Generic Machine Learning Inference on Heterogeneous Treatment Effects Using the Package `GenericML`

Max Welz[1,2] Andreas Alfons[1] Mert Demirer[3]
Victor Chernozhukov[3]

[1]Erasmus School of Economics, Erasmus University Rotterdam
[2]Erasmus University Medical Center (Erasmus MC)
[3]Massachusetts Institute of Technology

useR!, June 21, 2022

Motivation

Recent literature in causal inference is focused on heterogeneous treatment effects

- Often based on Machine Learning (ML) techniques
- Goal: Consistent estimation and uniformly valid inference on conditional average treatment effect (CATE)

⟶ Difficult w/o strong assumptions, especially in high dimensions!

⟶ Generic Machine Learning Inference (Generic ML; Chernozhukov, Demirer, Duflo, and Fernández-Val, 2020) remedies this in randomized experiments

Motivation

Recent literature in causal inference is focused on heterogeneous treatment effects

- Often based on Machine Learning (ML) techniques
- Goal: Consistent estimation and uniformly valid inference on conditional average treatment effect (CATE)

⟶ Difficult w/o strong assumptions, especially in high dimensions!

⟶ Generic Machine Learning Inference (Generic ML; Chernozhukov, Demirer, Duflo, and Fernández-Val, 2020) remedies this in randomized experiments

Motivation

Recent literature in causal inference is focused on heterogeneous treatment effects

- Often based on Machine Learning (ML) techniques
- Goal: Consistent estimation and uniformly valid inference on conditional average treatment effect (CATE)

⟶ Difficult w/o strong assumptions, especially in high dimensions!

⟶ Generic Machine Learning Inference (Generic ML; Chernozhukov, Demirer, Duflo, and Fernández-Val, 2020) remedies this in randomized experiments

Setup

Let

- Y be the outcome
- Z be a possibly high-dimensional vector of covariates
- D be a binary treatment assignment variable

$\longrightarrow$ Observe $(Y_i, Z_i, D_i)_{i=1}^{N}$ as i.i.d. copies of (Y, Z, D)

$\longrightarrow$ Assume unconfoundedness and random treatment assignment

A Very General Model

We consider the very general model

$$Y = b_0(Z) + Ds_0(Z) + U, \qquad \mathrm{E}[U \mid Z, D] = 0,$$

where

$$b_0(Z) = \mathrm{E}[Y \mid D = 0, Z]$$

is the baseline conditional average (BCA), and

$$s_0(Z) = \mathrm{E}[Y \mid D = 1, Z] - \mathrm{E}[Y \mid D = 0, Z]$$

is the conditional average treatment effect (CATE)

A Very General Model

We consider the very general model

$$Y = b_0(Z) + Ds_0(Z) + U, \qquad \mathrm{E}[U \mid Z, D] = 0,$$

where

$$b_0(Z) = \mathrm{E}[Y \mid D = 0, Z]$$

is the baseline conditional average (BCA), and

$$s_0(Z) = \mathrm{E}[Y \mid D = 1, Z] - \mathrm{E}[Y \mid D = 0, Z]$$

is the conditional average treatment effect (CATE)

A Very General Model

We consider the very general model

$$Y = b_0(Z) + Ds_0(Z) + U, \qquad \mathrm{E}[U \mid Z, D] = 0,$$

where

$$b_0(Z) = \mathrm{E}[Y \mid D = 0, Z]$$

is the baseline conditional average (BCA), and

$$s_0(Z) = \mathrm{E}[Y \mid D = 1, Z] - \mathrm{E}[Y \mid D = 0, Z]$$

is the conditional average treatment effect (CATE)

Focus of Generic ML

Generic ML focuses on estimation and inference on

key features of $s_0(Z)$ rather than $s_0(Z)$ itself

$\longrightarrow$ No need for consistent estimation of $s_0(Z)$ or $b_0(Z)$!

Focus of Generic ML

Generic ML focuses on estimation and inference on

key features of $s_0(Z)$ rather than $s_0(Z)$ itself

$\longrightarrow$ No need for consistent estimation of $s_0(Z)$ or $b_0(Z)$!

