# Simulation.rewrite.rst

# 1 Scenario 1

- $W_1$ ,  $W_2$  and  $W_3$  are all continuous random variables
- no interaction term in  $Y \sim A + W$ , i.e.,  $\tau(W)$  is a constant

$$\begin{split} W_1 \sim Unif(-1,1) \\ W_2 \sim Unif(-1,1) \\ W_3 \sim Unif(-1,1) \\ A \sim Bernoulli(\pi_0) \ where \ \pi_0 = expit(0.5 + \frac{1}{3}W_1) \\ Y \sim N(\mu_0,1) \\ \mu_0(A,W) = 0.1 + 0.2 * A + 0.5 * W_1 - 0.3 * W_2 + 0.1 * W_3 \\ \mu_0(1,W) = 0.3 + 0.5 * W_1 - 0.3 * W_2 + 0.1 * W_3 \\ \mu_0(0,W) = 0.1 + 0.5 * W_1 - 0.3 * W_2 + 0.1 * W_3 \\ \tau(W) = 0.2 \\ \psi_0 = 0.04 \\ \theta_0 = 0 \end{split}$$

#### 1.1 Result

- Simulation setting:
  - -n = 2000
  - repeat 1000 times

Table 1:  $\sqrt{n} * \frac{1}{1000} \sum (\psi_n - \psi_0)$  when n = 2000

est	${\bf Super Learner}$	glm.all
plug.in1	0.057	0.0829
os.est1	<b>0.131</b>	0.0849
plug.in2	0.461	0.3585
os.est2	0.747	0.3583

#### **Explanation:**

- Estimator
  - estimator labeled with 1 means estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  all together in one model
  - estimator labeled with 2 means estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  in separate models
- Model
  - SuperLearner means: using SuperLearner() for both propensity score and outcome regression
     \* SL.library = c("SL.mean", "SL.glm", "SL.gam", "SL.earth")
  - glm.all means: using glm() for both propensity score and outcome regression

• Bias is calculated by  $\sqrt{2000} * \frac{1}{1000} \sum (\psi_n - \psi_0)$  and the code is

```
sqrt(n)*mean(rst$psi.plug.in - psi0)
sqrt(n)*mean(rst$psi.one.step.est - psi0)
```

- Findings (more details will be given in the following section 1.2 Detail)
  - the plug-in estimator converge to 0 faster than the one-step estimator
  - estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  in separate models always includes more bias
  - the one-step estimator using SuperLearner() failed to converge to 0 even when n = 2000

Table 2: estimated standard error and empirical standard deviation of the estimator

est	${\bf Super Learner}$	$_{\mathrm{glm.all}}$
plug.in1	0.8165 (0.8175)	0.8269 (0.8238)
os.est1	$0.8165 \ (0.8371)$	$0.8269 \ (0.8228)$
plug.in2	$0.9076 \ (0.8564)$	0.8906 (0.8449)
os.est2	$0.9076 \ (0.9482)$	$0.8906 \ (0.8454)$

#### **Explanation:**

- Standard error
  - the value outside the parentheses is the mean of the estimate of the standard error, which is essentially mean(se(eif.hat))
  - the value inside the parentheses is the empirical standard deviation of the estimator

```
mean(rst$psi.se) # 0.8269
sd(sqrt(n)*(rst$psi.plug.in - psi0)) # 0.8238
```

- Findings (more details will be given in the following section 1.2 Detail)
  - When the glm model is correct, the estimated standard error is close to the empirical standard deviation
  - estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  in separate models always increases the value of estimated standard error
  - the one-step estimator using SuperLearner() underestimates the empirical standard deviation

#### 1.2 Detail

#### Why does the plug-in estimator converge to 0 faster than the one-step estimator?

Our guess is that the model used for estimating the outcome regression is correctly specified. So tau.hat is asymptotically unbiased and psi.plug.in <- mean(tau.hat^2) is also asymptotically unbiased.

$$\hat{\mu}(A, W) = 0.0836 + 0.2289 * A + 0.4083 * W_1 - 0.3607 * W_2 + 0.1312 * W_3$$

This is actually very close to the correct model.

$$\mu_0(A, W) = 0.1 + 0.2 * A + 0.5 * W_1 - 0.3 * W_2 + 0.1 * W_3$$

What phenomenon will support our guess?

