Day 1, Practical 1, Hely's solution

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1 Simulating data

Task 1.

```r
library(data.table)

sim.fun <- function(n) {

    X1 <- runif(n, -2, 2)
    X2 <- rnorm(n)
    X3 <- rbinom(n, 1, prob=0.2)
    A <- rbinom(n, 1, prob=plogis(-0.25+0.8*X1+0.25*X3))
    Y <- rbinom(n, 1, prob=plogis(-0.9+1.9*X1^2+0.6*X2+0.5*A))

    return(data.table(X1=X1, X2=X2, X3=X3, A=A, Y=Y))

}
```

2 Computing the true value of the ATE

Task 2.

```r
library(data.table)

sim.fun <- function(n, a=NULL) {
    X1 <- runif(n, -2, 2)
    X2 <- rnorm(n)
    X3 <- rbinom(n, 1, 0.2)
    if (length(a)>0) {
    A  <- a
    } else {
    A  <- rbinom(n, 1, prob=plogis(-0.25 + 0.8*X1 + 0.25*X3))
    }
    Y <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X1^2 + 0.6*X2 + 0.5*A))
    if (length(a)>0) {
    return(mean(Y))
    } else {
    return(data.table(id=1:n,X1=X1,X2=X2,X3=X3,A=A,Y=Y))
    }
}
```

```
set.seed(12)
message(paste0("EY1 = ", E.Y1 <- sim.fun(1e6, a=1)))
message(paste0("EY0 = ", E.Y0 <- sim.fun(1e6, a=0)))
message(paste0("ATE = ", ATE <- E.Y1 - E.Y0))
```

```
EY1 = 0.749921
EY0 = 0.68208
ATE = 0.0678409999999999
```

3 Estimation

Task 3.

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

```
   id         X1          X2 X3 A Y
1:  1  0.4084562  0.38996075  0 0 0
2:  2 -1.2198243 -1.67449303  1 0 0
3:  3  1.8658349 -2.22881407  0 1 1
4:  4  0.6036221 -0.01388672  0 0 0
5:  5 -0.5317124  0.57686435  0 0 0
6:  6  1.9554368  0.15718650  0 0 1
```

```
message("fitted model for the outcome regression:")
summary(fit.f <- glm(Y~A+X1+X2+X3, family=binomial, data=sim.data))
message("-------------------------------------")
message("fitted model for the propensity score:")
summary(fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data))
```

```
fitted model for the outcome regression:

Call:
glm(formula = Y ~ A + X1 + X2 + X3, family = binomial, data = sim.data)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2530  -1.2483   0.6745   0.8255   1.3174

Coefficients:
            Estimate Std. Error z value          Pr(>|z|)
(Intercept)  0.76917    0.10360   7.424 0.000000000000113 ***
A            0.46609    0.16396   2.843           0.00447 **
X1          -0.01980    0.06944  -0.285           0.77554
X2           0.45090    0.07413   6.083 0.000000001180179 ***
X3           0.23320    0.19117   1.220           0.22253
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

```
(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1170.5  on 999  degrees of freedom
Residual deviance: 1121.4  on 995  degrees of freedom
AIC: 1131.4

Number of Fisher Scoring iterations: 4
---------------------------------------
fitted model for the propensity score:

Call:
glm(formula = A ~ X1 + X2 + X3, family = binomial, data = sim.data)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.9285  -0.9355  -0.5552   0.9638   2.0656

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.314837   0.079178  -3.976  0.00007 ***
X1           0.843342   0.066527  12.677  < 2e-16 ***
X2          -0.004127   0.068828  -0.060   0.9522
X3           0.379385   0.179716   2.111   0.0348 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1380.8  on 999  degrees of freedom
Residual deviance: 1182.2  on 996  degrees of freedom
AIC: 1190.2

Number of Fisher Scoring iterations: 4
```

```r
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
message(paste0("g-formula estimate = ", round(sim.data[, mean(pred.EY1 - pred.EY0)],
    5)))
##-- ipw;
sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
message(paste0("ipw estimate = ", round(sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred
    .pi1))], 5)))
```

```
g-formula estimate = 0.08732
ipw estimate = 0.05979
```

Task 4.

```r
fit.f2 <- glm(Y~A+X1.squared+X2+X3, family=binomial, data=sim.data[, X1.squared:=X1
    ^2])
```

```r
fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data)
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])]
message(paste0("g-formula estimate = ", round(sim.data[, mean(pred.EY1 - pred.EY0)],
    5)))
##-- ipw;
sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
message(paste0("ipw estimate = ", round(sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred
    .pi1))], 5)))
```

```
g-formula estimate = 0.06703
ipw estimate = 0.05979
```

Task 5.

```r
library(randomForestSRC)
fit.rf <- rfsrc(Y~A+X1+X2+X3, data=sim.data)
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=1])$
    predicted]
sim.data[, pred.EY0:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=0])$
    predicted]
message(paste0("g-formula estimate (RF) = ", round(sim.data[, mean(pred.EY1 - pred.EY0
    )], 5)))
```

```
g-formula estimate (RF) = 0.06118
```

Task 6.

```r
sim.data[, pred.EY1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
sim.data[, mean(A/pred.pi1*(Y-pred.EY1) - (1-A)/(1-pred.pi1)*(Y-pred.EY0) + pred.EY1 -
     pred.EY0)]
```

```
[1] 0.06638761
```

Task 7.

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

```
[1] 0.06626344
```

```r
tmle.fit$Qinit$coef
fit.f$coef
```

```
(Intercept)           A          X1          X2          X3 
 0.76917331  0.46609109 -0.01979933  0.45089688  0.23320073 
(Intercept)           A          X1          X2          X3 
 0.76917331  0.46609109 -0.01979933  0.45089688  0.23320073 
```

Task 8.

