

Day 2, Lecture 2

Targeting: Changing the target

# Targeted learning framework

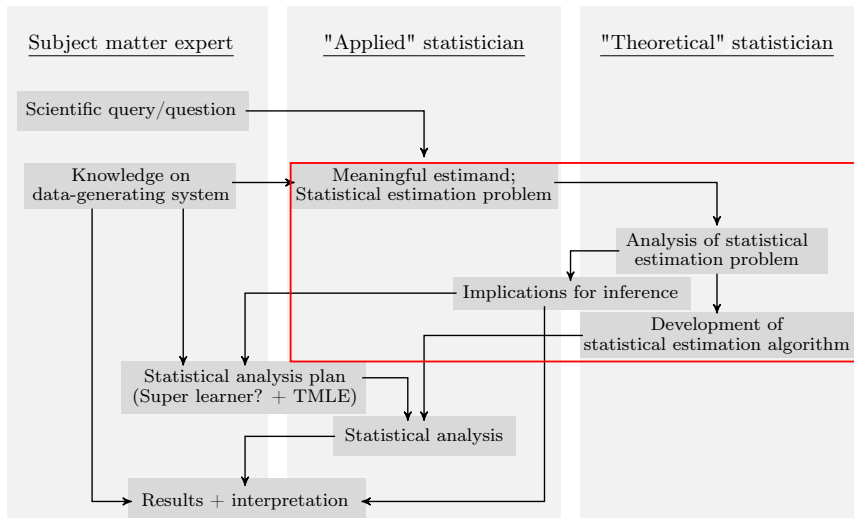
In this lecture, our goal is to:

1. Summarize the steps involved in analyzing and constructing Targeted Minimum Loss-based Estimation (TMLE) estimators for a new estimation problem, using a specific example as a reference point.

# Targeted learning framework



# Targeted learning framework



# Changing the target

## ATE: Statistical estimation problem

$O_1, \dots, O_n \stackrel{iid}{\sim} P_0$ ,  $O_i$  is the observation for individual  $i$  of the dataset, consists of

- ▶ Covariates:  $X_i \in \mathcal{X} \subseteq \mathbb{R}^d$
- ▶ Exposure/treatment:  $A_i \in \{0, 1\}$
- ▶ Outcome:  $Y_i \in \{0, 1\}$  or  $Y \in \mathbb{R}$

We are interested in:

$$\Psi(P) = \tilde{\Psi}(f, \mu_X) = \int_{\mathbb{R}} (f(1, x) - f(0, x)) d\mu_X(x),$$

where  $f(a, x) = \mathbb{E}_P[Y \mid A = a, X = x]$ .

A plug-in estimator requires an estimator  $\hat{f}_n$  for  $f$ :

$$\hat{\psi}_n = \tilde{\Psi}(\hat{f}_n, \mathbb{P}_n) = \frac{1}{n} \sum_{i=1}^n (\hat{f}_n(1, X_i) - \hat{f}_n(0, X_i)).$$

# Changing the target

What is the interpretation?

**Causal interpretation ATE:** The risk difference, had everyone in the population been treated versus had everyone in the population been untreated.

## Changing the target

In an observational study, the de facto treated and the de facto untreated groups may differ quite a lot.

Sometimes we may be interested in the effect averaged with respect to the distribution of covariates *in the treated population*.

⇒ the average treatment effect among the treated.

## Changing the target: Average treatment effect among the treated

**Causal interpretation ATE:** The risk difference, had everyone in the population been treated versus had everyone in the population been untreated.

**Causal interpretation ATT:** The risk difference, had everyone in the treated population been treated versus had everyone in the untreated population been untreated.



## Changing the target: Average treatment effect among the treated

The relevance of this is linked to heterogeneity in treatment effects.