If there exists an interaction term A\*W in data generating process, then a simple glm model is not a correct model. The one-step estimator should converge to 0 faster than the plug-in estimator. See Section 2.2.

# Why estimating $\hat{\mu}_1$ and $\hat{\mu}_0$ in separate models always include more bias?

My guess is that when estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  separately,  $\hat{\tau}$  will be a function of W.  $\tau$  in this case is actually a constant. So more bias is included.

```
AW1 <- cbind(data.frame(Y=Y[which(A==1)]), data.frame(W[which(A==1),]))
mu1.reg <- glm(Y ~ ., data=AW1, family='gaussian')</pre>
# Coefficients:
# (Intercept)
       0.3138
                     0.3825
                                 -0.3379
                                                0.1827
AWO <- cbind(data.frame(Y=Y[which(A==0)]), data.frame(W[which(A==0),]))
mu0.reg <- glm(Y ~ ., data=AWO, family='gaussian')</pre>
# Coefficients:
# (Intercept)
                         W1
                                                     W3
      0.08462
                    0.45018
                                -0.39852
```

$$\hat{\tau} = 0.2292 + \hat{\gamma}_1 * W_1 + \hat{\gamma}_2 * W_2 + \hat{\gamma}_3 * W_3$$

 $E(\hat{\tau}) = 0.2292$  but the variance and covariance of W will be included in  $E(\hat{\tau}^2)$ .

But this only explain the bias in the plug-in estimator I guess. I still can not figure out why does the one-step estimator fail to converge.

Why did the one-step estimator using SuperLearner() failed to converge to 0 even when n = 2000?

I am not sure whether 0.131 should be considered as converging to 0 or not. (Add a plot maybe) But from my understanding, the bias from the one-step estimator should be very close to the one from the plug-in estimator like the result from using glm() (0.0829 vs 0.0849 in Table 1). But right now it was like 0.057 vs 0.131.

# the one-step estimator using SuperLearner() underestimates the empirical standard deviation

This is actually also the biggest issue we faced when we were trying to do our previous complicated simulation setting. (underestimating the empirical standard deviation leads to the undercoverage of the Confidence Intervals)

My initial guess is that **SuperLearner()** use a couple of models, hence the variance of the estimator is decreasing especially when the model is weakly correlated. But the contradictory issue is that the empirical standard deviation is also the variance of the estimator, it should be decreasing at the same time. So confusing and still working on this part.

Table 3: estimate mul.hat and mul.hat in one model

est	earth	gam	glm	-earth	all
plug.in1 os.est1 se	0.061		0.0524 0.0518 0.94		

- When the true model is glm, SL.earth will bring bias to the one-step estimator.
- When we use a couple of SL models, we will have a smaller se estimate.

# 2 Scenario 2

- $W_1$ ,  $W_2$  and  $W_3$  are all continuous random variables
- add interaction term in  $Y \sim A + W_1 + W_2 + W_3 + AW_1$ , i.e.,  $\tau(W)$  is a function of  $W_1$

$$W_1 \sim Unif(-1,1)$$

$$W_2 \sim Unif(-1,1)$$

$$W_3 \sim Unif(-1,1)$$

$$A \sim Bernoulli(\pi_0) \ where \ \pi_0 = expit(0.5 + \frac{1}{3}W_1)$$

$$Y \sim N(\mu_0, 1)$$

$$\mu_0(A, W) = 0.1 + 0.2 * A + 0.5 * A * W_1 - 0.3 * W_2 + 0.1 * W_3$$

$$\mu_0(1, W) = 0.3 + 0.5 * W_1 - 0.3 * W_2 + 0.1 * W_3$$

$$\mu_0(0, W) = 0.1 - 0.3 * W_2 + 0.1 * W_3$$

$$\tau(W) = 0.2 + 0.5 * W_1$$

$$\psi_0 = 0.2^2 + (0.5^2)/3 = 0.1233$$

$$\theta_0 = (0.5^2)/3 = 0.083$$

#### 2.1 Result

- Simulation setting:
  - -n = 2000
  - repeat 1000 times

#### model1:

- 1. SL.glm.interaction + SL.gam.interaction + SL.earth, params = list(penalty=-1)
- 2. SL.gam