```
tmle.fit2 <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$X3
    ),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1.squared+X2+X3, ## outcome model
          family="binomial",
          cvQinit=FALSE)
#-- get the ATE estimate:
tmle.fit2$estimates$ATE$psi
```

```
[1] 0.06791028
```

```
tmle.fit2$Qinit$coef
fit.f2$coef
```

```
(Intercept)           A  X1.squared          X2          X3 
 -0.8362875   0.5140438   1.8457299   0.5762989   0.1435289 
(Intercept)           A  X1.squared          X2          X3 
 -0.8362875   0.5140438   1.8457299   0.5762989   0.1435289 
```

```
sim.data[, pred.EY1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])]
sim.data[, mean(A/pred.pi1*(Y-pred.EY1) - (1-A)/(1-pred.pi1)*(Y-pred.EY0) + pred.EY1 -
     pred.EY0)]
```

```
[1] 0.06790105
```

4 Changed data setting

Task 9.

```
new.sim.fun <- function(n, a=NULL) {
    X1 <- runif(n, -2, 2)
    X2 <- rnorm(n)
    X3 <- rbinom(n, 1, 0.2)
    if (length(a)>0) {
    A <- a
    } else {
    A <- rbinom(n, 1, prob=plogis(-0.25 + 2.8*X1 + 0.25*X3))
    }
    Y <- rbinom(n, 1, prob=plogis(-0.9 + 1.9*X1^2 + 0.6*X2 + 0.5*A))
    if (length(a)>0) {
    return(mean(Y))
    } else {
    return(data.table(id=1:n,X1=X1,X2=X2,X3=X3,A=A,Y=Y))
    }
}
```

Task (9)3.

```
set.seed(15)
head(sim.data <- new.sim.fun(1000))
```

```
   id         X1          X2 X3 A Y
1:  1  0.4084562  0.38996075  0 1 1
2:  2 -1.2198243 -1.67449303  1 0 0
3:  3  1.8658349 -2.22881407  0 1 1
4:  4  0.6036221 -0.01388672  0 0 0
5:  5 -0.5317124  0.57686435  0 0 0
6:  6  1.9554368  0.15718650  0 1 1
```

```
message("fitted model for the outcome regression:")
summary(fit.f <- glm(Y~A+X1+X2+X3, family=binomial, data=sim.data))
message("----------------------------------------")
message("fitted model for the propensity score:")
summary(fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data))
```

```
fitted model for the outcome regression:

Call:
glm(formula = Y ~ A + X1 + X2 + X3, family = binomial, data = sim.data)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.4128  -1.1028   0.6456   0.8032   1.3819

Coefficients:
            Estimate Std. Error z value        Pr(>|z|)
(Intercept)  0.72501    0.13638   5.316 0.0000001061167 ***
A            0.72655    0.24014   3.026         0.00248 **
X1          -0.11379    0.10283  -1.107         0.26847
X2           0.51261    0.07640   6.710 0.0000000000195 ***
X3           0.09166    0.19105   0.480         0.63138
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1146.1  on 999  degrees of freedom
Residual deviance: 1085.4  on 995  degrees of freedom
AIC: 1095.4

Number of Fisher Scoring iterations: 4
---------------------------------------
fitted model for the propensity score:

Call:
glm(formula = A ~ X1 + X2 + X3, family = binomial, data = sim.data)
```

```
Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.6536  -0.3012   0.0803   0.3409   3.3465

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.26425    0.12320  -2.145   0.0320 *
X1           2.98819    0.18819  15.879   <2e-16 ***
X2          -0.07899    0.10454  -0.756   0.4499
X3           0.58430    0.28893   2.022   0.0431 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 1385.72  on 999  degrees of freedom
Residual deviance:  538.79  on 996  degrees of freedom
AIC: 546.79

Number of Fisher Scoring iterations: 6
```

```
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
message(paste0("g-formula estimate = ", round(sim.data[, mean(pred.EY1 - pred.EY0)],
    5)))
##-- ipw;
sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
message(paste0("ipw estimate = ", round(sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred
    .pi1))], 5)))
```

```
g-formula estimate = 0.13182
ipw estimate = 0.39891
```

Task (9)4.

```
fit.f2 <- glm(Y~A+X1.squared+X2+X3, family=binomial, data=sim.data[, X1.squared:=X1
    ^2])
fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data)
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])]
message(paste0("g-formula estimate = ", round(sim.data[, mean(pred.EY1 - pred.EY0)],
    5)))
##-- ipw;
sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
message(paste0("ipw estimate = ", round(sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred
    .pi1))], 5)))
```

```
g-formula estimate = 0.07055
ipw estimate = 0.39891
```

Task (9)5.

```
library(randomForestSRC)
fit.rf <- rfsrc(Y~A+X1+X2+X3, data=sim.data)
##-- g-formula;
sim.data[, pred.EY1:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=1])$
    predicted]
sim.data[, pred.EY0:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=0])$
    predicted]
message(paste0("g-formula estimate (RF) = ", round(sim.data[, mean(pred.EY1 - pred.EY0
    )], 5)))
```

```
g-formula estimate (RF) = 0.05446
```

Task (9)6.

```
sim.data[, pred.EY1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
sim.data[, mean(A/pred.pi1*(Y-pred.EY1) - (1-A)/(1-pred.pi1)*(Y-pred.EY0) + pred.EY1 -
     pred.EY0)]
```

```
[1] 0.1742685
```

Task (9)7.

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

```
[1] 0.1401536
```

How much weight truncation is going on?