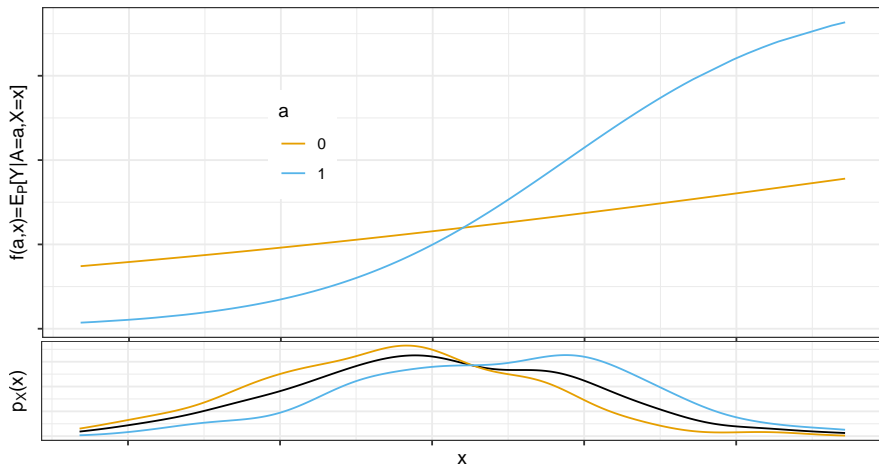
- ▶ Treated and untreated subjects may be very different, and may benefit very differently from treatment.

This is what we would put under the term "interaction effects" in classical parametric regression analysis.

(This is not about confounding, but rather about understanding how the treatment interacts with different characteristics of the population).

In many real-world settings, we may care more about how effective a treatment is for the specific group of individuals who are treated, rather than the general population (e.g., those who chose to be vaccinated, patients receiving a new cancer therapy, or individuals with a particular genetic profile).

## Changing the target: Average treatment effect among the treated



The **X-standardized ATE** is the average of the difference between the two lines  $x \mapsto \mu_P(1, x)$  and  $x \mapsto \mu_P(0, x)$  (upper panel), with the average taken with respect to the marginal distribution of  $X$  (lower panel).

## Changing the target: Average treatment effect among the treated

### Average treatment effect (ATE)

- ▶  $O = (X, A, Y) \in \mathbb{R}^d \times \{0, 1\} \times \{0, 1\}$
- ▶ The ATE is defined for  $P \in \mathcal{M}$  as

$$\Psi(P) = \mathbb{E}_P[\mathbb{E}_P[Y \mid A = 1, X] - \mathbb{E}_P[Y \mid A = 0, X]]$$

- ▶ Under causal assumptions:

$$\Psi(P) = \mathbb{E}_P[Y^1] - \mathbb{E}_P[Y^0]$$

## Changing the target: Average treatment effect among the treated

### Average treatment effect among the treated (ATT)

- ▶  $O = (X, A, Y) \in \mathbb{R}^d \times \{0, 1\} \times \{0, 1\}$
- ▶ The ATT is defined for  $P \in \mathcal{M}$  as

$$\Psi(P) = \mathbb{E}_P[\mathbb{E}_P[Y \mid A = 1, X] - \mathbb{E}_P[Y \mid A = 0, X] \mid A = 1]$$

- ▶ Under causal assumptions:

$$\Psi(P) = \mathbb{E}_P[Y^1 \mid A = 1] - \mathbb{E}_P[Y^0 \mid A = 1]$$

This changes the statistical estimation problem and thus the TMLE.