Table 4:  $\sqrt{n} * \frac{1}{1000} \sum (\psi_n - \psi_0)$  when n = 2000

est	$\operatorname{glm}$	model1
plug.in1	-3.8729	0.3846
os.est1	-3.6471	0.4617
plug.in2	0.4239	0.4705
os.est2	0.4199	0.56

Table 5: estimated standard error and empirical standard deviation of the estimator

est	$\operatorname{glm}$	model1
plug.in1	0.78 (0.77)	1.53 (1.49)
os.est1	0.78(0.82)	1.53(1.48)
plug.in2	1.53(1.47)	1.54(1.48)
os.est2	1.53(1.47)	1.54 (1.49)

# 2.2 Detail

# Support our guess in Section 1.2

This time a simple glm model is not a correct model. The one-step estimator has smaller bias than the plug-in estimator. Also, estimating  $\hat{\mu}_1$  and  $\hat{\mu}_0$  in separate models can provide a tau.hat more close to the true  $\tau(W)$ .

When we tried simple glm for mu1.hat and mu0.hat separately, we can actually have a better one-step estimator, which means, it is actually possible to get a reasonable one-step estimator by estimating mu1.hat and mu0.hat separately. So the issue that the one-step estimator failed to converge to 0 we faced in our previous complicated simulation might be solved by using the appropriate

model.

# 3 Scenario 3

$$\begin{split} W_1 \sim Unif(-1,1) \\ W_2 \sim Unif(-1,1) \\ W_3 \sim Bernoulli(0.5) \\ A \sim Bernoulli(\pi_0) \ where \ \pi_0 = expit(0.5 + \frac{1}{3}W_1) \\ Y \sim N(\mu_0,1) \ where \ \mu_0 = 0.1 + 0.25 * A + 0.75A(W_1^2 + W_3) + W_1 + W_2^2 \\ \tau(W) = 0.25 + 0.75 * (W_1^2 + W_3) \\ \psi_0 = 0.956 \\ \theta_0 = 0.191 \end{split}$$

- Simulation setting:
  - -n = 2000
  - repeat 1000 times

#### model1:

- 1.  $glm(Y \sim .^2)$
- 2. SL.glm + SL.gam

#### model2:

- 1. SL.glm.interaction + SL.gam.interaction + SL.earth, params = list(penalty=-1)
- 2. SL.gam

#### model3:

- 1. SL.glm.interaction + SL.gam.interaction
- 2. SL.glm

### model4:

 $1. \ \, SL.glm.interaction + SL.earth, \, params = list(penalty \!\!=\!\! -1)$ 

2.

Table 6: 
$$\sqrt{n} * \frac{1}{1000} \sum (\psi_n - \psi_0)$$
 when  $n = 2000$ 

est	model1	model2	model3	model4
plug.in1	-1.956	-1.13	-2.09	-0.040
os.est1	-1.891	0.152	-1.95	0.54
plug.in2	-0.889	-0.889	-1.94	
os.est2	0.294	0.294	-1.87	

Table 7: estimated standard error and empirical standard deviation of the estimator

est	model1	model2	model3	model4
plug.in1	4.2 (4.14)	4.06(3.85)	4.04 (3.94)	4.1 (3.88)
os.est1	4.2(4.15)	4.06 (4.03)	4.04(3.95)	4.1 (4.05)
plug.in2	4.1 (3.9)	4.1(3.95)	4.21(4.14)	
os.est2	4.1 (4)	4.1 (4.01)	4.21(4.15)	

Table 8:  $\sqrt{n} * \frac{1}{1000} \sum (\theta_n - \theta_0)$  when n = 2000

est	model1	model2	model3	model4
plug.in1 os.est1	-1.937 -1.98	-1.09 <b>0.124</b>	-1.98 -1.99	-0.042 0.5183
plug.in2 os.est2	-0.91 $0.236$	-0.91 0.236	-1.94 -1.98	

Table 9: estimated standard error and empirical standard deviation of the estimator

est	model1	model2	model3	model4
plug.in1 os.est1 plug.in2 os.est2	1.66 (1.65) 1.66 (1.64) 1.71 (1.61) 1.71 (1.75)	1.68 (1.40) <b>1.68 (1.82)</b> 1.71 (1.61) 1.71 (1.76)	1.59 (1.57) 1.59 (1.59) 1.66 (1.65) 1.66 (1.65)	1.79 (1.46) 1.46 (1.85)

# Explanation: \* Models \* Findings