOC(u; \hat{\tau}) du$$

where the TARGETING OPERATOR CHARACTERISTIC (TOC) is defined as

$$TOC(u; \hat{\tau}) := \underbrace{E[\tau(X) \mid F(\hat{\tau}(X)) \geq 1 - u]}_{\text{average effect of highest } 100u\%} - \underbrace{E[\tau(X)]}_{ATE}$$

with $F(\cdot)$ the cumulative distribution function of $\hat{\tau}(X)$, $0 < u \leq 1$, and $\alpha : (0, 1] \to \mathcal{R}$ a generic weight function.

The RATE provides a measure of the ability of estimated CATEs to prioritize units to treatment in terms of treatment benefit (assuming higher outcomes are better)

The idea is to regard $\hat{\tau}(X)$ as a "prioritization rule" sorting units according to their estimated CATEs

The $TOC(u; \hat{\tau}) := \mathbb{E}[Y(1) - Y(0) \mid F(\hat{\tau}(X)) \geq 1 - u] - \mathbb{E}[Y(1) - Y(0)]$ contrasts the average effect in the subgroup with the $100u\%$ highest estimated CATEs and ATE

If the estimated CATEs capture systematic heterogeneity, we expect that the TOC is positive throughout and largest for low values of u

Furthermore, $TOC(1; \hat{\tau}) = 0$ because $\mathbb{E}[Y(1) - Y(0) \mid F(\hat{\tau}(X)) \geq 0] = \mathbb{E}[Y(1) - Y(0)]$
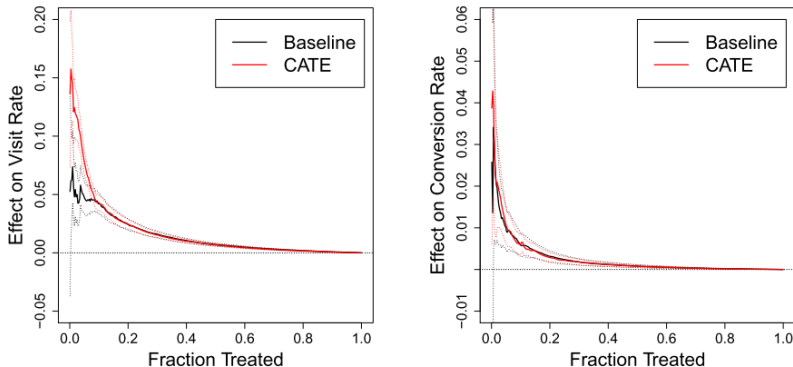
Example from Yadlowsky et al. (2024)

Figure 2. TOC curves for two prioritization rules (baseline- and CATE-based) and two outcomes (rate of visits and rate of conversion) on Criteo Uplift benchmark dataset.

Different ways to weight TOCs

Yadlowsky et al. (2024) consider three different ways to aggregate the TOCs into RATEs:

1. **High-vs-all**: Gives all weight to a particular TOC and requires to fix which fraction u of the estimated CATEs are defined as "high"

2. **Area under TOC (AUTOC)**: Takes integral under TOC curve

$$AUTOC(\hat{\tau}) = \int_0^1 TOC(u; \hat{\tau}(X))du$$

3. **Qini:** Qini coefficient gives linear weight to the TOCs

$$QINI(\hat{\tau}) = \int_0^1 uTOC(u; \hat{\tau}(X))du$$

Unifying framework

Note that all parameters defined so far can be considered as defining a new target parameter of the general form

$$\theta_{wc} = \mathbb{E}[\omega(\hat{\tau}(X))(Y(1) - Y(0))] = \mathbb{E}[\omega(\hat{\tau}(X))\tau(X)] \tag{1}$$

where $\omega(\hat{\tau}(X))$ is some weighting function that depends on some CATEs function $\hat{\tau}(X)$ being estimated in a training sample

In all cases we discussed above, we could show that $\mathbb{E}[\omega(\hat{\tau}(X))] = 0$

Therefore, we call these parameters CENTERED WEIGHTED ATE (CWATE)

The Centered Weighted ATEs perspective is instructive because

$$\theta_{wc} := \mathbb{E}[\omega(\hat{\tau}(X))\tau(X)]$$
$$= \underbrace{\mathbb{E}[\omega(\hat{\tau}(X))]}_{=0} \mathbb{E}[\tau(X)] + Cov(\omega(\hat{\tau}(X)), \tau(X))$$
$$= Cov(\omega(\hat{\tau}(X)), \tau(X))$$

$\Rightarrow$ they check whether some function of estimated CATE covaries with true CATE

We can think about all introduced strategies as testing $H_0 : \theta_{cw} = 0$

Form of the weights function

BLP: $\beta_2 = \frac{Cov[\tau(X),\hat{\tau}(X)]}{Var[\hat{\tau}(X)]} = \frac{\mathbb{E}[(\hat{\tau}(X)-\mathbb{E}[\hat{\tau}(X)])\tau(X)]}{Var[\hat{\tau}(X)]} = \mathbb{E}\left[\underbrace{\frac{\hat{\tau}(X)-\mathbb{E}[\hat{\tau}(X)]}{Var[\hat{\tau}(X)]}}_{=\omega(\hat{\tau}(X))}\tau(X)\right]$

GATES: $\gamma_K - \gamma_1 = \mathbb{E}\left[\underbrace{(\mathbb{1}[G_K]-\mathbb{1}[G_1])}_{=\omega(\hat{\tau}(X))}\tau(X)\right]$