## Changing the target: Average treatment effect among the treated

The ATT parameter is a difference of two parts

$$\Psi(P) = \underbrace{\mathbb{E}_P[\mathbb{E}_P[Y \mid A = 1, X] \mid A = 1]}_{\Psi^1(P)} - \underbrace{\mathbb{E}_P[\mathbb{E}_P[Y \mid A = 0, X] \mid A = 1]}_{=\Psi^0(P)}$$

where  $\Psi^0(P)$  is the interesting/challenging part. We rewrite this as

$$\begin{aligned}\Psi^0(P) &= \mathbb{E}_P[\mathbb{E}_P[Y \mid A = 0, X] \mid A = 1] \\ &= \int_{\mathcal{X}} f_P(0, x) P(X \in dx \mid A = 1) \\ &= \int_{\mathcal{X}} f_P(0, x) \frac{P(X \in dx, A = 1)}{P(A = 1)} \\ &= \int_{\mathcal{X}} f_P(0, x) \frac{\pi_P(1 \mid x)}{\bar{\pi}} d\mu_X(x),\end{aligned}$$

with  $\bar{\pi}(a) = P(A = a)$  is the marginal distribution of  $A$ .

## Changing the target: Average treatment effect among the treated

Thus, the ATT can be identified as the statistical parameter:

$$\begin{aligned}\Psi(P) &= \mathbb{E}_P[\mathbb{E}_P[Y \mid A = 1, X] - \mathbb{E}_P[Y \mid A = 0, X] \mid A = 1] \\ &= \int_{\mathbb{R}^d} (f(1, x) - f(0, x)) \frac{\pi(1 \mid x)}{\bar{\pi}(1)} d\mu_X(x)\end{aligned}$$

where:

- ▶  $f(a, x) = \mathbb{E}_P[Y \mid A = a, X = x]$
- ▶  $\pi(a \mid x) = P(A = a \mid X = x)$
- ▶  $\bar{\pi}(a) = P(A = a)$  is the marginal distribution of  $A$
- ▶  $\mu_X$  is the marginal distribution of  $X$

## Targeting step: Average treatment effect on the treated

### EXAMPLE: Average treatment effect (ATE)

**Step 1** Construct initial estimators  $\hat{f}_n, \hat{\pi}_n$  for  $f, \pi$

**Step 2** Update the estimator  $\hat{f}_n \mapsto \hat{f}_n^*$  for  $f$  such that  $\hat{f}_n^*$  for the fixed  $\hat{\pi}_n$  solves the efficient influence curve equation

For the ATE, Step 2 is simply just an additional logistic regression step.

## Targeting step: Average treatment effect on the treated

EXAMPLE: Average treatment effect among the treated (ATT)

Step 1 Construct initial estimators  $\hat{f}_n, \hat{\pi}_n$  for  $f, \pi$

Step 2 Update the estimator  $\hat{f}_n \mapsto \hat{f}_n^*$  for  $f$  and the estimator  $\hat{\pi}_n \mapsto \hat{\pi}_n^*$  for  $\pi$  such that  $\hat{f}_n^*, \hat{\pi}_n^*$  solves the efficient influence curve equation

For the ATE, Step 2 is simply just an additional logistic regression step.

For the ATT, Step 2 is an iterative algorithm with recursive steps of additional logistic regressions.



## Targeting step: Average treatment effect on the treated

We can write the ATT target parameter as

$$\begin{aligned}\Psi(P) &= \mathbb{E}_P[\mathbb{E}_P[Y \mid A = 1, X] - \mathbb{E}_P[Y \mid A = 0, X] \mid A = 1] \\ &= \int_{\mathbb{R}^d} (f(1, x) - f(0, x)) \frac{\pi(1 \mid x)}{\bar{\pi}(1)} d\mu_X(x) \\ &= \tilde{\Psi}(\mu_X, \pi, f).\end{aligned}$$

We could construct an estimator as

$$\tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n, \hat{\mu}_n) = \frac{1}{n} \sum_{i=1}^n \frac{\hat{\pi}_n(1 \mid X_i)}{\frac{1}{n} \sum_{i=1}^n \hat{\pi}_n(1 \mid X_i)} (\hat{f}_n(1, X_i) - \hat{f}_n(0, X_i)).$$