```
summary(tmle.fit$g$g1W)
tmle.fit$gbound
mean(tmle.fit$g$g1W<tmle.fit$gbound)
```

```
    Min.  1st Qu.   Median     Mean  3rd Qu.     Max.
0.001739 0.049518 0.533751 0.512000 0.952438 0.998164
[1] 0.02288933 1.00000000
[1] 0.601
```

Changing the gbound argument to avoid truncation of weights:

```
library(tmle)
tmle.fit <- 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
```

```r
         Qform=Y~A+X1+X2+X3, ## outcome model
         family="binomial",
         gbound=c(0,1),
         cvQinit=FALSE)
#-- get the ATE estimate:
tmle.fit$estimates$ATE$psi
```

```
[1] 0.1776457
```

Task (9)8.
Without changing the weight truncation:

```r
tmle.fit2 <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$X3
    ),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1.squared+X2+X3, ## outcome model
          family="binomial",
          cvQinit=FALSE)
#-- get the ATE estimate:
tmle.fit2$estimates$ATE$psi
```

```
[1] 0.08152813
```

Changing the gbound argument to avoid truncation of weights:

```r
tmle.fit2 <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$X3
    ),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1.squared+X2+X3, ## outcome model
          family="binomial",
          gbound=c(0,1),
          cvQinit=FALSE)
#-- get the ATE estimate:
tmle.fit2$estimates$ATE$psi
```

```
[1] 0.08330816
```

For comparison, the estimating equation (ee) estimator is:

```r
sim.data[, pred.EY1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])]
sim.data[, pred.EY0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])]
sim.data[, mean(A/pred.pi1*(Y-pred.EY1) - (1-A)/(1-pred.pi1)*(Y-pred.EY0) + pred.EY1 -
     pred.EY0)]
```

```
[1] 0.08379974
```

5 Simulation study

Task 10.

```
library(here)

fit.g.glm1 <- list()
fit.g.glm2 <- list()
fit.g.rf <- list()
fit.ipw <- list()
fit.ipw2 <- list()
fit.ipw.rf <- list()
fit.tmle <- list()
fit.tmle.var <- list()
fit.ee <- list()
fit.ee.var <- list()
fit.tmle2 <- list()
fit.tmle2.var <- list()
fit.ee2 <- list()
fit.ee2.var <- list()

for (m in 1:500) {

  set.seed(m+110)
  sim.data <- sim.fun(1000)

  fit.f <- glm(Y~A+X1+X2+X3, family=binomial, data=sim.data)
  fit.f2 <- glm(Y~A+X1.squared+X2+X3, family=binomial, data=sim.data[, X1.squared:=X1
    ^2])
  fit.rf <- rfsrc(Y~A+X1+X2+X3, data=sim.data)
  fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data)
  fit.pi2 <- glm(A~X2+X3, family=binomial, data=sim.data)
  fit.rf.pi <- rfsrc(A~X1+X2+X3, data=sim.data)

  ##-- g-formula (misspecified);
  sim.data[, pred.f1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
  sim.data[, pred.f0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
  fit.g.glm1[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

  ##-- ipw (correctly specified);
  sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
  fit.ipw[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]

  ##-- tmle (misspecified f);
  tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
           cbind(X1=sim.data$X1,X2=sim.data$X2,X3=sim.data$X3),
           gform=A~X1+X2+X3, ## treatment model
           Qform=Y~A+X1+X2+X3, ## outcome model
           family="binomial",
           cvQinit=FALSE)
  fit.tmle[[m]] <- tmle.fit$estimates$ATE$psi
  fit.tmle.var[[m]] <- tmle.fit$estimates$ATE$var

  ##-- estimating equation estimator (misspecified f);
  sim.data[, pred.f1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
  sim.data[, pred.f0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
  sim.data[, pred.f:=predict(fit.f, type="response", newdata=sim.data)]
  sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
```

```
fit.ee[[m]] <- sim.data[, mean((A/pred.pi1 - (1-A)/(1-pred.pi1))*(Y - pred.f) +
               pred.f1 - pred.f0)]
fit.ee.var[[m]] <- sim.data[, mean((A/pred.pi1*(Y-pred.f1) - (1-A)/(1-pred.pi1)*(Y-
  pred.f0) + pred.f1 - pred.f0)^2)/nrow(sim.data)]

##-- g-formula (correctly specified);
sim.data[, pred.f1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])
  ]
sim.data[, pred.f0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])
  ]
fit.g.glm2[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

##-- tmle (correctly specified f);
tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
         cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$
  X3),
         gform=A~X1+X2+X3, ## treatment model
         Qform=Y~A+X1.squared+X2+X3, ## outcome model
         family="binomial",
         cvQinit=FALSE)
fit.tmle2[[m]] <- tmle.fit$estimates$ATE$psi
fit.tmle2.var[[m]] <- tmle.fit$estimates$ATE$var

##-- estimating equation estimator (correctly specified f);
sim.data[, pred.f1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])
  ]
sim.data[, pred.f0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])
  ]
sim.data[, pred.f:=predict(fit.f2, type="response", newdata=sim.data)]
sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
fit.ee2[[m]] <- sim.data[, mean((A/pred.pi1 - (1-A)/(1-pred.pi1))*(Y - pred.f) +
                pred.f1 - pred.f0)]
fit.ee2.var[[m]] <- sim.data[, mean((A/pred.pi1*(Y-pred.f1) - (1-A)/(1-pred.pi1)*(Y-
  pred.f0) + pred.f1 - pred.f0)^2)/nrow(sim.data)]

##-- g-formula based on RF;
sim.data[, pred.f1:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=1])
  $predicted]
sim.data[, pred.f0:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=0])
  $predicted]
fit.g.rf[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