Generic ML

1. Randomly partition the data in two disjoint sets A and M
2. On set A, use some machine learner to obtain estimates $B(Z)$ and $S(Z)$ of $b_0(Z)$ and $s_0(Z)$, respectively
3. On set M, calculate the key features of $s_0(Z)$

Two sources of uncertainty:

- Estimation uncertainty (conditional on set A) from Step 2
- Splitting uncertainty from the sample splitting in Step 1

⟶ Address by repeating Steps 1–3 many times

Generic ML

1. Randomly partition the data in two disjoint sets A and M
2. On set A, use some machine learner to obtain estimates $B(Z)$ and $S(Z)$ of $b_0(Z)$ and $s_0(Z)$, respectively
3. On set M, calculate the key features of $s_0(Z)$

Two sources of uncertainty:

- Estimation uncertainty (conditional on set A) from Step 2
- Splitting uncertainty from the sample splitting in Step 1

⟶ Address by repeating Steps 1–3 many times

Generic ML

1. Randomly partition the data in two disjoint sets A and M
2. On set A, use some machine learner to obtain estimates $B(Z)$ and $S(Z)$ of $b_0(Z)$ and $s_0(Z)$, respectively
3. On set M, calculate the key features of $s_0(Z)$

Two sources of uncertainty:

- Estimation uncertainty (conditional on set A) from Step 2
- Splitting uncertainty from the sample splitting in Step 1

⟶ Address by repeating Steps 1–3 many times

Inference

Variational Estimation and Inference (VEIN):

- Fix significance level $\alpha \in (0, 0.5)$
- Calculate the key features across *S* splits of the data
- Take medians across the *S* splits of each key feature parameter

$\longrightarrow$ Inference on each key feature parameter with size control of level 2α

$\longrightarrow$ Can be repeated for many machine learners (report the "best" one)

Software Implementation

Package `GenericML` (Welz, Alfons, Demirer, and Chernozhukov, 2022)

- CRAN: `https://CRAN.R-project.org/package=GenericML`
- GitHub: `https://github.com/mwelz/GenericML`

⟶ Flexible, user-friendly, fast, object-oriented

⟶ Based on `mlr3` ecosystem of Lang et al. (2019)

Empirical Example: Setup

We revisit Crépon et al.'s (2015) study on the effects of microcredits[1]

⟶ Sample: 162 villages in rural Morocco, divided into 81 similar pairs

⟶ Randomly select one village in each pair and make microcredits available for the residents

⟶ Measure if total borrowing changes

---

[1] We thank Esther Duflo for making the data available to us

Empirical Example: Data

Household-level data on $N = 5,513$ households

- Dependent variable Y: total volume of borrowing
- Treatment indicator D: 1 if household can access microcredits
- Covariates Z: 97 variables (after encoding), among which

  ⟶ `head_age_bl` is age of household's head

- Grouping variables:

  ⟶ `demi_paire` is a factor of village membership
  ⟶ `vil_pair` is a factor of village pair membership

Empirical Example: Loading Data

⟶ The data are available on GitHub in repo `"mwelz/GenericML"`

⟶ Slides and replication files are in the subfolder `"slides"` of this repo

```
R> ## load data, available in GitHub repo mwelz/GenericML
R> url_data <-
+    url(paste0(
+      "https://github.com/mwelz/GenericML/blob/main/slides",
+      "/data/morocco_preprocessed.Rdata?raw=true"
+    ))
R> load(url_data)
```

Empirical Example: Baseline Results

Crépon et al. (2015) find that microcredit availability has…

- low take-up (17% in treatment group)
- significant effect on total borrowing: ATE of MAD[2] 1,206 ($p < 0.01$)

⟶ Use `GenericML` to investigate heterogeneity in this effect!

---

[2] MAD = Moroccan Dirham

Empirical Example: Specification of Learners

⟶ Specify a suite of learners with `mlr3` syntax

⟶ Here: random forest, elastic net, support vector machine, gradient boosting

```
R> # install version 0.2.3 which is not yet on CRAN
R> # devtools::install_github("mwelz/GenericML")
R> library("GenericML")
R>
R> # specify learners
R> learners <-
+    c("random_forest",
+      "mlr3::lrn('cv_glmnet', s = 'lambda.min', alpha = 0.5)",
+      "mlr3::lrn('svm')",
+      "mlr3::lrn('xgboost')")
```