## Targeting step: Average treatment effect on the treated

... but also note that the parameter can be further rewritten as

$$\Psi(P) = \int_{\mathbb{R}^d} (f(1, x) - f(0, x)) \frac{P(X \in dx, A = 1)}{P(A = 1)},$$

and we can plug in the empirical distributions for  $P(X \in dx, A = 1)$  and  $P(A = 1)$  to construct an estimator as

$$\tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n, \hat{f}_n) = \frac{1}{n} \sum_{i=1}^n \frac{A_i}{\hat{\pi}_n} (\hat{f}_n(1, X_i) - \hat{f}_n(0, X_i)),$$

with  $\hat{\pi}_n = \frac{1}{n} \sum_{i=1}^n A_i$ .

After the TMLE algorithm has been applied, these two representations can be used interchangeably.

## Targeting step: Average treatment effect on the treated

The efficient influence curve decomposed into scores of  $f, \pi, \mu_X$ :

$$\begin{aligned}\phi_P(O) &= \left( \frac{A}{\bar{\pi}(1)} - \frac{(1-A)\pi(1|X)}{\bar{\pi}(1)\pi(0|X)} \right) (Y - f(A, X)) \\ &\quad + \frac{A}{\bar{\pi}(1)} (f(1, X) - f(0, X) - \Psi(P)) \quad (\pi, \mu_X) \\ &= \left( \frac{A}{\bar{\pi}(1)} - \frac{(1-A)\pi(1|X)}{\bar{\pi}(1)\pi(0|X)} \right) (Y - f(A, X)) \\ &\quad + \frac{f(1, X) - f(0, X) - \Psi(P)}{\bar{\pi}(1)} (A - \pi(1|X)) \quad (\pi) \\ &\quad + \frac{\pi(1|X)}{\bar{\pi}(1)} (f(1, X) - f(0, X) - \Psi(P)) \quad (\mu_X)\end{aligned}$$

## Targeting step: Average treatment effect on the treated

We can proceed with:

(i) Parametric submodel  $\{f_{P,\varepsilon_1}, \pi_{P,\varepsilon_2}, \tau_{P,\varepsilon_3} : \varepsilon_1, \varepsilon_2, \varepsilon_3 \in \mathbb{R}\}$

(ii) Loss function

$$\mathcal{L}(f, \pi, \mu_X)(O) = \mathcal{L}_1(f)(O) + \mathcal{L}_2(\pi)(O) + \mathcal{L}_3(\mu_X)(O)$$

such that: (1)  $f_{P,\varepsilon_1=0} = f, \pi_{P,\varepsilon_2=0} = \pi, \tau_{P,\varepsilon_3=0} = \mu_X$

$$(2) \left. \frac{d}{d\varepsilon_j} \right|_{\varepsilon=0} \mathcal{L}(f_{P,\varepsilon_1}, \pi_{P,\varepsilon_2}, \tau_{P,\varepsilon_3})(O) = \phi_P^j(O), j = 1, 2, 3,$$

where:

$$\begin{aligned}\phi_P^1(O) &= \left( \frac{A}{\bar{\pi}(1)} - \frac{(1-A)\pi(1|X)}{\bar{\pi}(1)\pi(0|X)} \right) (Y - f(A, X)), \\ \phi_P^2(O) &= \frac{f(1, X) - f(0, X) - \Psi(P)}{\bar{\pi}(1)} (A - \pi(1|X)), \\ \phi_P^3(O) &= \frac{\pi(1|X)}{\bar{\pi}(1)} (f(1, X) - f(0, X) - \Psi(P)).\end{aligned}$$

## Targeting step: Average treatment effect on the treated

(i) Loss functions:

$$\mathcal{L}_1(f)(O) = -\left(Y \log(f(A, X)) + (1 - Y) \log(1 - f(A, X))\right)$$

$$\mathcal{L}_2(\pi)(O) = -\left(A \log(\pi(1 | X)) + (1 - A) \log(1 - \pi(1 | X))\right)$$