##-- ipw (misspecified);
sim.data[, pred.pi1:=predict(fit.pi2, type="response", newdata=sim.data)]
fit.ipw2[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]

##-- rf (misspecified);
sim.data[, pred.pi1:=predict(fit.rf.pi, type="response", newdata=sim.data)$predicted
  ]
fit.ipw.rf[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]

saveRDS(list(fit.g.glm1 = fit.g.glm1,
         fit.g.glm2 = fit.g.glm2,
         fit.g.rf = fit.g.rf,
         fit.ipw = fit.ipw,
           fit.ipw2 = fit.ipw2,
           fit.ipw.rf = fit.ipw.rf,
           fit.tmle = fit.tmle,
           fit.tmle.var = fit.tmle.var,
           fit.ee = fit.ee,
           fit.ee.var = fit.ee.var,
           fit.tmle2 = fit.tmle2,
           fit.tmle2.var = fit.tmle2.var,
           fit.ee2 = fit.ee2,
           fit.ee2.var = fit.ee2.var),
      file=paste0(here(), "/data/sim-data-output/",
              "save-est-sim-setting-1",
              ".rds"))

}
```

Task 11. See Figure 1.

```
library(ggplot2)

estimator.list <- readRDS(file=paste0(here(), "/data/sim-data-output/",
                      "save-est-sim-setting-1",
                      ".rds"))

pdat <- data.table(estimator=c(rep("g-formula estimator (misspecified)",
                   length(estimator.list$fit.g.glm1)),
                   rep("g-formula estimator (correctly specified)",
                   length(estimator.list$fit.g.glm2)),
                   rep("g-formula estimator (random forest)",
                   length(estimator.list$fit.g.rf)),
                   rep("IPW estimator (correctly specified)",
                   length(estimator.list$fit.ipw)),
                   rep("IPW estimator (misspecified)",
                   length(estimator.list$fit.ipw2)),
                   rep("IPW estimator (random forest)",
                   length(estimator.list$fit.ipw.rf)),
                   rep("TMLE estimator (misspecified initial)",
                   length(estimator.list$fit.tmle)),
                   rep("EE estimator (misspecified initial)",
                   length(estimator.list$fit.ee))),
           est=c(unlist(estimator.list$fit.g.glm1),
             unlist(estimator.list$fit.g.glm2),
             unlist(estimator.list$fit.g.rf),
             unlist(estimator.list$fit.ipw),
             unlist(estimator.list$fit.ipw2),
             unlist(estimator.list$fit.ipw.rf),
             unlist(estimator.list$fit.tmle),
             unlist(estimator.list$fit.ee)))

pdat[, estimator.factor := factor(estimator, levels=pdat[, unique(estimator)], order=
    TRUE)]

ggplot(pdat) +
  theme_bw(base_size=25) +
  geom_boxplot(aes(x=est)) +
facet_wrap(. ~ estimator.factor, ncol=2) +
geom_vline(aes(xintercept=ATE), linetype="dashed", color="red") +
xlab(expression(hat(psi)[n])) + ylab("")
```

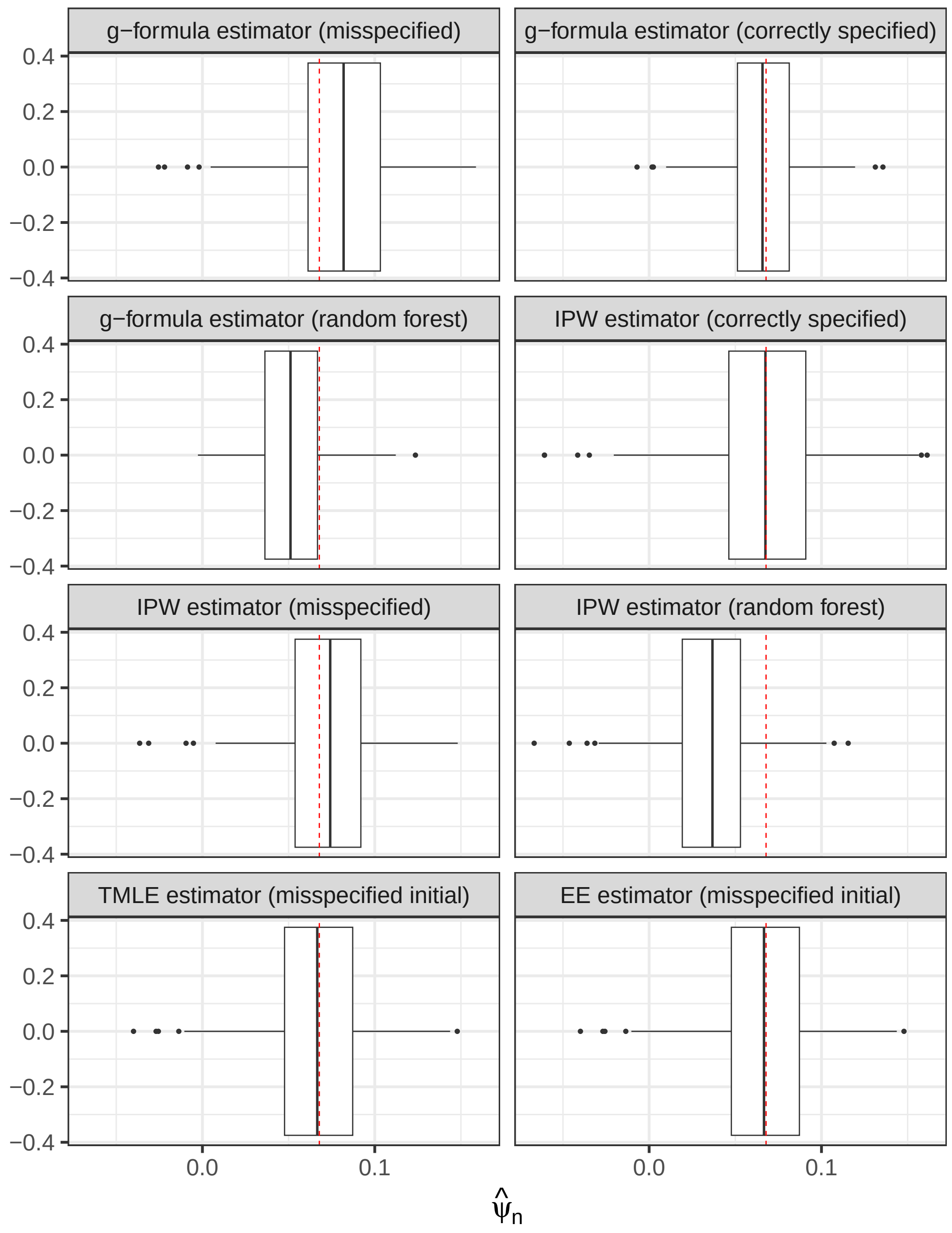

g−formula estimator (misspecified)
g−formula estimator (correctly specified)
g−formula estimator (random forest)
IPW estimator (correctly specified)
IPW estimator (misspecified)
IPW estimator (random forest)
TMLE estimator (misspecified initial)
EE estimator (misspecified initial)
0.4
0.2
0.0
−0.2
−0.4
0.0
0.1
$\hat{\psi}_n$

Figure 1

6 Simulation study for new data setting (with positivity issues)

Task 10. Same as **Task 9** but changing the distribution of A as follows: $\mathbb{E}[A \mid X_1, X_2, X_3] = \text{logit}(-0.25 + 2.8X_1 + 0.25X_3)$ (Section 4). Results are shown in Figure 2.

