Estimating the target
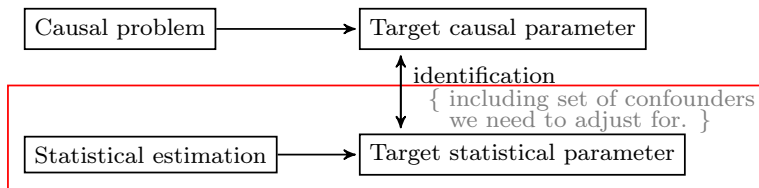
Estimating the target

- one estimator is not more causal than another.
- different estimators are based on different nuisance parameters and have different statistical properties (bias/variance).

G-formula versus IP-weighting

G-formula
1. Estimate nuisance parameters $f(a, x) = \mathbb{E}[Y \mid A = a, X = x]$ and the average over the marginal distribution μ_X of X
2. Plug in to estimate the ATE:

$$\hat{\psi}_n^{\text{g-formula}} = \tilde{\Psi}(\hat{f}_n, \hat{\mu}_X) = \int_{\mathbb{R}^d} \left(\hat{f}_n(1, x) - \hat{f}_n(0, x) \right) d\hat{\mu}_X(x)$$

IP-weighting
1. Estimate nuisance parameters $\pi(a \mid x) = P(A = a \mid X = x)$ and the average over the distribution P of O
2. Plug in to estimate the ATE:

$$\hat{\psi}_n^{\text{ipw}} = \tilde{\Psi}_{\text{ipw}}(\hat{\pi}_n, \hat{P}_n) = \int_{\mathbb{R}^d} \left(\frac{ay}{\hat{\pi}_n(a \mid x)} - \frac{(1-a)y}{\hat{\pi}_n(a \mid x)} \right) d\hat{P}_n(x)$$

One-step estimation

One-step 1. Estimate nuisance parameters
$f(a, x) = \mathbb{E}[Y \mid A = a, X = x]$, $\pi(a \mid x) = \mathbb{E}[A \mid X = x]$
and the average over the distribution P of O
2. Plug in to estimate the ATE:

$$\hat{\psi}_n^{\text{one}} = \tilde{\Psi}_{\text{one}}(\hat{f}_n, \hat{\pi}_n, \hat{P}_n) = \int_{\mathbb{R}^d} \sum_{a=0,1} \sum_{y=0,1} \left\{ \left(\frac{a}{\hat{\pi}_n(a \mid x)} - \frac{1-a}{\hat{\pi}_n(a \mid x)} \right) \left(y - \hat{f}_n(a, x) \right) \right.$$
$$\left. + \hat{f}_n(1, x) - \hat{f}_n(0, x) \right\} d\hat{P}_n(o)$$

G-formula versus IP-weighting

Estimation of the averages over μ_X and P is straightforward using the empirical average over the observed data.

This yields:

G-formula estimator: $\quad \hat{\psi}_n^{\text{g-formula}} = \dfrac{1}{n} \sum_{i=1}^n \left\{ \hat{f}_n(1, X_i) - \hat{f}_n(0, X_i) \right\}$

IP-weighted estimator: $\quad \hat{\psi}_n^{\text{ipw}} = \dfrac{1}{n} \sum_{i=1}^n \left\{ \dfrac{A_i Y_i}{\hat{\pi}_n(A_i \mid X_i)} - \dfrac{(1 - A_i) Y_i}{\hat{\pi}_n(A_i \mid X_i)} \right\}$

One-step estimator: $\quad \hat{\psi}_n^{\text{one}} = \dfrac{1}{n} \sum_{i=1}^n \left\{ \dfrac{A_i}{\hat{\pi}_n(A_i \mid X_i)} - \dfrac{(1 - A_i)}{\hat{\pi}_n(A_i \mid X_i)} \big(Y_i - \hat{f}_n(A_i, X_i) \big) \right.$

$$\left. + \, \hat{f}_n(1, X_i) - \hat{f}_n(0, X_i) \right\}.$$

G-formula versus IP-weighting versus one-step/TMLE

Properties of the different estimators:

G-formula versus IP-weighting versus one-step/TMLE

Properties of the different estimators:

G-formula estimator requires estimator $\hat{f}_n$ for conditional expectation f.
- consistent if $\hat{f}_n$ is consistent.

IP-weighted estimator requires estimator $\hat{\pi}_n$ for the propensity score π.
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One-step estimator requires estimators $\hat{f}_n$ and $\hat{\pi}_n$ for conditional expectation f and propensity score π.

