

# Assignment 1

*Statistics and Data Science 365/565*

*Due: Monday February 3rd 11:59pm*

## Problem 1: Two views of linear regression (10 points)

### Problem 1 View 1

$$\hat{\beta} = \operatorname{argmin} \|Y - X\beta\|^2$$

where  $\beta \in \mathbf{R}^P$

To minimize this, we can solve the partial derivative by  $\beta = 0$

$$\frac{\partial \|Y - X\beta\|^2}{\partial \beta} = X^T(Y - X\beta) = 0$$

$$X^TY - X^TX\beta = 0$$

$$\hat{\beta} = (X^TX)^{-1}X^TY$$

### Problem 1 View 2

we have the density of  $y$  as

$$f(y) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left(-\frac{1}{2}(y - X\beta)^T\Sigma^{-1}(y - X\beta)\right)$$

then we consider the log density of  $y$ , use mle, maximized the likelihood of  $\beta$

$$\begin{aligned} L(\beta) &= \log(f(x_1)f(x_2)\dots f(x_n)) = \sum_{i=1}^n \left(-\frac{1}{2}(y_i - x_i\beta)^T\Sigma^{-1}(y_i - x_i\beta)\right) - \log(\sqrt{|2\pi\Sigma|}) \\ &= \sum_{i=1}^n \left(-\frac{1}{2}(y_i - x_i\beta)^T(y_i - x_i\beta)\right) - \log(\sqrt{|2\pi\sigma|}) \\ \frac{\partial L(\beta)}{\partial \beta} &= -\frac{1}{2}(\sum_{i=1}^n (y_i - x_i\beta)x_i) = 0 \end{aligned}$$

$$\hat{\beta} = \frac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}$$



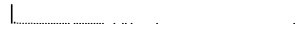

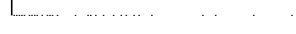


the  $\beta$  solved in this way is exactly same as view 1 since  $\sum_{i=1}^n (-\frac{1}{2}(y_i - x_i \beta)^T (y_i - x_i \beta))$  can also be written as  $(-\frac{1}{2}(Y - X\beta)^T (Y - X\beta))$  and  $\sum_{i=1}^n x_i y_i = X^T Y \sum_{i=1}^n x_i^2 = X^T X$  # Problem 2: Linear regression and classification (30 points)

## Problem 2 Part a.

The summary statistics, the scatter plot, box plot shows as follows, we can find some extreme values and outliers

- Strange stations number distributions

the density function of the station numbers have two peak, with 75% of days the total number of the stations below 331, while the 20% days the total number of the stations within the range of 424 ~ 475

citi_train													
11 Variables							1001 Observations						
trips													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	987	1	25022	13187	5401	8645	15545	26629	34208	38485	42170	
lowest : 876 1107 1144 1214 1459, highest: 50285 50705 51179 51368 52706													
n_stations													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	91	0.996	354.2	48.7	319	321	324	327	331	465	470	
lowest : 292 298 303 307 311, highest: 471 472 473 474 475													
PRCP													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	103	0.685	0.1193	0.2104	0.00	0.00	0.00	0.00	0.04	0.36	0.73	
lowest : 0.00 0.01 0.02 0.03 0.04, highest: 1.95 1.98 2.10 2.54 4.97													
SNWD													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	21	0.321	0.8932	1.647	0.0	0.0	0.0	0.0	0.0	2.0	7.9	
lowest : 0.0 1.0 1.2 2.0 3.1, highest: 15.0 16.1 16.9 18.1 18.9													
SNOW													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	30	0.129	0.1131	0.2216	0	0	0	0	0	0	0	
lowest : 0.0 0.1 0.2 0.3 0.4, highest: 5.5 7.5 8.0 9.5 11.0													
TMAX													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	83	1	62.62	21.9	31	36	46	64	80	86	89	
lowest : 15 17 18 19 20, highest: 94 95 96 97 98													
TMIN													
n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95	
1001	0	82	1	48.12	20.65	17	23	35	50	64	71	73	
lowest : -1 2 3 4 5, highest: 78 79 81 82 83													

## AWND

n	missing	distinct	Info	Mean	Gmd	.05	.10	.25	.50	.75	.90	.95
1001	0	59	0.999	-24.61	62.37	2.2	2.7	3.8	4.9	6.7	8.5	9.8
Value	-10000	0	20									
Frequency	3	948	50									
Proportion	0.003	0.947	0.050									

---

## Outliers

### • PRCP SNWD SNOW

Rainfall and snowfall belong to the small probability event, most days of our data there will be no snow or rain, thus the distribution of PRCP SNWD SNOW should be a skewed distribution naturally. However, we still need to discriminate the outliers. To acquire rigorous decision, we referred to the **nyuweather** and distribution of *non zero PRCP SNWD SNOW*, the precipitation should be smaller than 2, SNOW should be smaller than 8.0, outliers imputed with the average precipitation within the month

### • WIND

from the descriptive statistics and the boxplot, we find there is an observation has a -10000 windspeed, which contradicts the definition of the windspeed, wind doesn't have such strong seasonality, thus we remove this single outlier. After removing the unreasonable value, we recheck the outlier, eliminate the 24 outliers (with windspeed > 10).