Empirical Example: Specification of Learners

⟶ Specify a suite of learners with `mlr3` syntax

⟶ Here: random forest, elastic net, support vector machine, gradient boosting

```
R> # install version 0.2.3 which is not yet on CRAN
R> # devtools::install_github("mwelz/GenericML")
R> library("GenericML")
R>
R> # specify learners
R> learners <-
+    c("random_forest",
+      "mlr3::lrn('cv_glmnet', s = 'lambda.min', alpha = 0.5)",
+      "mlr3::lrn('svm')",
+      "mlr3::lrn('xgboost')")
```

Empirical Example: Customization

Spatial data of 81 village pairs

⟶ Include fixed effects for each pair

⟶ Cluster standard errors on the village level

⟶ `GenericML` allows this through setup functions

⟶ Support for `sandwich` covariance estimators (Zeileis, 2004)

Empirical Example: Customization

`setup_X1()` customizes inclusion of controls and fixed effects

```
R> # include BCA and CATE controls
R> # add fixed effects along variable "vil_pair"
R> X1 <- setup_X1(funs_Z = c("B", "S"),
+                  fixed_effects = vil_pair)
```

`setup_vcov()` customizes covariance estimation

```
R> # calls functions from the "sandwich" package
R> # cluster standard errors along "demi_paire"
R> vcov <- setup_vcov(estimator = "vcovCL",
+                      arguments = list(cluster = demi_paire))
```

Empirical Example: Customization

`setup_X1()` customizes inclusion of controls and fixed effects

```
R> # include BCA and CATE controls
R> # add fixed effects along variable "vil_pair"
R> X1 <- setup_X1(funs_Z = c("B", "S"),
+                  fixed_effects = vil_pair)
```

`setup_vcov()` customizes covariance estimation

```
R> # calls functions from the "sandwich" package
R> # cluster standard errors along "demi_paire"
R> vcov <- setup_vcov(estimator = "vcovCL",
+                      arguments = list(cluster = demi_paire))
```

Empirical Example: Customization

`setup_X1()` customizes inclusion of controls and fixed effects

```
R> # include BCA and CATE controls
R> # add fixed effects along variable "vil_pair"
R> X1 <- setup_X1(funs_Z = c("B", "S"),
+                 fixed_effects = vil_pair)
```

`setup_vcov()` customizes covariance estimation

```
R> # calls functions from the "sandwich" package
R> # cluster standard errors along "demi_paire"
R> vcov <- setup_vcov(estimator = "vcovCL",
+                     arguments = list(cluster = demi_paire))
```

Empirical Example: Customization

`setup_X1()` customizes inclusion of controls and fixed effects

```
R> # include BCA and CATE controls
R> # add fixed effects along variable "vil_pair"
R> X1 <- setup_X1(funs_Z = c("B", "S"),
+                  fixed_effects = vil_pair)
```

`setup_vcov()` customizes covariance estimation

```
R> # calls functions from the "sandwich" package
R> # cluster standard errors along "demi_paire"
R> vcov <- setup_vcov(estimator = "vcovCL",
+                      arguments = list(cluster = demi_paire))
```

`GenericML` Interface

```
R> genML <- GenericML(
+    Z = Z, D = D, Y = Y,                      # observed data
+    learners_GenericML = learners,            # learners
+    learner_propensity_score = "constant",    # = 0.5 (RCT)
+    num_splits = 100L,                        # number splits
+    quantile_cutoffs = c(0.2, 0.4, 0.6, 0.8), # grouping
+    significance_level = 0.05,                # significance level
+    X1_BLP = X1, X1_GATES = X1,               # regression setup
+    vcov_BLP = vcov, vcov_GATES = vcov,       # covariance setup
+    parallel = TRUE, num_cores = 6L,          # parallelization
+    seed = 20220621)                          # RNG seed
```

…and many more arguments for fine-tuning!

⟶ stratified sampling, Horvitz-Thompson transformation…

`GenericML` Interface

```
R> genML <- GenericML(
+    Z = Z, D = D, Y = Y,                        # observed data
+    learners_GenericML = learners,              # learners
+    learner_propensity_score = "constant",      # = 0.5 (RCT)
+    num_splits = 100L,                          # number splits
+    quantile_cutoffs = c(0.2, 0.4, 0.6, 0.8), # grouping
+    significance_level = 0.05,                  # significance level
+    X1_BLP = X1, X1_GATES = X1,                 # regression setup
+    vcov_BLP = vcov, vcov_GATES = vcov,         # covariance setup
+    parallel = TRUE, num_cores = 6L,            # parallelization
+    seed = 20220621)                            # RNG seed
```

…and many more arguments for fine-tuning!