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  - the one-step estimator and the TMLE estimator share the same large-sample properties.

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One-step estimator requires estimators $\hat{f}_n$ and $\hat{\pi}_n$ for conditional expectation f and propensity score π.

- the one-step estimator and the TMLE estimator share the same large-sample properties.
- one thing they have in common is an additional bias correction leads to consistency if either $\hat{f}_n$ or $\hat{\pi}_n$ is consistent (commonly known as double robustness).

G-formula versus IP-weighting versus TMLE

SMALL EXERCISE:

By the law of large numbers, the one-step estimator converges in probability to:

$$\mathbb{E}_{P_0}\left[\left(\frac{A}{\pi(A\,|\,X)} - \frac{1-A}{\pi(A\,|\,X)}\right)\left(Y - f(A,X)\right) + f(1,X) - f(0,X)\right] \quad (1)$$

where (f, π) denotes the limit of $(\hat{f}_n, \hat{\pi}_n)$. Compute the right hand side of (1) when

1. $f = f_0$ (i.e., the outcome regression is consistently estimated), and

2. $\pi = \pi_0$ (i.e., the propensity score is consistently estimated).

G-formula versus IP-weighting versus TMLE

TMLE estimator requires estimators $\hat{f}_n$ and $\hat{\pi}_n$ for conditional expectation f and propensity score π.

- consistent if either $\hat{f}_n$ or $\hat{\pi}_n$ is consistent.

G-formula versus IP-weighting versus TMLE

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- consistent if either $\hat{f}_n$ or $\hat{\pi}_n$ is consistent.

Some other things we will see/explore:

- if $\hat{\pi}_n$ is modeled correctly, the TMLE estimator will have lower variance than the IP-weighted estimator.

G-formula versus IP-weighting versus TMLE

TMLE estimator requires estimators $\hat{f}_n$ and $\hat{\pi}_n$ for conditional expectation f and propensity score π.

▸ consistent if either $\hat{f}_n$ or $\hat{\pi}_n$ is consistent.

Some other things we will see/explore:

▸ if $\hat{\pi}_n$ is modeled correctly, the TMLE estimator will have lower variance than the IP-weighted estimator.

▸ the TMLE estimator may have larger variance than the g-formula estimator based on a correctly modeled $\hat{f}_n$ (but it gives protection against the case that it is not).

G-formula versus IP-weighting versus TMLE

Can't we just construct a good g-formula estimator???

G-formula versus IP-weighting versus TMLE

Can't we just construct a good g-formula estimator???

- a logistic regression — great if correctly specified, but horrible if not.
- a random forest — properly tuned?

A random forest — properly tuned?

Predictive performance of an estimator can be measured in terms of some distance[1] between:

   1) the observed outcome: Y_i

   2) and the predicted conditional expectation: $\hat{f}_n(A_i, X_i)$

---

[1]Measured in terms of a *loss function*.

A random forest — properly tuned?

Predictive performance of an estimator can be measured in terms of some distance[1] between:

1. the observed outcome: Y_i
2. and the predicted conditional expectation: $\hat{f}_n(A_i, X_i)$

One example of a loss function $\mathscr{L}(f)(O)$ is the negative log-likelihood loss:

$$\mathscr{L}(\hat{f}_n)(Y_i, A_i, X_i) = -(Y_i \log(\hat{f}_n(A_i, X_i)) + (1 - Y_i) \log(1 - \hat{f}_n(A_i, X_i))).$$

---

[1] Measured in terms of a *loss function*.

A random forest — properly tuned?

Predictive performance of an estimator can be measured in terms of some distance[1] between:

1) the observed outcome: Y_i

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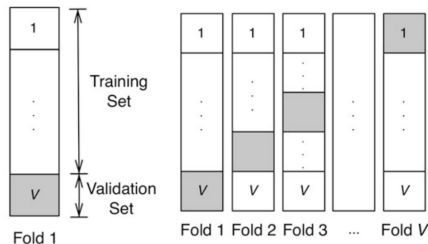One example of a loss function $\mathscr{L}(f)(O)$ is the negative log-likelihood loss:

$$\mathscr{L}(\hat{f}_n)(Y_i, A_i, X_i) = -(Y_i \log(\hat{f}_n(A_i, X_i)) + (1 - Y_i) \log(1 - \hat{f}_n(A_i, X_i))).$$

The estimator $\hat{f}_n$ closest to the true f_0 minimizes the risk:

$$\mathbb{E}_{P_0}[\mathscr{L}(\hat{f}_n)(Y_i, A_i, X_i)].$$

---

[1] Measured in terms of a *loss function*.

