PM591 Assignment01

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1/26/2022

```
options(scipen = 1, digits = 4)
```

Analysis

1. Re-analysis of the brain weight data

a. Read in (`read.table`) the Brain weight dataset. Examine (`head`) and summarize (`summary`) the data.

```
brain <- read.table("brain.csv", header = TRUE)
head(brain)
```

```
##   Sex Age Head.size Brain.weight
## 1   1   1      4512         1530
## 2   1   1      3738         1297
## 3   1   1      4261         1335
## 4   1   1      3777         1282
## 5   1   1      4177         1590
## 6   1   1      3585         1300
```

```
summary(brain)
```

```
##       Sex            Age         Head.size     Brain.weight
##  Min.   :1.00   Min.   :1.00   Min.   :2720   Min.   : 955
##  1st Qu.:1.00   1st Qu.:1.00   1st Qu.:3389   1st Qu.:1207
##  Median :1.00   Median :2.00   Median :3614   Median :1280
##  Mean   :1.43   Mean   :1.54   Mean   :3634   Mean   :1283
##  3rd Qu.:2.00   3rd Qu.:2.00   3rd Qu.:3876   3rd Qu.:1350
##  Max.   :2.00   Max.   :2.00   Max.   :4747   Max.   :1635
```

b. Convert Sex and Age to factor variables so that `lm` can properly deal with them.

```
brain$Sex <- factor(brain$Sex, levels = 1:2, labels = c("Male","Female"))
brain$Age <- factor(brain$Age, levels = 1:2, labels = c("20-46","46+"))
```

c. Split the data into training (70%) and test (30%) sets.

```r
set.seed(2018)
n <- nrow(brain)
trainset <- sample(1:n, floor(0.7*n))
brain_train <- brain[trainset,]
brain_test <- brain[-trainset,]
```

d. Fit a linear regression model with brain weight as the outcome and head Size, Sex, and Age as predictors. What is the interpretation of the coefficients for Sex and Age? Compute the training and test RMSE and R^2. Does adding Age improves *prediction performance* over the model with Sex and Head size alone?

```r
model_alone <- lm(Brain.weight~Sex+Head.size, data = brain_train)
RMSE_train_alone <-sqrt(sum(residuals(model_alone)^2)/nrow(brain_train))
RSS_alone <- sum(residuals(model_alone)^2)
TSS_alone <- sum((brain_train$Brain.weight-mean(brain_train$Brain.weight))^2)
R2_train_alone <- 1-RSS_alone/TSS_alone
pred_alone <- predict(model_alone, newdata = brain_test)
RMSE_test_alone <- sqrt(sum((brain_test$Brain.weight-pred_alone)^2)/nrow(brain_test))
R2_test_alone <- 1-sum((brain_test$Brain.weight-pred_alone)^2)/sum((brain_test$Brain.weight-mean(brain_t
```

```r
model_all <- lm(Brain.weight~Sex+Head.size+Age, data = brain_train)
coef(model_all)
```

```
## (Intercept)   SexFemale   Head.size      Age46+
##    482.4972    -21.3368      0.2264    -25.0911
```

```r
RMSE_train_all <-sqrt(sum(residuals(model_all)^2)/nrow(brain_train))
RSS_all <- sum(residuals(model_all)^2)
TSS_all <- sum((brain_train$Brain.weight-mean(brain_train$Brain.weight))^2)
R2_train_all <- 1-RSS_all/TSS_all
pred_all <- predict(model_all, newdata = brain_test)
RMSE_test_all <- sqrt(sum((brain_test$Brain.weight-pred_all)^2)/nrow(brain_test))
R2_test_all <- 1-sum((brain_test$Brain.weight-pred_all)^2)/sum((brain_test$Brain.weight-mean(brain_test$
```

```r
tab_rmse <- data.frame(RMSE_train_all,RMSE_train_alone,RMSE_test_all,RMSE_test_alone)
knitr::kable(tab_rmse)
```

RMSE_train_all	RMSE_train_alone	RMSE_test_all	RMSE_test_alone
70.64	71.69	72.07	73.06

```r
tab_r2 <- data.frame(R2_train_all,R2_train_alone,R2_test_all,R2_test_alone)
knitr::kable(tab_r2)
```