⟶ stratified sampling, Horvitz-Thompson transformation…

Analysis of `GenericML` Objects

Methods for the analysis of the *key features* of CATE

- `get_BLP()`
- `get_GATES()`
- `get_CLAN()`

⟶ linked to rich `plot()` and `print()` methods

Empirical Example: `get_BLP()`

Best Linear Predictor (BLP): Estimates some (β_1, β_2) via OLS:

- $\beta_1 = \mathrm{E}s_0(Z)$ is the ATE
- $\beta_2 \neq 0$ if there is heterogeneity in $s_0(Z)$ and $S(Z)$ predicts it well

```
R> results_BLP <- get_BLP(genML, plot = TRUE)
R> results_BLP # print method
BLP generic targets
---
         Estimate   CI lower CI upper p value
beta.1 1113.50155  273.02645 1935.274 0.00945 **
beta.2    0.35315   -0.04384    0.698 0.08613 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

Empirical Example: `get_BLP()`

Best Linear Predictor (BLP): Estimates some (β_1, β_2) via OLS:

- $\beta_1 = \mathrm{E}s_0(Z)$ is the ATE
- $\beta_2 \neq 0$ if there is heterogeneity in $s_0(Z)$ and $S(Z)$ predicts it well

```
R> results_BLP <- get_BLP(genML, plot = TRUE)
R> results_BLP # print method
BLP generic targets
---
         Estimate   CI lower CI upper p value
beta.1 1113.50155  273.02645 1935.274 0.00945 **
beta.2    0.35315   -0.04384    0.698 0.08613 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

Empirical Example: `get_BLP()`

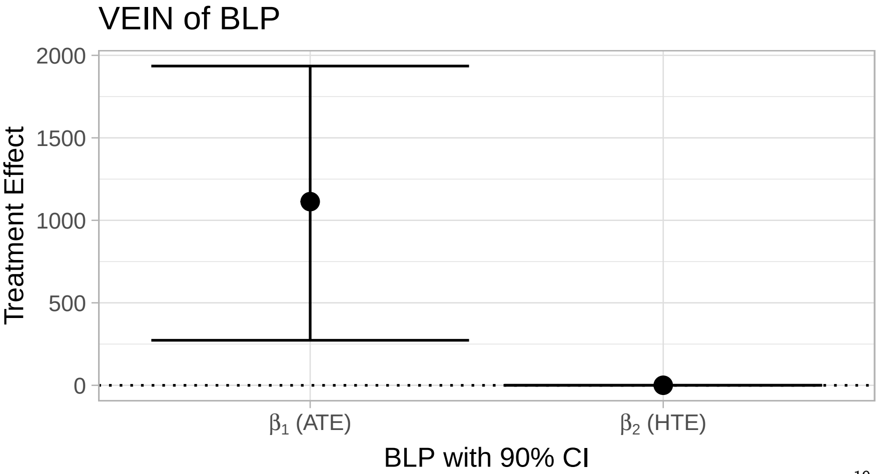
Best Linear Predictor (BLP): Estimates some (β_1, β_2) via OLS:

- $\beta_1 = \mathrm{E}s_0(Z)$ is the ATE
- $\beta_2 \neq 0$ if there is heterogeneity in $s_0(Z)$ and $S(Z)$ predicts it well

```
R> results_BLP <- get_BLP(genML, plot = TRUE)
R> results_BLP # print method
BLP generic targets
---
          Estimate   CI lower CI upper p value
beta.1 1113.50155  273.02645 1935.274 0.00945 **
beta.2    0.35315   -0.04384    0.698 0.08613 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

Empirical Example: `get_BLP()`