A random forest — properly tuned?

Fold 1

Fold 1 Fold 2 Fold 3 ... Fold V

The risk can be estimated in a cross-validation scheme.[a]

I.e., for each sample split:

1. Each model is created and fitted on the training data: $\hat{f}_n^{\text{train}}$.

2. The quality of the model is checked on the validation data
   - Average of $\mathscr{L}(\hat{f}_n^{\text{train}})(O_i)$ in the validation sample.

---

[a]To measure performance on independent data.

A random forest — properly tuned?

Simulated example

- $X \sim \text{Unif}(-2, 2)$
- $X_1^{\text{noise}}, \ldots, X_5^{\text{noise}} \sim N(0, 1)$
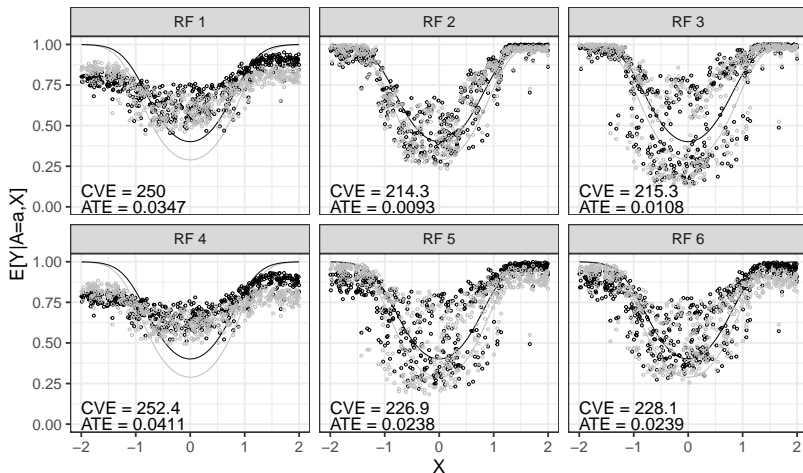- $A \in \{0, 1\}$ with distribution given X given by:

$$\text{logit}\,\mathbb{E}[A \mid X] = \gamma_0 + \gamma_X^\top X$$

- $Y \in \{0, 1\}$ with distribution given X and A given by:

$$\text{logit}\,\mathbb{E}[Y \mid A, X] = \beta_0 + \beta_A A + \beta_X^\top X^2$$
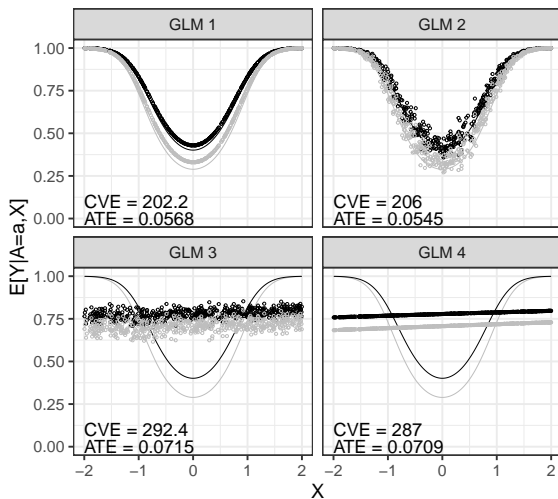
A random forest — properly tuned?

RF fitted with different values of tuning parameters (`nodesize`, `mtry`):

value of a ∘ 0 + 1

Different GLM models

GLM models fitted with different covariates and functional form of covariates:

A random forest — properly tuned?

This is all about constructing a good estimator for the conditional expectation f.

This does not necessarily translate into a good estimator for the target $\tilde{\Psi}(f, \mu_X)$.

A random forest — properly tuned?

This is all about constructing a good estimator for the conditional expectation f.

This does not necessarily translate into a good estimator for the target $\tilde{\Psi}(f, \mu_X)$.

TMLE is all about constructing a g-formula estimator which is a good estimator for *the target*.