```
fit.g.glm1 <- list()
fit.g.glm2 <- list()
fit.g.rf <- list()
fit.ipw <- list()
fit.ipw2 <- list()
fit.ipw.rf <- list()
fit.tmle <- list()
fit.tmle.var <- list()
fit.wt.tmle <- list()
fit.wt.tmle.var <- list()
fit.ee <- list()
fit.ee.var <- list()
fit.tmle2 <- list()
fit.tmle2.var <- list()
fit.wt.tmle2 <- list()
fit.wt.tmle2.var <- list()
fit.ee2 <- list()
fit.ee2.var <- list()

for (m in 1:500) {

  set.seed(m+110)
  sim.data <- new.sim.fun(1000)

  fit.f <- glm(Y~A+X1+X2+X3, family=binomial, data=sim.data)
  fit.f2 <- glm(Y~A+X1.squared+X2+X3, family=binomial, data=sim.data[, X1.squared:=X1
    ^2])
  fit.rf <- rfsrc(Y~A+X1+X2+X3, data=sim.data)
  fit.pi <- glm(A~X1+X2+X3, family=binomial, data=sim.data)
  fit.pi2 <- glm(A~X2+X3, family=binomial, data=sim.data)
  fit.rf.pi <- rfsrc(A~X1+X2+X3, data=sim.data)

  ##-- g-formula (misspecified);
  sim.data[, pred.f1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
  sim.data[, pred.f0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
  fit.g.glm1[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

  ##-- ipw (correctly specified);
  sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
  fit.ipw[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]

  ##-- tmle (misspecified f);
  tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
           cbind(X1=sim.data$X1,X2=sim.data$X2,X3=sim.data$X3),
           gform=A~X1+X2+X3, ## treatment model
           Qform=Y~A+X1+X2+X3, ## outcome model
           gbound=c(0,1),
           family="binomial",
           cvQinit=FALSE)
  fit.tmle[[m]] <- tmle.fit$estimates$ATE$psi
```

```
 fit.tmle.var[[m]] <- tmle.fit$estimates$ATE$var

 #-- *with* weight truncation:
 tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1,X2=sim.data$X2,X3=sim.data$X3),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1+X2+X3, ## outcome model
          family="binomial",
          cvQinit=FALSE)
 fit.wt.tmle[[m]] <- tmle.fit$estimates$ATE$psi
 fit.wt.tmle.var[[m]] <- tmle.fit$estimates$ATE$var

 ##-- estimating equation estimator (misspecified f);
 sim.data[, pred.f1:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=1])]
 sim.data[, pred.f0:=predict(fit.f, type="response", newdata=copy(sim.data)[, A:=0])]
 sim.data[, pred.f:=predict(fit.f, type="response", newdata=sim.data)]
 sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
 fit.ee[[m]] <- sim.data[, mean((A/pred.pi1 - (1-A)/(1-pred.pi1))*(Y - pred.f) +
               pred.f1 - pred.f0)]
 fit.ee.var[[m]] <- sim.data[, mean((A/pred.pi1*(Y-pred.f1) - (1-A)/(1-pred.pi1)*(Y-
   pred.f0) + pred.f1 - pred.f0)^2)/nrow(sim.data)]

##-- g-formula (correctly specified);
 sim.data[, pred.f1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])
   ]
 sim.data[, pred.f0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])
   ]
 fit.g.glm2[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

 ##-- tmle (correctly specified f);
 tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$
   X3),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1.squared+X2+X3, ## outcome model
          gbound=c(0,1),
          family="binomial",
          cvQinit=FALSE)
 fit.tmle2[[m]] <- tmle.fit$estimates$ATE$psi
 fit.tmle2.var[[m]] <- tmle.fit$estimates$ATE$var