```
R> plot(results_BLP) # plot method
```



Empirical Example: `get_GATES()`

Sorted Group Average Treatment Effects (GATES): Build groups

$$G_k := \{S(Z) \in I_k\}, \quad k = 1, \dots, K,$$

where $I_k = [\ell_{k-1}, \ell_k)$ divide the support of $S(Z)$ into regions

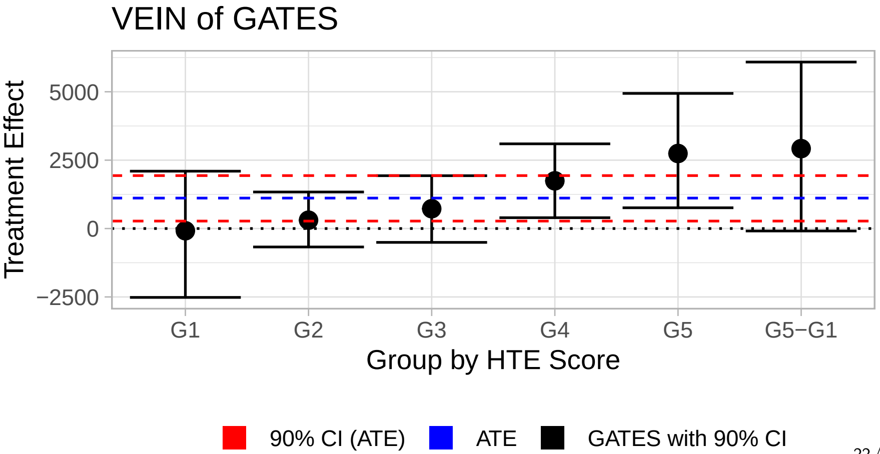
$\longrightarrow$ Estimate group-ATE $\gamma_k := \mathrm{E}[s_0(Z) \mid G_k]$ via OLS

Empirical Example: `get_GATES()`

```
R> results_GATES <- get_GATES(genML, plot = TRUE)
R> results_GATES
GATES generic targets
---
                Estimate CI lower CI upper p value
gamma.1           -80.44 -2517.30     2097 0.93525
gamma.2           305.50  -674.10     1336 0.49251
gamma.3           725.63  -505.53     1932 0.19349
gamma.4          1744.51   395.93     3097 0.01225 *
gamma.5          2743.76   759.85     4940 0.00911 **
gamma.5-gamma.1  2922.13   -89.43     6087 0.05536 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

Empirical Example: `get_GATES()`

```
R> plot(results_GATES)
```



Empirical Example: `get_CLAN()`

Classification Analysis (CLAN): Observed within-group averages, δ_k, of a variable for groups G_k

```
R> results_CLAN <-
+    get_CLAN(genML, variable = "head_age_bl", plot = TRUE)
R> results_CLAN
CLAN generic targets for variable 'head_age_bl'
---
                Estimate CI lower CI upper  p value
delta.1            36.49    34.46   38.554  < 2e-16 ***
delta.2            43.66    42.12   45.210  < 2e-16 ***
delta.3            41.40    39.50   43.258  < 2e-16 ***
delta.4            34.75    32.55   36.853  < 2e-16 ***
delta.5            23.85    21.53   26.151  < 2e-16 ***
delta.5-delta.1   -12.52   -15.61   -9.514 4.44e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

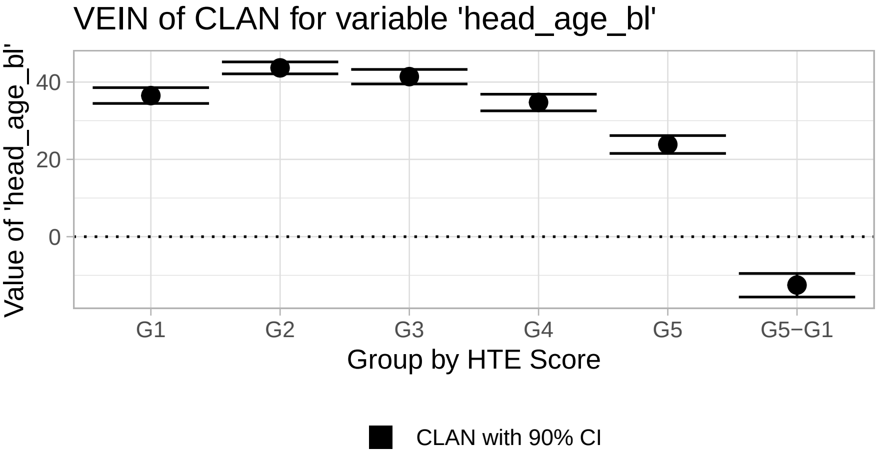
Empirical Example: `get_CLAN()`

Classification Analysis (CLAN): Observed within-group averages, δ_k, of a variable for groups G_k