R2_train_all	R2_train_alone	R2_test_all	R2_test_alone
0.5895	0.5773	0.7348	0.7275

The interpretation of coefficients of Age and Sex is that Brain size will increase in 0.2264196 unit as sex increases in one unit and Brain size will decrease in 25.0911009 units as age increases in one unit. Adding Age improves prediction performance over the model with Sex and Head size alone

e. Explore whether fitting a linear regression model with separate intercepts and separate slopes for $20 \leq$ Age < 46 and Age ≥ 46 improves prediction performance over the model *Brain.weight ~ Age + Brain.size* (hint: you can, for example, specify an interaction between Sex and Head size including `Head.Size:Age` in the model formula.

```
model3 <- lm(Brain.weight~Age+Head.size+Head.size:Age, data = brain_train)
RMSE_train3 <-sqrt(sum(residuals(model3)^2)/nrow(brain_train))
RSS3 <- sum(residuals(model3)^2)
TSS3 <- sum((brain_train$Brain.weight-mean(brain_train$Brain.weight))^2)
R2_train3 <- 1-RSS3/TSS3
pred3 <- predict(model3, newdata = brain_test)
RMSE_test3 <- sqrt(sum((brain_test$Brain.weight-pred3)^2)/nrow(brain_test))
R2_test3 <- 1-sum((brain_test$Brain.weight-pred3)^2)/sum((brain_test$Brain.weight-mean(brain_test$Brain
```

```
model3_alone <- lm(Brain.weight~Age+Head.size, data = brain_train)
RMSE_train3_alone <-sqrt(sum(residuals(model3_alone)^2)/nrow(brain_train))
RSS3_alone <- sum(residuals(model3_alone)^2)
TSS3_alone <- sum((brain_train$Brain.weight-mean(brain_train$Brain.weight))^2)
R2_train3_alone <- 1-RSS3_alone/TSS3_alone
pred3_alone <- predict(model3_alone, newdata = brain_test)
RMSE_test3_alone <- sqrt(sum((brain_test$Brain.weight-pred3_alone)^2)/nrow(brain_test))
R2_test3_alone <- 1-sum((brain_test$Brain.weight-pred3_alone)^2)/sum((brain_test$Brain.weight-mean(brai
```

```
tab_rmse <- data.frame(RMSE_train3,RMSE_train3_alone,RMSE_test3,RMSE_test3_alone)
knitr::kable(tab_rmse)
```

RMSE_train3	RMSE_train3_alone	RMSE_test3	RMSE_test3_alone
70.97	71.25	73.34	72.91

```
tab_r2 <- data.frame(R2_train3,R2_train3_alone,R2_test3,R2_test3_alone)
knitr::kable(tab_r2)
```

R2_train3	R2_train3_alone	R2_test3	R2_test3_alone
0.5858	0.5825	0.7254	0.7286

It improves in trainset but not in testset.