(ii) Logistic regression models:

$$f_{P,\varepsilon}(A, X) = \text{expit}(\text{logit}(f(A, X)) + \varepsilon H_1(\pi)(A, X))$$

$$\pi_{P,\varepsilon}(X) = \text{expit}(\text{logit}(\pi(1 | X)) + \varepsilon H_2(f, \pi, \mu_X)(X))$$

with the clever covariates:

$$H_1(\pi)(A, X) = \left( \frac{A}{\bar{\pi}(1)} - \frac{(1 - A)\pi(1 | X)}{\bar{\pi}(1)\pi(0 | X)} \right),$$

$$H_2(f, \pi, \mu_X)(X) = \frac{f(1, X) - f(0, X) - \tilde{\Psi}(\mu_X, \pi_P, f)}{\bar{\pi}(1)}.$$

## Targeting step: Average treatment effect on the treated

For the marginal distribution of  $X$ , we can define the submodel  $\{\mu_{X,\varepsilon_3} : \varepsilon_3 \in \mathbb{R}\}$  as

$$d\mu_{X,\varepsilon} = (1 + \varepsilon\phi_3^*(P))d\mu_X,$$

and the log-likelihood loss  $\mathcal{L}_3(\mu_X) = -\log(d\mu_X)$ .

But again, we will see that this does not matter.

## Targeting step: Average treatment effect on the treated

Iterative algorithm:

Given initial estimators  $\hat{f}_n^0, \hat{\pi}_n^0$ :

- ▶ Obtain estimate  $\hat{\varepsilon}_1^0$  for  $\varepsilon$ :

$$\hat{f}_{n,\varepsilon}(A, X) = \text{expit}(\text{logit}(\hat{f}_n^0(A, X)) + \varepsilon H_1(\hat{\pi}_n^0)(A, X))$$

(regress  $Y$  on covariate  $H_1(\hat{\pi}_n^0)(A, X)$  with offset  $\text{logit}(\hat{f}_n^0(A, X))$ )

- ▶ Update:  $\hat{f}_n^1 := \hat{f}_{n,\hat{\varepsilon}_1^0}^0$ .

- ▶ Obtain estimate  $\hat{\varepsilon}_2^0$  for  $\varepsilon$ :

$$\hat{\pi}_{n,\varepsilon}(X) = \text{expit}(\text{logit}(\hat{\pi}_n^0(1 | X)) + \varepsilon H_2(\hat{f}_n^1, \hat{\pi}_n^1, \hat{\mu}_{X,n})(X))$$

(regress  $A$  on covariate  $H_2(\hat{f}_n^1, \hat{\pi}_n^1, \hat{\mu}_{X,n})(X)$  with offset  $\text{logit}(\hat{\pi}_n^0(1 | X))$ )

- ▶ Update:  $\hat{\pi}_n^1 := \hat{\pi}_{n,\hat{\varepsilon}_2^0}^0$ .

## Targeting step: Average treatment effect on the treated

Iterative algorithm:

Iteratively from  $k$  to  $k + 1$ , given current estimators  $\hat{f}_n^k, \hat{\pi}_n^k$ :

- ▶ Obtain estimate  $\hat{\varepsilon}_1^k$  for  $\varepsilon$ :

$$\hat{f}_{n,\varepsilon}^k(A, X) = \text{expit}(\text{logit}(\hat{f}_n^k(A, X)) + \varepsilon H_1(\hat{\pi}_n^k)(A, X))$$

(regress  $Y$  on covariate  $H_1(\hat{\pi}_n^k)(A, X)$  with offset  $\text{logit}(\hat{f}_n^k(A, X))$ )

- ▶ Update:  $\hat{f}_n^{k+1} := \hat{f}_{n,\hat{\varepsilon}_1^k}^k$ .