```
R> results_CLAN <-
+    get_CLAN(genML, variable = "head_age_bl", plot = TRUE)
R> results_CLAN
CLAN generic targets for variable 'head_age_bl'
---
                Estimate CI lower CI upper  p value
delta.1            36.49    34.46   38.554  < 2e-16 ***
delta.2            43.66    42.12   45.210  < 2e-16 ***
delta.3            41.40    39.50   43.258  < 2e-16 ***
delta.4            34.75    32.55   36.853  < 2e-16 ***
delta.5            23.85    21.53   26.151  < 2e-16 ***
delta.5-delta.1   -12.52   -15.61   -9.514 4.44e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
---
Confidence level of confidence interval [CI lower, CI upper]: 90 %
```

Empirical Example: `get_CLAN()`

```
R> plot(results_CLAN)
```



Conclusions and Discussion

Conclusions

- ⟶ High-dimensional uniformly valid inference on CATE is hard
- ⟶ Generic ML can do so under minimal assumptions by focusing on key features of CATE instead of CATE itself
- ⟶ R package `GenericML` available on CRAN

Future work

- ⟶ Implement monotonization of confidence bounds
- ⟶ Enable support for deep learning, perhaps via `mlr3keras`

Conclusions and Discussion

Conclusions

- ⟶ High-dimensional uniformly valid inference on CATE is hard
- ⟶ Generic ML can do so under minimal assumptions by focusing on key features of CATE instead of CATE itself
- ⟶ R package `GenericML` available on CRAN

Future work

- ⟶ Implement monotonization of confidence bounds
- ⟶ Enable support for deep learning, perhaps via `mlr3keras`

References

Victor Chernozhukov, Mert Demirer, Esther Duflo, and Iván Fernández-Val. Generic Machine Learning Inference on Heterogenous Treatment Effects in Randomized Experiments. **arXiv preprint: arXiv:1712.04802**, 2020.

Bruno Crépon, Florencia Devoto, Esther Duflo, and William Parienté. Estimating the Impact of Microcredit on Those Who Take It Up: Evidence from a Randomized Experiment in Morocco. **American Economic Journal: Applied Economics**, 7(1):123–150, 2015.

Michel Lang, Martin Binder, Jakob Richter, Patrick Schratz, Florian Pfisterer, Stefan Coors, Quay Au, Giuseppe Casalicchio, Lars Kotthoff, and Bernd Bischl. `mlr3`: A Modern Object-Oriented Machine Learning Framework in R. **Journal of Open Source Software**, 4 (44):1903, 2019.

Max Welz, Andreas Alfons, Mert Demirer, and Victor Chernozhukov. **`GenericML`: Generic Machine Learning Inference**, 2022. URL `https://CRAN.R-project.org/package=GenericML`. R package version 0.2.2.

Achim Zeileis. Econometric Computing with HC and HAC Covariance Matrix Estimators. **Journal of Statistical Software**, 11(10):1–17, 2004.

Algorithm 1 in Chernozhukov et al. (2020)

```
 IN: Data = $(Y_i, Z_i, D_i)_{i=1}^{N}$, significance level $\alpha$, a suite of ML methods, number of
     splits $S$
OUT: $p$-values and $(1-2\alpha)$ confidence intervals of point estimates of each target
     parameter in GATES, BLP, and CLAN

❶ Compute propensity scores $p(Z_i), i = 1, \ldots, N$
❷ Do $S$ splits of $\{1, \ldots, N\}$ into disjoint sets $A$ and $M$ of same size
❸ for each ML method and each split $s = 1, \ldots, S$, do
    ⓐ Tune and train each ML method to learn $B(\cdot)$ and $S(\cdot)$ on $A$
    ⓑ On $M$, use $B(\cdot)$ and $S(\cdot)$ to estimate the BLP, GATES, CLAN target
      parameters
    ⓒ Compute some performance measures for the ML methods
❹ Choose the best ML method based on the medians of the performance measures
❺ Calculate the medians of the confidence bounds, $p$-values, and point estimates of
  each target parameter
❻ Adjust the confidence bounds and $p$-values
```

Best Learner

Compute two performance measures for each learner

$$\widehat{\Lambda} = |\widehat{\beta}_2|^2 \ \widehat{\mathsf{Var}}(S(Z)), \qquad \widehat{\bar{\Lambda}} = \frac{1}{K}\sum_{k=1}^{K} \widehat{\gamma}_k^2$$

$\longrightarrow$ Best learner maximizes their median across S splits
$\longrightarrow$ In the empirical example, that's random forest (get via `get_best()`)