f. Compare your results from e. to fitting two separate models: Brain.weight ~ Age + Brain.size for individuals $20 \leq$ Age < 46 and 'Brain.weight ~ Age + Brain.size" for individuals Age ≥ 46. Is this equivalent to the single model you fitted in e.? Explain (hint: think about the residual sum of squares being minimized in each case to obtain the model coefficients).

```
brain_train_young <- dplyr::filter(brain_train, brain_train$Age=="20-46")
brain_test_young <- dplyr::filter(brain_test, brain_test$Age=="20-46")
model4 <- lm(Brain.weight~Head.size, data = brain_train_young)
```

```r
brain_train_old <- dplyr::filter(brain_train, brain_train$Age=="46+")
brain_test_old <- dplyr::filter(brain_test, brain_test$Age=="46+")
model5 <- lm(Brain.weight~Head.size, data = brain_train_old)
```

```r
summary(model3_alone)
```

```
##
## Call:
## lm(formula = Brain.weight ~ Age + Head.size, data = brain_train)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -152.7  -43.2    0.0   41.7  257.1
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 421.0135    60.3974    6.97  7.6e-11 ***
## Age46+      -21.7441    11.3493   -1.92    0.057 .
## Head.size     0.2403     0.0163   14.76  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 71.9 on 162 degrees of freedom
## Multiple R-squared:  0.582,  Adjusted R-squared:  0.577
## F-statistic:  113 on 2 and 162 DF,  p-value: <2e-16
```

```r
summary(model4)
```

```
##
## Call:
## lm(formula = Brain.weight ~ Head.size, data = brain_train_young)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -152.36  -54.25    5.25   38.46  237.71
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 503.7849    99.9011    5.04  3.6e-06 ***
## Head.size     0.2178     0.0271    8.04  1.9e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 75.7 on 68 degrees of freedom
## Multiple R-squared:  0.487,  Adjusted R-squared:  0.48
## F-statistic: 64.6 on 1 and 68 DF,  p-value: 1.89e-11
```

```r
summary(model5)
```

```
##
## Call:
```

```
## lm(formula = Brain.weight ~ Head.size, data = brain_train_old)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -161.3  -49.3    2.7   40.1  253.4
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 344.7871    73.4016     4.7  9.1e-06 ***
## Head.size     0.2554     0.0201    12.7  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 68.9 on 93 degrees of freedom
## Multiple R-squared:  0.633,  Adjusted R-squared:  0.629
## F-statistic:  161 on 1 and 93 DF,  p-value: <2e-16
```

They are different since coefficients are obtained by minimizing residual sum of squares, when more data evolved in the model, residual sum of squares of the original model will increase and maynot be the minimum one, hence the coefficients will change and then prodece a new model.

2. Write a R function Rsq to compute R^2.

The function should take two vector arguments observed and predicted and return R^2. Given the correct inputes it should be able to compute training and test R^2s.

```
Rsq <- function(obs,pred){
  RSS = sum((obs-pred)^2)
  TSS = sum((obs-mean(obs))^2)
  R2 = 1-RSS/TSS
}
```

Simulation

1.Simulation study

You will perform a small simulation study to investigate the degree to which assessing prediction performance in *the same data* used to train/fit a model – rather than using a separate test dataset – leads to an overly optimistic assessment of prediction performance. Of particular interest is to investigate how the degree of overoptimistic assessment is affected by i) the size of the training data and ii) the level of noise in the data. The simulation will loosely mimic the brain weight data.

1. Set the training sample size to `n_train=100`, the test sample size to `n_test=50`, and the total sample size to `n = n_train + n_test = 150` (the train/test split is 2/3 train to 1/3 test rather than the more usual 0.8 to 0.2 to prevent the test set from being too small).

```
n_train <- 100
n_test <- 50
n <- n_train + n_test
```

2. Generate a variable/vector `Head.size` of size `n` drawn from a normal distribution with population mean and population standard deviations equal to the sample mean and sample standard deviation, respectively, of the Head.Size variable in the real brain weight data.

```
Head.size <- rnorm(n, mean = mean(brain$Head.size), sd = sd(brain$Head.size))
```

3. Generate a binary variable/vector `Sex`= Female/Male of size `n` with a population frequency of Sex==Female/Male matching the observed frequencies of the variable Sex in the real brain weight data (hint: use `rbinom` to generate samples form a binomial distribution: `rbinom(n, size=1, prob=Malefreq)`, where `Malefreq` was previously computed).

```
Malefreq <- sum(brain$Sex == "Male")/length(brain$Sex)
Sex <- rbinom(n, size = 1, prob = Malefreq)
```

4. Similarly, generate a binary variable/vector `Age`= $<= 46/ > 46$ with population frequencies for $<=$ 46 and $>$ 46 matching the observed frequencies of the variable Age in the the real brain weight data.

```
youngfreq <- sum(brain$Age == "20-46")/length(brain$Age)
Age <- rbinom(n, size = 1, prob = youngfreq)
```

5. Generate a variable/vector `Brain.weight` of size `n` according to the linear model `Brain.weight = b0 + ba * Age + bs * Sex + bh * Head.size`. Use the coefficients beta_0, beta_{A}, beta_S, and beta_H obtained from fitting the corresponding linear regression model to the full real brain weight dataset.

```
lm_model <- lm(Brain.weight~Age+Sex+Head.size, data = brain)
beta_0 <- summary(lm_model)$coefficients[1,1]
beta_A <- summary(lm_model)$coefficients[2,1]
beta_S <- summary(lm_model)$coefficients[3,1]
beta_H <- summary(lm_model)$coefficients[4,1]
Brain.weight <- beta_0 + beta_A*Age + beta_S*Sex + beta_H * Head.size
```