 #-- *with* weight truncation:
 tmle.fit <- tmle(Y=sim.data$Y, A=sim.data$A,
          cbind(X1=sim.data$X1, X1.squared=sim.data$X1^2,X2=sim.data$X2,X3=sim.data$
   X3),
          gform=A~X1+X2+X3, ## treatment model
          Qform=Y~A+X1.squared+X2+X3, ## outcome model
          family="binomial",
          cvQinit=FALSE)
 fit.wt.tmle2[[m]] <- tmle.fit$estimates$ATE$psi
 fit.wt.tmle2.var[[m]] <- tmle.fit$estimates$ATE$var

 ##-- estimating equation estimator (correctly specified f);
 sim.data[, pred.f1:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=1])
   ]
```

```
  sim.data[, pred.f0:=predict(fit.f2, type="response", newdata=copy(sim.data)[, A:=0])
    ]
  sim.data[, pred.f:=predict(fit.f2, type="response", newdata=sim.data)]
  sim.data[, pred.pi1:=predict(fit.pi, type="response", newdata=sim.data)]
  fit.ee2[[m]] <- sim.data[, mean((A/pred.pi1 - (1-A)/(1-pred.pi1))*(Y - pred.f) +
                 pred.f1 - pred.f0)]
  fit.ee2.var[[m]] <- sim.data[, mean((A/pred.pi1*(Y-pred.f1) - (1-A)/(1-pred.pi1)*(Y-
    pred.f0) + pred.f1 - pred.f0)^2)/nrow(sim.data)]

 ##-- g-formula based on RF;
  sim.data[, pred.f1:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=1])
    $predicted]
  sim.data[, pred.f0:=predict(fit.rf, type="response", newdata=copy(sim.data)[, A:=0])
    $predicted]
  fit.g.rf[[m]] <- sim.data[, mean(pred.f1 - pred.f0)]

  ##-- ipw (misspecified);
  sim.data[, pred.pi1:=predict(fit.pi2, type="response", newdata=sim.data)]
  fit.ipw2[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]

  ##-- rf (misspecified);
  sim.data[, pred.pi1:=predict(fit.rf.pi, type="response", newdata=sim.data)$predicted
    ]
  fit.ipw.rf[[m]] <- sim.data[, mean(A*Y/pred.pi1 - (1-A)*Y/(1-pred.pi1))]


  saveRDS(list(fit.g.glm1 = fit.g.glm1,
          fit.g.glm2 = fit.g.glm2,
          fit.g.rf = fit.g.rf,
          fit.ipw = fit.ipw,
          fit.ipw2 = fit.ipw2,
          fit.ipw.rf = fit.ipw.rf,
          fit.tmle = fit.tmle,
          fit.tmle.var = fit.tmle.var,
          fit.wt.tmle = fit.wt.tmle,
          fit.wt.tmle.var = fit.wt.tmle.var,
          fit.ee = fit.ee,
          fit.ee.var = fit.ee.var,
          fit.tmle2 = fit.tmle2,
          fit.tmle2.var = fit.tmle2.var,
          fit.wt.tmle2 = fit.wt.tmle2,
          fit.wt.tmle2.var = fit.wt.tmle2.var,
          fit.ee2 = fit.ee2,
          fit.ee2.var = fit.ee2.var),
      file=paste0(here(), "/data/sim-data-output/",
              "save-est-sim-setting-2",
              ".rds"))

}
```

```
library(ggplot2)

estimator.list <- readRDS(file=paste0(here(), "/TMLE-course/data/sim-data-output/",
                      "save-est-sim-setting-2",
                      ".rds"))
```

```
pdat <- data.table(estimator=c(rep("g-formula estimator (misspecified)",
                   length(estimator.list$fit.g.glm1)),
                   rep("g-formula estimator (correctly specified)",
                   length(estimator.list$fit.g.glm2)),
                   rep("g-formula estimator (random forest)",
                   length(estimator.list$fit.g.rf)),
                   rep("IPW estimator (correctly specified)",
                   length(estimator.list$fit.ipw)),
                   rep("IPW estimator (misspecified)",
                   length(estimator.list$fit.ipw2)),
                   rep("IPW estimator (random forest)",
                   length(estimator.list$fit.ipw.rf)),
                   rep("TMLE estimator (misspecified initial)",
                   length(estimator.list$fit.tmle)),
                   rep("EE estimator (misspecified initial)",
                   length(estimator.list$fit.ee))),
           est=c(unlist(estimator.list$fit.g.glm1),
             unlist(estimator.list$fit.g.glm2),
             unlist(estimator.list$fit.g.rf),
             unlist(estimator.list$fit.ipw),
             unlist(estimator.list$fit.ipw2),
             unlist(estimator.list$fit.ipw.rf),
             unlist(estimator.list$fit.tmle),
             unlist(estimator.list$fit.ee)))

pdat[, estimator.factor := factor(estimator, levels=pdat[, unique(estimator)], order=
    TRUE)]

ggplot(pdat) +
  theme_bw(base_size=25) +
  geom_boxplot(aes(x=est)) +
  facet_wrap(. ~ estimator.factor, ncol=2) +
  geom_vline(aes(xintercept=ATE), linetype="dashed", color="red") +
  xlab(expression(hat(psi)[n])) + ylab("")
```

7 Extra: Tuning the random forest

```
setwd("~/Undervisning/TMLE/TMLE-course/practicals/day1/")
library(ggplot2)
library(data.table)
library(randomForestSRC)

ate.rf.models.list <- list()
V <- 5 # <- number of folds.
loss.fun <- function(Y, fit) -Y*log(fit)-(1-Y)*log(1-fit) # <- loss function.