Simulating simple data structure in R

Fix randomness:

```
set.seed(5)
```

Fix a sample size:

```
n <- 500
```

Generate covariate $X \in [-2, 2]$:

```
X <- runif(n, -2, 2)
```

Generate binary treatment decision A:

```
A <- rbinom(n, 1, prob=plogis(-0.25 + 1.2*X))
```

(corresponding to logit $\mathbb{E}[A \mid X] = \gamma_0 + \gamma_X X$)

Simulating simple data structure in R

Generate binary outcome Y according to

$$\operatorname{logit} \mathbb{E}[Y \mid A, X] = \beta_0 + \beta_A A + \beta_X X^2$$

Simulating simple data structure in R

Generate binary outcome Y according to

$$\text{logit}\, \mathbb{E}[Y \mid A, X] = \beta_0 + \beta_A A + \beta_X X^2$$

First generate counterfactuals:

```
Y1 <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*1))
Y0 <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*0))
```

Simulating simple data structure in R

Generate binary outcome Y according to

$$\text{logit}\,\mathbb{E}[Y \mid A, X] = \beta_0 + \beta_A A + \beta_X X^2$$

First generate counterfactuals:

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Y1 <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*1))
Y0 <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*0))
```

We only observe the counterfactual outcome corresponding to the observed treatment level:

```
Y <- A*Y1 + (1-A)*Y0
```

Simulating simple data structure in R

Observed data:

```
              X A Y
  1: -1.1991422 0 0
  2:  0.7408744 1 0
  3:  1.6675031 1 1
  4: -0.8624022 0 1
  5: -1.5813995 0 1
 ---
496: -0.3978523 1 0
497: -1.5069379 0 1
498:  1.8340120 1 1
499:  0.6349484 1 1
500: -0.5214807 0 1
```

Simulating simple data structure in R

Observed data:

```
            X A Y
  1: -1.1991422 0 0
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496: -0.3978523 1 0
497: -1.5069379 0 1
498:  1.8340120 1 1
499:  0.6349484 1 1
500: -0.5214807 0 1
```

Counterfactual data:

```
            X Y1 Y0
  1: -1.1991422 0  1
  2:  0.7408744 1  0
  3:  1.6675031 1  1
  4: -0.8624022 0  1
  5: -1.5813995 1  1
 ---
496: -0.3978523 0  1
497: -1.5069379 0  1
498:  1.8340120 1  1
499:  0.6349484 0  0
500: -0.5214807 0  0
```

Simulating simple data structure in R

Simulating many observations of counterfactuals allows us to approximate the true ATE:

```
X <- runif(1e6, -2, 2)
Y1 <- rbinom(1e6, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*1))
Y0 <- rbinom(1e6, 1, prob=plogis(-0.9 + 1.9*X^2 + 0.5*0))
```

The true ATE is then approximately:

```
(true.ate <- mean(Y1 - Y0))
```

[1] 0.070292

since ATE $= \mathbb{E}_{P_0}[Y^1] - \mathbb{E}_{P_0}[Y^0]$.

Simulating simple data structure in R

Fit correctly specified parametric model:

```
fit.glm <- glm(Y~A+X.squared, data=dt[, X.squared:=X^2],
    family=binomial)
```

Use model to estimate $f(1, X)$ for all subjects:

```
dt[, pred.glm.A1:=predict(fit.glm, type="response", newdata=
    copy(dt)[, A:=1])]
```

And similarly $f(0, X)$ for all subjects:

```
dt[, pred.glm.A0:=predict(fit.glm, type="response", newdata=
    copy(dt)[, A:=0])]
```

Then we can estimate the ATE by:

```
(fit.glm <- dt[, mean(pred.glm.A1-pred.glm.A0)])
```

[1] 0.04322891

Simulating simple data structure in R

Using a random forest (no tuning):

```
library(randomForestSRC)
fit.rf <- rfsrc(Y~A+X, data=dt)
dt[, pred.rf.A1:=predict(fit.rf, type="response", newdata=
    copy(dt)[, A:=1])$predicted]
dt[, pred.rf.A0:=predict(fit.rf, type="response", newdata=
    copy(dt)[, A:=0])$predicted]
(fit.rf <- dt[, mean(pred.rf.A1-pred.rf.A0)])
```

[1] 0.07005063

Simulating simple data structure in R

Using a misspecified parametric model:

```
fit.glm.mis <- glm(Y~A+X, data=dt, family=binomial)
dt[, pred.glm.mis.A1:=predict(fit.glm.mis, type="response",
    newdata=copy(dt)[, A:=1])]
dt[, pred.glm.mis.A0:=predict(fit.glm.mis, type="response",
    newdata=copy(dt)[, A:=0])]
(fit.glm.mis <- dt[, mean(pred.glm.mis.A1-pred.glm.mis.A0)])
```

[1] 0.09127889

Simulating simple data structure in R

We can investigate the properties of different estimators —

- We know the true value of ATE: $\psi_0 \approx 0.0702$
- We have generated the outcome Y according to

$$\text{logit}\, \mathbb{E}[Y \mid A, X] = \beta_0 + \beta_A A + \beta_X X^2$$

- We have generated the treatment A according to

$$\text{logit}\, \mathbb{E}[A \mid X] = \gamma_0 + \gamma_X X$$

If we repeat the experiment of drawing n observations we would every time end up with a different realization of the particular estimator.

Different estimators

G-formula estimator Using an estimator $\hat{f}_n$ for
$f(a, X) = \mathbb{E}[Y \mid A = a, X]$, estimate the ATE by:

$$\hat{\psi}_n^{\text{g−formula}} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \hat{f}_n(1, X_i) - \hat{f}_n(0, X_i) \right\}$$

Inverse probability weighted estimator Using an estimator $\hat{\pi}_n$ for
$\pi(a \mid X) = P(A = a \mid X)$, estimate the ATE by:

$$\hat{\psi}_n^{\text{ipw}} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{A_i Y_i}{\hat{\pi}_n(A_i \mid X_i)} - \frac{(1 - A_i) Y_i}{\hat{\pi}_n(A_i \mid X_i)} \right\}$$

TMLE estimator Update the estimator $\hat{f}_n \mapsto \hat{f}_n^*$ in a "targeted way"
using the information from the estimator $\hat{\pi}_n$, then
estimate the ATE by: Helene

$$\hat{\psi}_n^{\text{tmle}} = \frac{1}{n} \sum_{i=1}^{n} \left\{ \hat{f}_n^*(1, X_i) - \hat{f}_n^*(0, X_i) \right\}$$

Different estimators — `tmle` implementation

Today we will just (more or less blindly) use software to estimate TMLE.

Different estimators — `tmle` implementation

Today we will just (more or less blindly) use software to estimate TMLE.

```
library(tmle)
```

```
tmle(Y, A, X,
     gform,
     Qform,
     SL.library,
     family="binomial",
     cvQinit=FALSE,
     ...
     )
```

- $Y \in \mathbb{R}$ or $Y \in \{0,1\}$
- $A \in \{0,1\}$
- X a vector, matrix or a data frame

Different estimators — `tmle` implementation

- `gform`
  - optional regression formula for the propensity score π
  - on the form `A~X1+X2`
  - (overrides call to SuperLearner)

- `Qform`
  - optional regression formula for the conditional expectation f
  - on the form `Y~X1+X2`
  - (overrides call to SuperLearner)

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  - (overrides call to `SuperLearner`)

- `cvQinit=FALSE`
  - default is `TRUE` which means cross-validated predicted values are estimated

- `gbound`
  - truncation of predicted probabilities of treatment

Different estimators — `tmle` implementation

- `Q.SL.library`
    - optional vector of prediction algorithms to use for SuperLearner in initial estimation of f

- `g.SL.library`
    - optional vector of prediction algorithms to use for SuperLearner in initial estimation of π

- `Q.discreteSL`
    - if `TRUE`, a discrete super learner is used (rather than ensemble)
    - default is `FALSE`

- `g.discreteSL`
    - if `TRUE`, a discrete super learner is used (rather than ensemble)
    - default is `FALSE`

Note: The discrete super learner simply picks an algorithm from its library by minimizing the cross-validated empirical risk with respect a loss function.

Different estimators — `tmle` implementation

What were the estimated IP weights?

```
summary(fit.tmle$g$g1W)
```

```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
0.04751 0.19441 0.49405 0.49400 0.79710 0.94109
```

Note that weights close to 0 or to 1 would indicate positivity issues.

Different estimators — `tmle` implementation

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summary(fit.tmle$g$g1W)
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```
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```

Note that weights close to 0 or to 1 would indicate positivity issues.

What truncation level was used?

```
fit.tmle$gbound
```

```
[1] 0.03598084 1.00000000
```

I.e., no weights were truncated.

Explorations based on simulated data

As part of the exercise we want to explore —

1. Comparing g-formula estimators for different estimators for f; either different logistic regressions or different machine learning algorithms.

2. Properties of the g-formula estimator and the IP-weighted estimator, compared to the TMLE estimator.

3. Double robustness: Misspecification of the outcome regression (f).

The exercise is described in detail in: **day1-practical1.pdf**.