6. Generate a noise/error vector `noise` of size `n` drawn from a normal distribution with mean 0 and variance equal to that of the residual variance in the linear regression model fitted above on the full real brain weight dataset. Add the noise to Brain.weight: `Brain.weight = Brain.weight + noise`.

```
noise <- rnorm(n, mean=0, sd = summary(lm_model)$sigma)
Brain.weight <- Brain.weight + noise
```

7. Construct a dataframe containing the generated variables `Sex`, `Age`, `Brain.weight`, and `Head.size`

```
brain_new <- data.frame(Sex, Age, Brain.weight, Head.size)
```

8. Split the data into training (`size n_train`) and test (`size n_test`) sets.

```
train <- sample(1:n, n_train)
train_set <- brain_new[train,]
test_set <- brain_new[-train,]
```

9. Fit the model `Brain.weight ~ b0 + ba * Age + bs * Sex + bh * Head.size` to the training data.

```r
model2 <- function(Sex, Age, Head.size){
  pred = beta_0 + beta_A*Age + beta_S*Sex + beta_H*Head.size
}
```

```r
rmse <- function(obs,pred){
  sqrt(mean((obs-pred)^2))
}
```

```r
train_set$pred <- model2(train_set$Sex, train_set$Age, train_set$Head.size)
test_set$pred <- model2(test_set$Sex, test_set$Age, test_set$Head.size)
```

10. Compute the training and test RMSE and R^2.

```r
rmse_train <- rmse(train_set$Brain.weight, train_set$pred)
r2_train <- Rsq(train_set$Brain.weight, train_set$pred)
rmse_test <- rmse(test_set$Brain.weight, test_set$pred)
r2_test <- Rsq(test_set$Brain.weight, test_set$pred)
tab <- data.frame(rmse_train, rmse_test, r2_train, r2_test)
knitr::kable(tab)
```

rmse_train	rmse_test	r2_train	r2_test
73.91	57.16	0.5813	0.7233

11. Repeat steps 2 to 10 100 times (save the RMSE's and R^2's from each simulation replicate).

```r
result <- data.frame(1:100,0,0,0,0)
colnames(result) <- c("NO_sim","rmse_train", "rmse_test", "r2_train", "r2_test")
for (i in 1:100){
  Head.size <- rnorm(n, mean = mean(brain$Head.size), sd = sd(brain$Head.size))
  Malefreq <- sum(brain$Sex == "Male")/length(brain$Sex)
Sex <- rbinom(n, size = 1, prob = Malefreq)
  youngfreq <- sum(brain$Age == "20-46")/length(brain$Age)
  Age <- rbinom(n, size = 1, prob = youngfreq)
  lm_model <- lm(Brain.weight~Age+Sex+Head.size, data = brain)
  beta_0 <- summary(lm_model)$coefficients[1,1]
  beta_A <- summary(lm_model)$coefficients[2,1]
  beta_S <- summary(lm_model)$coefficients[3,1]
  beta_H <- summary(lm_model)$coefficients[4,1]
  Brain.weight <- beta_0 + beta_A*Age + beta_S*Sex + beta_H * Head.size
  noise <- rnorm(n, mean=0, sd = summary(lm_model)$sigma)
  Brain.weight <- Brain.weight + noise
  brain_new <- data.frame(Sex, Age, Brain.weight, Head.size)
  train <- sample(1:n, n_train)
  train_set <- brain_new[train,]
  test_set <- brain_new[-train,]
  model2 <- function(Sex, Age, Head.size){
    pred = beta_0 + beta_A*Age + beta_S*Sex + beta_H*Head.size
  }
  train_set$pred <- model2(train_set$Sex, train_set$Age, train_set$Head.size)
  test_set$pred <- model2(test_set$Sex, test_set$Age, test_set$Head.size)
```

```
  rmse_train <- rmse(train_set$Brain.weight, train_set$pred)
  r2_train <- Rsq(train_set$Brain.weight, train_set$pred)
  rmse_test <- rmse(test_set$Brain.weight, test_set$pred)
  r2_test <- Rsq(test_set$Brain.weight, test_set$pred)
  result[i,] <- data.frame(i, rmse_train, rmse_test, r2_train, r2_test)
}
```