for (m in 1:500) {

  set.seed(5+m)
  sim.data <- sim.fun(1000)
  sim.data[, id:=1:.N]
```

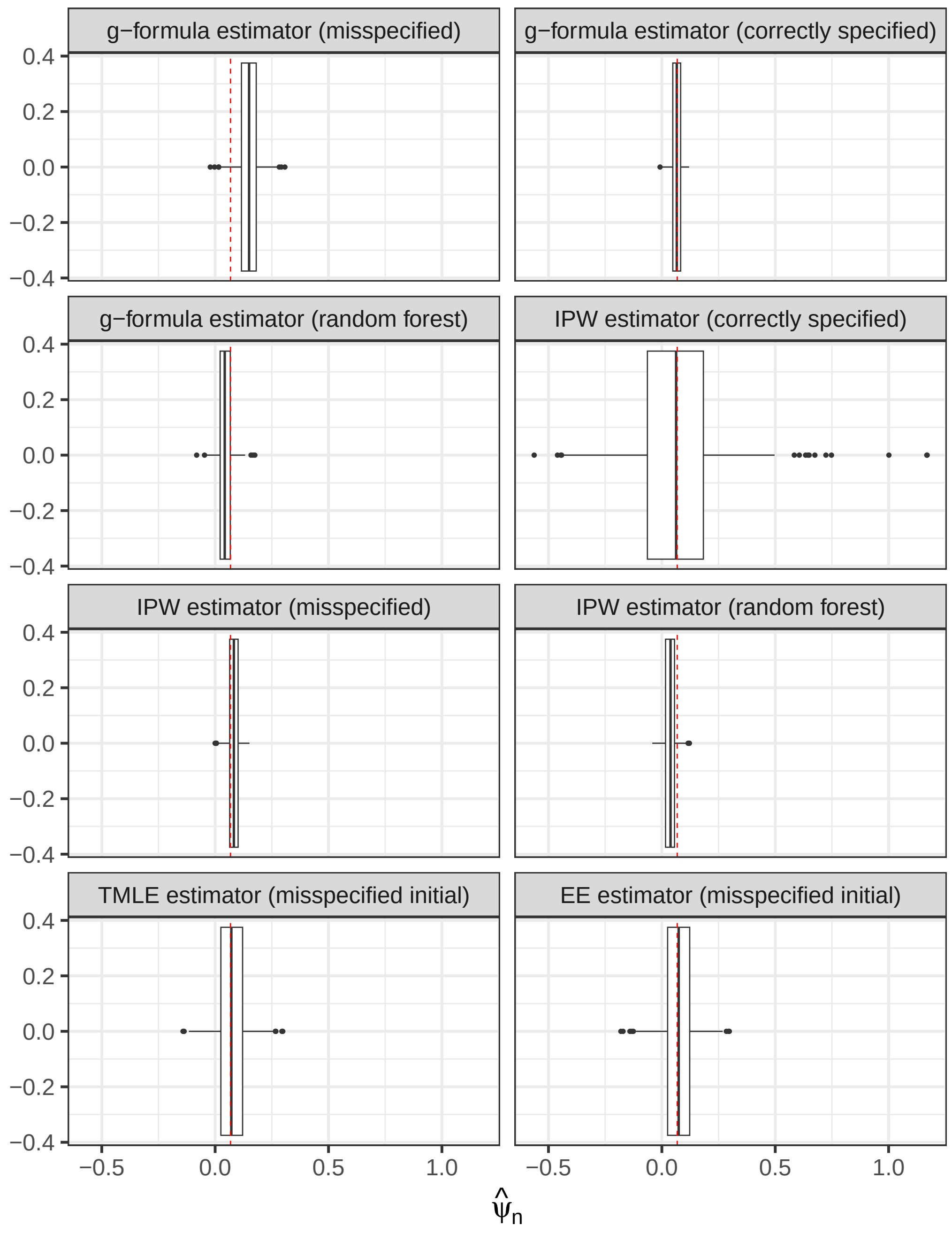

g−formula estimator (misspecified)
g−formula estimator (correctly specified)
g−formula estimator (random forest)
IPW estimator (correctly specified)
IPW estimator (misspecified)
IPW estimator (random forest)
TMLE estimator (misspecified initial)
EE estimator (misspecified initial)
0.4
0.2
0.0
−0.2
−0.4
−0.5
0.0
0.5
1.0
$\hat{\psi}_n$

Figure 2

```
#-- what random forests do we want to consider?
rf.models <- list(rf=c(nodesize=7, mtry=1),
          rf=c(nodesize=5, mtry=1),
          rf=c(nodesize=10, mtry=2),
          rf=c(nodesize=10, mtry=1),
          rf=c(nodesize=7, mtry=2)
          )

#-- for cross-validation;
cv.split <- matrix(sample(1:nrow(sim.data), size=nrow(sim.data)), ncol=V)

for (kk in 1:length(rf.models)) {
  rf.model <- rf.models[[kk]]
  for (vv in 1:V) {
    test.set <- cv.split[,vv]
    train.set <- sim.data[, id][!sim.data[, id] %in% test.set]
    sim.data.train <- sim.data[id%in%train.set]
    sim.data.test <- sim.data[id%in%test.set]
    train.fit <- rfsrc(formula(paste0("Y~A+X1+X2+X3")),
           data=sim.data.train,
           nodesize=rf.model["nodesize"],
           mtry=rf.model["mtry"])
    sim.data[id%in%test.set, (paste0("fit", kk)):=
               predict(train.fit,
                   newdata=sim.data[id%in%test.set],
                   type="response")$predicted]
  }
}

#-- compute cv error;
cve.rf.models <- unlist(lapply(1:length(rf.models), function(kk) {
  sum(loss.fun(sim.data$Y, sim.data[, get(paste0("fit", kk))]))
}))