- ▶ Obtain estimate  $\hat{\varepsilon}_2^k$  for  $\varepsilon$ :

$$\hat{\pi}_{n,\varepsilon}^k(X) = \text{expit}(\text{logit}(\hat{\pi}_n^k(1 | X)) + \varepsilon H_2(\hat{f}_n^{k+1}, \hat{\pi}_n^{k+1}, \hat{\mu}_{X,n})(X))$$

(regress  $A$  on covariate  $H_2(\hat{f}_n^{k+1}, \hat{\pi}_n^{k+1}, \hat{\mu}_{X,n})(X)$  with offset  $\text{logit}(\hat{\pi}_n^k(1 | X))$ )

- ▶ Update:  $\hat{\pi}_n^{k+1} := \hat{\pi}_{n,\hat{\varepsilon}_2^k}^k$ .



## Targeting step: Average treatment effect on the treated

In each step  $k$  note that:

$$\frac{1}{n} \sum_{i=1}^n \left( \frac{A_i}{\hat{\pi}_n(1)} - \frac{(1 - A_i) \hat{\pi}_n^{k-1}(1 | X_i)}{\hat{\pi}_n(1) \hat{\pi}_n^{k-1}(0 | X_i)} \right) (Y_i - \hat{f}_n^k(A_i, X_i)) \approx 0$$

and,

$$\frac{1}{n} \sum_{i=1}^n \frac{\hat{f}_n^k(1, X_i) - \hat{f}_n^k(0, X_i) - \tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^k, \hat{f}_n^k)}{\hat{\pi}_n(1)} (A_i - \hat{\pi}_n^k(1 | X_i)) \approx 0.$$

## Targeting step: Average treatment effect on the treated

Since

$$\tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^k, \hat{f}_n^k) = \sum_{i=1}^n \frac{A_i}{\hat{\pi}_n} (\hat{f}_n^k(1, X_i) - \hat{f}_n^k(0, X_i)),$$

then

$$\frac{1}{n} \sum_{i=1}^n \frac{A_i}{\hat{\pi}_n} (\hat{f}_n^k(1, X_i) - \hat{f}_n^k(0, X_i) - \tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^k, \hat{f}_n^k)) \approx 0$$

which combined with the 2nd display from the previous slide gives

$$\frac{1}{n} \sum_{i=1}^n \frac{\hat{\pi}_n^k(1 | X_i)}{\hat{\pi}_n(1)} (\hat{f}_n^k(1, X_i) - \hat{f}_n^k(0, X_i) - \tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^k, \hat{f}_n^k)) \approx 0,$$

i.e., (again), no updating of the estimator for  $\mu_X$  is needed.

## Targeting step: Average treatment effect on the treated

The TMLE algorithm is continued until solving:

$$\frac{1}{n} \sum_{i=1}^n \left( \frac{A_i}{\hat{\pi}_n(1)} - \frac{(1 - A_i) \hat{\pi}_n^{k*}(1 | X_i)}{\hat{\pi}_n(1) \hat{\pi}_n^{k*}(0 | X_i)} \right) (Y_i - \hat{f}_n^{k*}(A_i, X_i)) \approx 0$$

and,

$$\frac{1}{n} \sum_{i=1}^n \frac{\hat{f}_n^{k*}(1, X_i) - \hat{f}_n^{k*}(0, X_i) - \tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^{k*}, \hat{f}_n^{k*})}{\hat{\pi}_n(1)} (A_i - \hat{\pi}_n^{k*}(1 | X_i)) \approx 0;$$

and by that also solving:

$$\frac{1}{n} \sum_{i=1}^n \frac{\hat{\pi}_n^{k*}(1 | X_i)}{\hat{\pi}_n(1)} (\hat{f}_n^{k*}(1, X_i) - \hat{f}_n^{k*}(0, X_i) - \tilde{\Psi}(\hat{\mu}_{X,n}, \hat{\pi}_n^{k*}, \hat{f}_n^{k*})) \approx 0.$$

These together constitute the efficient influence curve equation.