12. Compute the average training and test RMSE (R^2) across the 100 simulation replicates.

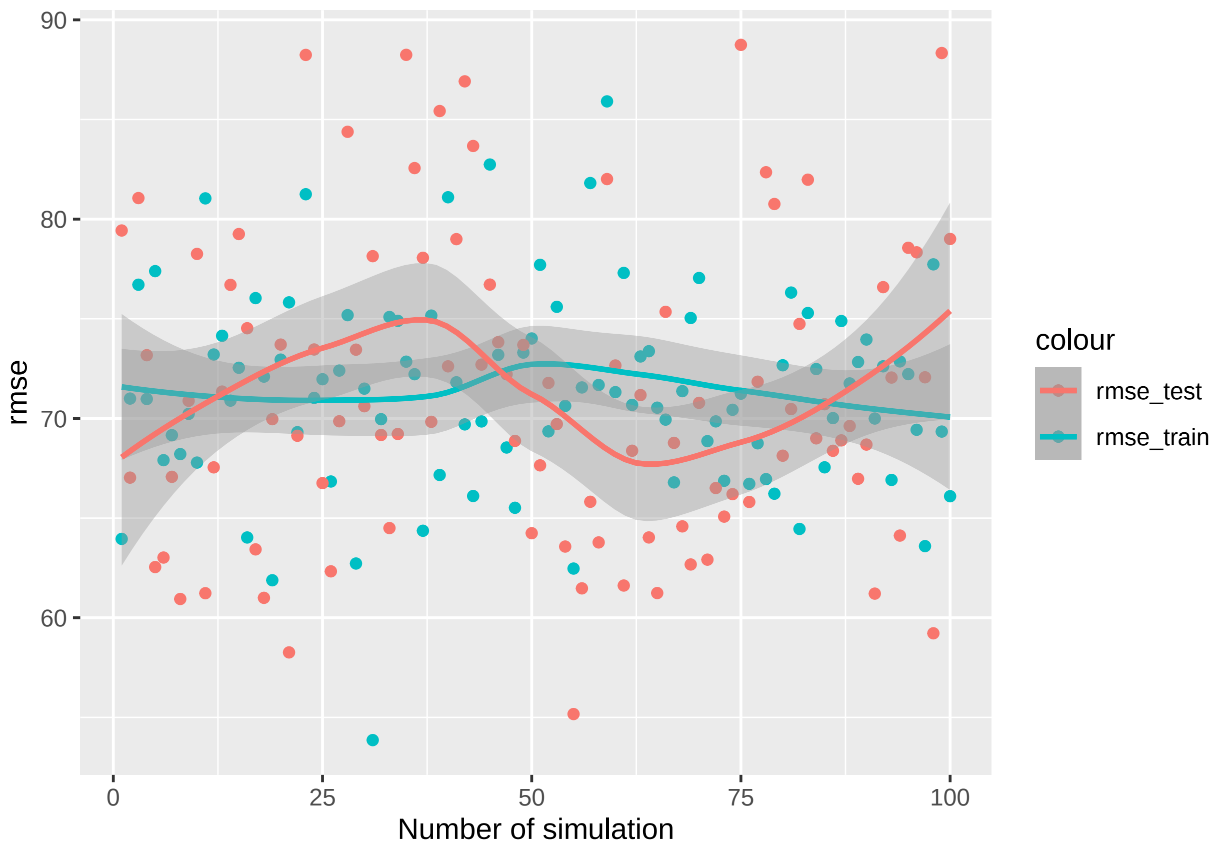
```
train_rmse_avg <- mean(result$rmse_train)
train_r2_avg <- mean(result$r2_train)
test_rmse_avg <- mean(result$rmse_test)
test_r2_avg <- mean(result$r2_test)
tab_mean <- data.frame(train_rmse_avg, train_r2_avg, test_rmse_avg, test_r2_avg)
knitr::kable(tab_mean)
```

train_rmse_avg	train_r2_avg	test_rmse_avg	test_r2_avg
71.34	0.6051	71.28	0.61

13. Visually (e.g. scatter plot, boxplot) evaluate the degree of optimistic assessment when training and testing on the same data.