#-- fit all random forest models;
for (kk in 1:length(rf.models)) {
  rf.model <- rf.models[[kk]]
  fit.rf <- rfsrc(formula(paste0("Y~A+X1+X2+X3")),
          data=sim.data,
          nodesize=rf.model["nodesize"],
          mtry=rf.model["mtry"])
  sim.data[, (paste0("pred.rf.", kk,".A1")):=predict(fit.rf, type="response",
  newdata=copy(sim.data)[, A:=1])$predicted]
  sim.data[, (paste0("pred.rf.", kk,".A0")):=predict(fit.rf, type="response",
  newdata=copy(sim.data)[, A:=0])$predicted]
}

cv.picked <- (1:length(rf.models))[(cve.rf.models==min(na.omit(cve.rf.models))) & !
  is.na(cve.rf.models)]

ate.rf.models.list[[m]] <- c(sapply(1:length(rf.models), function(kk) sim.data[,
  mean(get(paste0("pred.rf.", kk,".A1"))-
                                        get(paste0("pred.rf.", kk,".A0")))]),
                 sim.data[, mean(get(paste0("pred.rf.", cv.picked,".A1"))-
                         get(paste0("pred.rf.", cv.picked,".A0")))])
  saveRDS(ate.rf.models.list,
      file=paste0("~/Undervisning/TMLE/TMLE-course/data/sim-data-output/",
              "save-est-sim-setting-RF",
              ".rds"))
}
```

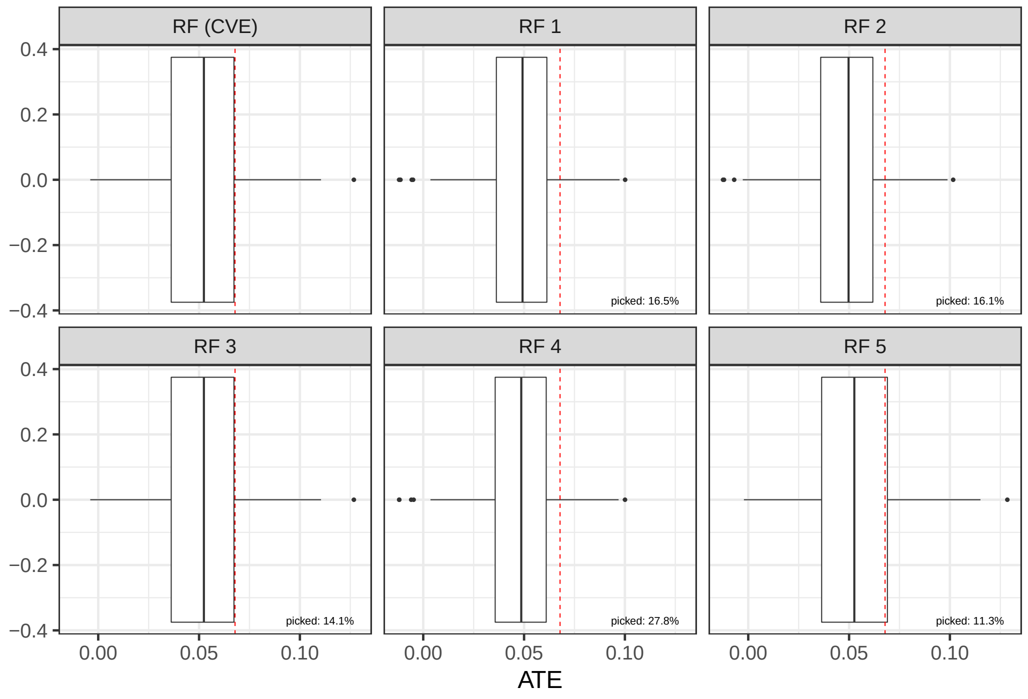
```
library(ggplot2)
library(data.table)

table.rf.picked <- data.table(rf.picked=as.numeric(table(unlist(lapply(ate.rf.models.
    list, function(rf.cve) {
    rf.picked <- (1:length(rf.cve))[rf.cve==min(rf.cve)]
}))))/sum(as.numeric(table(unlist(lapply(ate.rf.models.list, function(rf.cve) {
    rf.picked <- (1:length(rf.cve))[rf.cve==min(rf.cve)]
})))), which=paste0("RF ", 1:length(ate.rf.models.list[[1]])))

dplot <- data.table(ate=unlist(lapply(1:(length(rf.models)+1), function(kk) sapply(ate
    .rf.models.list, function(ate.rf) ate.rf[kk]))),
            which=unlist(lapply(1:(length(rf.models)+1), function(kk) rep(paste0("RF "
    , kk),
                                              length(ate.rf.models.list)))))
dplot[which==paste0("RF ", length(rf.models)+1), which:="RF (CVE)"]

dplot <- merge(dplot, table.rf.picked, by="which", all.x=TRUE)
dplot[, rf.picked:=paste0("picked: ", round(rf.picked*100, 1), "%")]
dplot[rf.picked=="picked: NA%", rf.picked:=""]

ggplot(dplot) +
    theme_bw(base_size=25) +
    geom_boxplot(aes(x=ate)) +
    geom_vline(aes(xintercept=ATE), color="red", linetype="dashed") +
    geom_text(data=unique(dplot, by="rf.picked"), aes(x=0.11, y=-0.37, label=rf.picked
    )) +
    facet_wrap(. ~ which) +
    ylab("") + xlab("ATE")
```



RF (CVE)
RF 1
RF 2
RF 3
RF 4
RF 5
picked: 16.5%
picked: 16.1%
picked: 14.1%
picked: 27.8%
picked: 11.3%
0.4
0.2
0.0
−0.2
−0.4
0.00
0.05
0.10
ATE

Figure 3