TOC: $\omega(\hat{\tau}(X)) = \mathbb{1}[F(\hat{\tau}(X)) \geq 1-u]/u$

AUTOC: $\omega(\hat{\tau}(X)) = -log(1-F(\hat{\tau}(X))) - 1$

QINI: $\omega(\hat{\tau}(X)) = F(\hat{\tau}(X)) - 1/2$

Unifying framework for estimation

One beautiful aspect of this common structure is that we can leverage a good old buddy for estimation, the pseudo-outcome $\tilde{Y}_{ATE}$

We know it is an unbiased signal of the CATE

Therefore estimation of all parameters introduced today can be cast in terms of the pseudo-outcome:

- BLP: $(\beta_1, \beta_2) = \arg\min_{b_1, b_2} \mathbb{E}\{[\tilde{Y}_{ATE} - b_1 - b_2(\hat{\tau}(X) - \mathbb{E}[\hat{\tau}(X)])]^2\}$
- GATES: $(\gamma_1, ..., \gamma_K) = \arg\min_g \mathbb{E}\{[\tilde{Y}_{ATE} - \sum_k g_k \mathbb{1}[G_k]]^2\}$
- TOC: $\widehat{TOC}(u; \hat{\tau}) = \frac{1}{\lfloor uN \rfloor} \sum_{j=1}^{\lfloor uN \rfloor} \tilde{Y}_{ATE, i(j)} - \frac{1}{N} \sum_{i=1}^{N} \tilde{Y}_{ATE, i}$
  where we sort units $i = 1, ..., N$ in order $j = 1, ..., N$
- RATE: $\frac{1}{N} \sum_{j=1}^{N} \alpha\left(\frac{j}{N}\right) \widehat{TOC}\left(\frac{j}{N}; \hat{\tau}\right)$

More ideas how to validate flexible CATE predictions:

- Calibration Error for Heterogeneous Treatment Effects (Xu & Yadlowsky, 2022)
- More on GATES in RCTs (Imai & Li, 2024)

How to describe/understand CATEs?

What "drives" heterogeneity?

If BLP and GATES indicate that our algorithms detect systematic effect heterogeneity, we usually would like to understand which covariates are most predictive

However, the causal ML methods do not produce seemingly easy to interpret OLS outputs or something similar

I am currently aware of two options:

1. Rely on classic variable importance measures from the supervised ML literature inheriting all their strengths and weaknesses (see e.g. Interpretable ML by Molnar or Explanatory Model Analysis by Biecek & Burzykowski)

2. Run a Classification Analysis of Chernozhukov et al. (2025)

Classification Analysis

Definition CLAN

CLASSIFICATION ANALYSIS (CLAN) compares the covariate values of the "least affected group" G_1 with the "most affected group" G_K defined for the GATES:

$$\delta_K - \delta_1$$

where $\delta_1 = \mathbb{E}[X \mid G_1]$ and $\delta_K = \mathbb{E}[X \mid G_K]$

This can be achieved by simple mean comparison in the test sample for a single train/test split

Again Chernozhukov et al. show how to aggregate results from repeated splits

Classification Analysis - example

TABLE 5. CLAN of Immunization Incentives

	Elastic Net			Nnet		
	20% Most (δ_5)	20% Least (δ_1)	Difference $(\delta_5 - \delta_1)$	20% Most (δ_5)	20% Least (δ_1)	Difference $(\delta_5 - \delta_1)$
Number of vaccines to pregnant mother	2.187 (2.115,2.259) -	2.277 (2.212,2.342) -	-0.081 (-0.180,0.015) [0.190]	2.174 (2.111,2.234) -	2.285 (2.224,2.345) -	-0.112 (-0.202,-0.028) [0.019]
Number of vaccines to child since birth	4.077 (3.858,4.304) -	4.639 (4.444,4.859) -	-0.562 (-0.863,-0.260) [0.001]	4.264 (4.091,4.434) -	4.734 (4.549,4.900) -	-0.490 (-0.739,-0.250) [0.000]
Fraction of children received polio drops	0.998 (0.995,1.001) -	1.000 (0.997,1.003) -	-0.002 (-0.006,0.002) [0.683]	1.000 (1.000,1.000) -	1.000 (1.000,1.000) -	0.000 (0.000,0.000) [0.943]
Number of polio drops to child	2.955 (2.935,2.974) -	2.993 (2.976,3.010) -	-0.037 (-0.063,-0.010) [0.013]	2.965 (2.953,2.977) -	2.998 (2.985,3.010) -	-0.032 (-0.049,-0.016) [0.000]
Fraction of children received immunization card	0.803 (0.754,0.851) -	0.926 (0.882,0.969) -	-0.121 (-0.187,-0.054) [0.001]	0.908 (0.881,0.932) -	0.927 (0.898,0.959) -	-0.027 (-0.059,0.007) [0.217]
Fraction of children received Measles vaccine by 15 months of age	0.133 (0.097,0.169) -	0.243 (0.209,0.276) -	-0.106 (-0.153,-0.056) [0.000]	0.126 (0.095,0.159) -	0.260 (0.228,0.291) -	-0.131 (-0.176,-0.085) [0.000]
Fraction of children received Measles vaccine at credible locations	0.293 (0.246,0.338) -	0.399 (0.358,0.444) -	-0.110 (-0.174,-0.045) [0.002]	0.289 (0.246,0.331) -	0.433 (0.391,0.475) -	-0.142 (-0.206,-0.084) [0.000]

Ceterum censeo a fancy method alone is not a credible identification strategy
$\Rightarrow$ separate identification and estimation