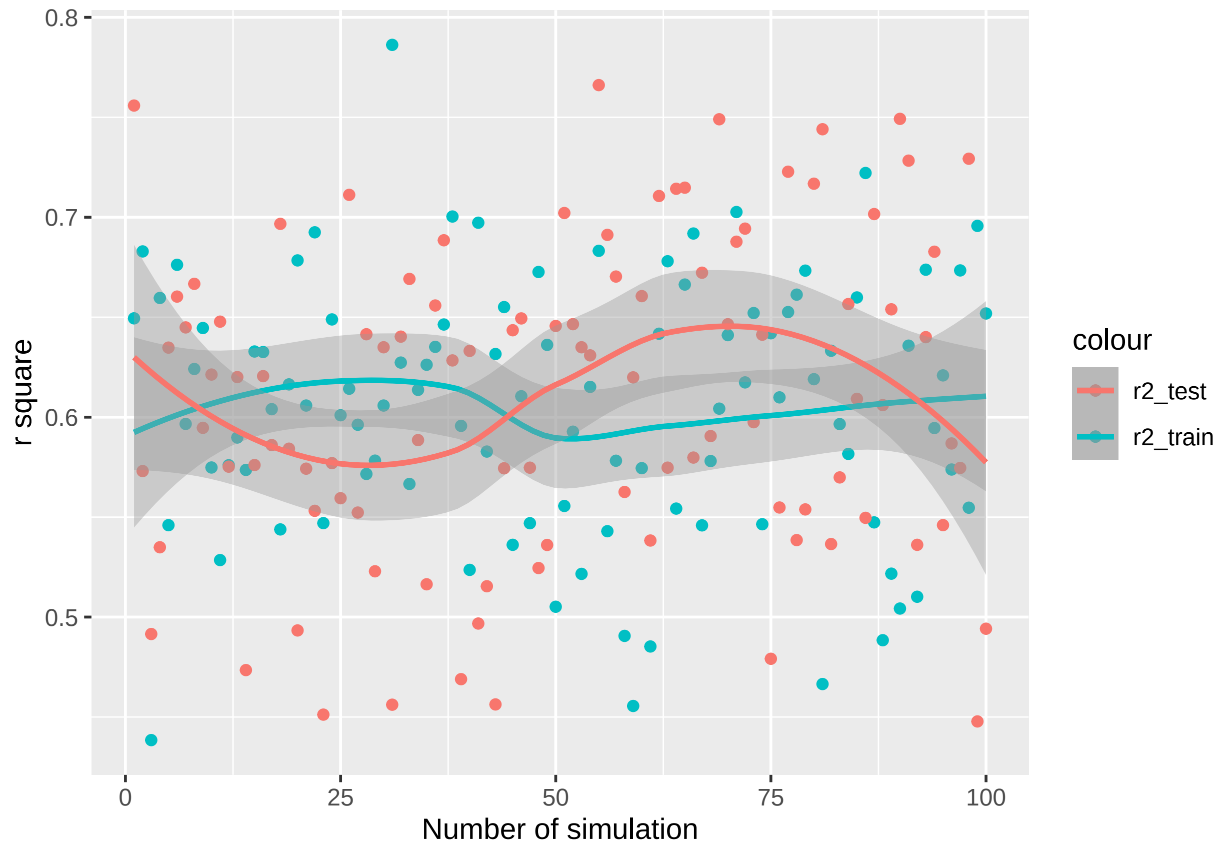
```
library("ggplot2")
ggplot(data = result)+
  geom_point(mapping = aes(x = NO_sim, y = rmse_train, color = "rmse_train"))+
  geom_point(mapping = aes(x = NO_sim, y = rmse_test, color = "rmse_test"))+
  geom_smooth(mapping = aes(x = NO_sim, y = rmse_train, color = "rmse_train"))+
  geom_smooth(mapping = aes(x = NO_sim, y = rmse_test, color = "rmse_test"))+
  labs(x = "Number of simulation", y = "rmse")
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```