## Average treatment effect on the treated

This was the targeting step: What we need procedurally to carry out the TMLE estimation.

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To finish the analysis, it remains to analyze the remainder term:

$$R(P, P_0) = \Psi(P) - \Psi(P_0) + P_0\phi^*(P).$$

## Average treatment effect on the treated

This was the targeting step: What we need procedurally to carry out the TMLE estimation.

To finish the analysis, it remains to analyze the remainder term:

$$R(P, P_0) = \Psi(P) - \Psi(P_0) + P_0\phi^*(P).$$

To derive this: Start from  $P_0\phi^*(P) = \mathbb{E}_{P_0}[\phi^*(P)(O)]$  and show that this can be written as [ something ] plus  $\Psi(P_0) - \Psi(P)$ . This [ something ] is the remainder term.

## Average treatment effect on the treated

For the ATT we can derive that:

$$\begin{aligned}\tilde{R}(f, \pi, \bar{\pi}, f_0, \pi_0, \bar{\pi}_n) = & \frac{1}{\bar{\pi}(1)} \left( \frac{\pi_0(1 | X) - \pi(1 | X)}{1 - \pi(1 | X)} \right) (f_0(0, X) - f(0, X)) \\ & + \left( \frac{\bar{\pi}_0(1) - \bar{\pi}(1)}{\bar{\pi}(1)} \right) (\psi(P_0) - \psi(P))\end{aligned}$$

Again we see the **double robust structure**.

## Average treatment effect on the treated

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## Average treatment effect on the treated

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Again we see the **double robust structure**.

This is a particularly nice result, since the parameter depends on both the outcome regression  $f$  and the propensity score  $\pi$ .

## Final comments — changing the target

For new parameters, we generally have to go through the whole machinery: canonical gradient (efficient influence curve) and second-order remainder term.

It depends very much on the target parameter and the structure of its efficient influence function how easy/hard estimation, and particularly targeting, becomes.

Some targets are easier — for example when they are defined as direct mappings of the treatment-specific mean outcomes  $\mathbb{E}[Y^1]$  and  $\mathbb{E}[Y^0]$ .

For many target parameters, all this work has already been done!

## Final comments — changing the target

The average treatment effect among the treated is implemented in the `tmle` package:

```
set.seed(15)
sim.data <- sim.fun(n=1000)
```

```
library(tmle)
fit.tmle <- tmle(Y=sim.data$Y, A=sim.data$A,
  cbind(X1=sim.data$X1,X2=sim.data$X2,
    X3=sim.data$X3),
  gform=A~X1+X2+X3, ## treatment model
  Qform=Y~A+X1+X2+X3, ## outcome model
  family="binomial",
  cvQinit=FALSE)
```

## Final comments — changing the target

### Additive Effect

Parameter Estimate: 0.066263  
Estimated Variance: 0.00085811  
p-value: 0.023694  
95% Conf Interval: (0.0088482, 0.12368)

### Additive Effect among the Treated

Parameter Estimate: 0.072104  
Estimated Variance: 0.0009739  
p-value: 0.020862  
95% Conf Interval: (0.010938, 0.13327)

### Additive Effect among the Controls

Parameter Estimate: 0.059976  
Estimated Variance: 0.0009839  
p-value: 0.055869  
95% Conf Interval: (-0.0015039, 0.12146)

### Relative Risk

Parameter Estimate: 1.0954

## Final comments — changing the target

Many other (!! ) interesting parameters<sup>1</sup>

- ▶ Controlled and natural direct and indirect effects (mediation analysis parameters)
- ▶ Effects among groups defined by specific covariate characteristics (effect modification)
- ▶ Dynamic interventions, stochastic interventions

⋮

We get back to examples of target parameters in longitudinal settings.

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<sup>1</sup>Newer software ecosystem: <https://tlverse.org/>.