```
ggplot(data = result)+
  geom_point(mapping = aes(x = NO_sim, y = r2_train, color = "r2_train"))+
  geom_point(mapping = aes(x = NO_sim, y = r2_test, color = "r2_test"))+
  geom_smooth(mapping = aes(x = NO_sim, y = r2_train, color = "r2_train"))+
  geom_smooth(mapping = aes(x = NO_sim, y = r2_test, color = "r2_test"))+
  labs(x = "Number of simulation", y = "r square")
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



14. Comment on the results of the simulation.

rmse of simulations in train and test are between 65 and 75 and r square of simulations in train and test are between 0.55 and 0.65. And they are stable in training set but not stable in testing set probably because of fewer data in test set.

15. Investigate how the results change as the standard deviation of the noise variable `noise` gets larger (say 1.5- and 2-fold lager than in the baseline simulation). Summarize and comment on your results.

```
result2 <- data.frame(1:10,0,0,0,0,0)
colnames(result2) <- c("NO_sim", "sd_noise" ,"rmse_train", "rmse_test", "r2_train", "r2_test")
for (i in 1:10){
  set.seed(2022)
  Head.size <- rnorm(n, mean = mean(brain$Head.size), sd = sd(brain$Head.size))
  Malefreq <- sum(brain$Sex == "Male")/length(brain$Sex)
  Sex <- rbinom(n, size = 1, prob = Malefreq)
  youngfreq <- sum(brain$Age == "20-46")/length(brain$Age)
  Age <- rbinom(n, size = 1, prob = youngfreq)
  lm_model <- lm(Brain.weight~Age+Sex+Head.size, data = brain)
  beta_0 <- summary(lm_model)$coefficients[1,1]
  beta_A <- summary(lm_model)$coefficients[2,1]
  beta_S <- summary(lm_model)$coefficients[3,1]
  beta_H <- summary(lm_model)$coefficients[4,1]
  Brain.weight <- beta_0 + beta_A*Age + beta_S*Sex + beta_H * Head.size
  sd_noise = summary(lm_model)$sigma * (0.5+i*0.5)
```

```r
  noise <- rnorm(n, mean=0, sd = sd_noise)
  Brain.weight <- Brain.weight + noise
  brain_new <- data.frame(Sex, Age, Brain.weight, Head.size)
  train <- sample(1:n, n_train)
  train_set <- brain_new[train,]
  test_set <- brain_new[-train,]
  model2 <- function(Sex, Age, Head.size){
    pred = beta_0 + beta_A*Age + beta_S*Sex + beta_H*Head.size
  }
  train_set$pred <- model2(train_set$Sex, train_set$Age, train_set$Head.size)
  test_set$pred <- model2(test_set$Sex, test_set$Age, test_set$Head.size)
  rmse_train <- rmse(train_set$Brain.weight, train_set$pred)
  r2_train <- Rsq(train_set$Brain.weight, train_set$pred)
  rmse_test <- rmse(test_set$Brain.weight, test_set$pred)
  r2_test <- Rsq(test_set$Brain.weight, test_set$pred)
  result2[i,] <- data.frame(i, sd_noise, rmse_train, rmse_test, r2_train, r2_test)
}
knitr::kable(result2)
```

NO_sim	sd_noise	rmse_train	rmse_test	r2_train	r2_test
1	71.36	72.68	56.13	0.5450	0.7387
2	107.04	109.02	84.20	0.2977	0.5766
3	142.72	145.36	112.27	0.1505	0.4511
4	178.40	181.70	140.33	0.0689	0.3589
5	214.08	218.04	168.40	0.0234	0.2912
6	249.76	254.38	196.47	-0.0026	0.2407
7	285.44	290.72	224.54	-0.0178	0.2022
8	321.12	327.06	252.60	-0.0268	0.1723
9	356.80	363.40	280.67	-0.0322	0.1486
10	392.48	399.74	308.74	-0.0352	0.1295

As the standard deviation of noise increases, both rmse of train and test increase and r square of train and test decrease.