## correlations within predictors

After manipulating the outlier, we finally start to analyze the relationship within predictors

### • TMAX is closely related to the TMIN

The maximum temperature for the day is positively correlated to the minimum temperature for the day, we can conclude both from common sense and the scatter plot ( $r = 0.967$ ), in the linear regression model we might need to consider removing multicollinearity of the two predictors, after reexamining the data we find out that during the September of 2015, there is an increase in the number of the stations, this might be due to the Citi Bike is expanding its scale at that time. Thus, even though in boxplot, many observations are marked as the outliers, we can't change its value or remove them.

### • Other strong relationships

Windspeed *AWND* has negative linear relationship with TMAX ( $r = -.502$ ) and TMIN ( $r = -.491$ ); Snowfall also has negative linear relationship with TMAX ( $r = -.43$ ) and TMIN ( $r = -.441$ )

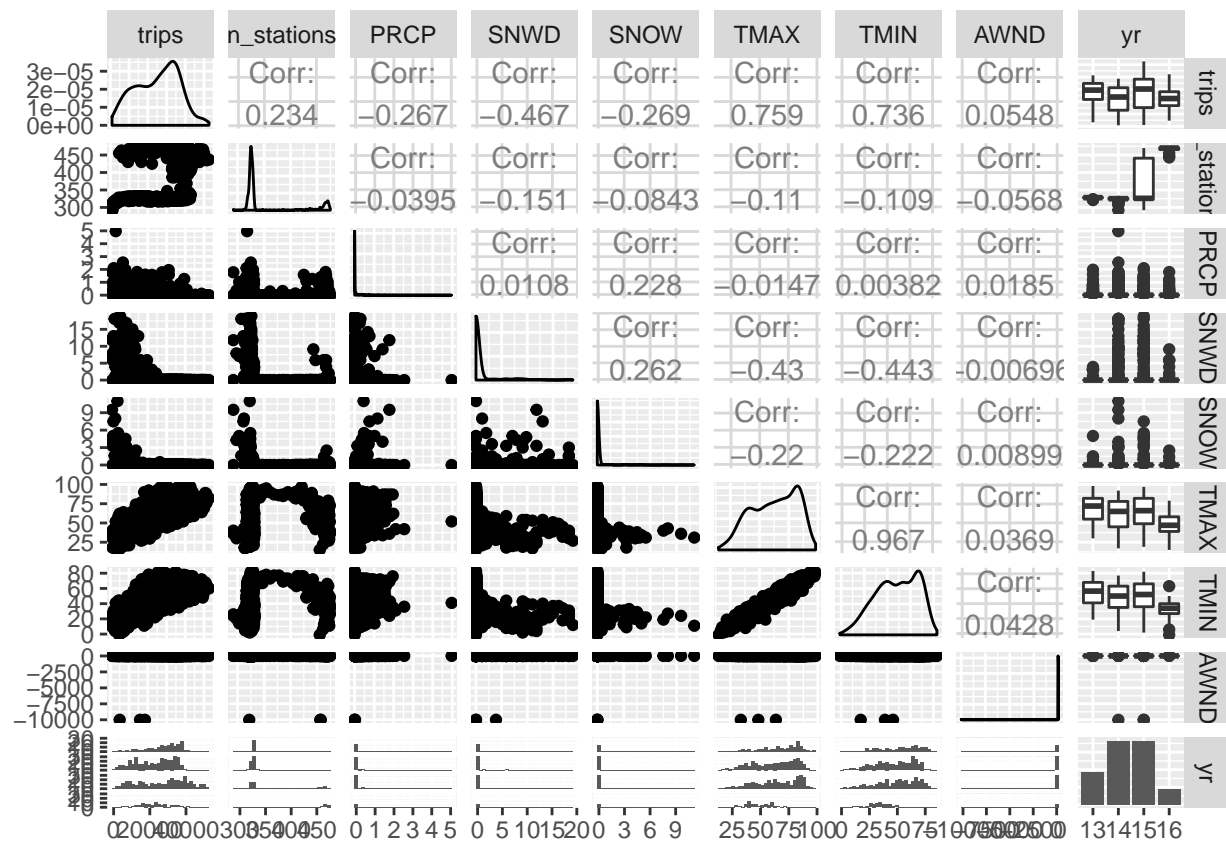
```
library(pacman)

p_load(dplyr,Hmisc,GGally,FNN,stringr,MASS,car,knitr,polynom)

citi_train <- read.csv("citibike_train.csv")
citi_test  <- read.csv("citibike_test.csv")
weather    <- read.csv("weather.csv")

citi_train <- citi_train%>%left_join(weather,by = 'date')%>%
  mutate(yr =str_sub(date,-2,-1))%>%dplyr::select(-date)
citi_test  <- citi_test%>%left_join(weather,by = 'date')%>%
  dplyr::select(-date)
#describe(citi_train)

ggpairs(citi_train%>%dplyr::select(-c(holiday,month,dayofweek)))
```

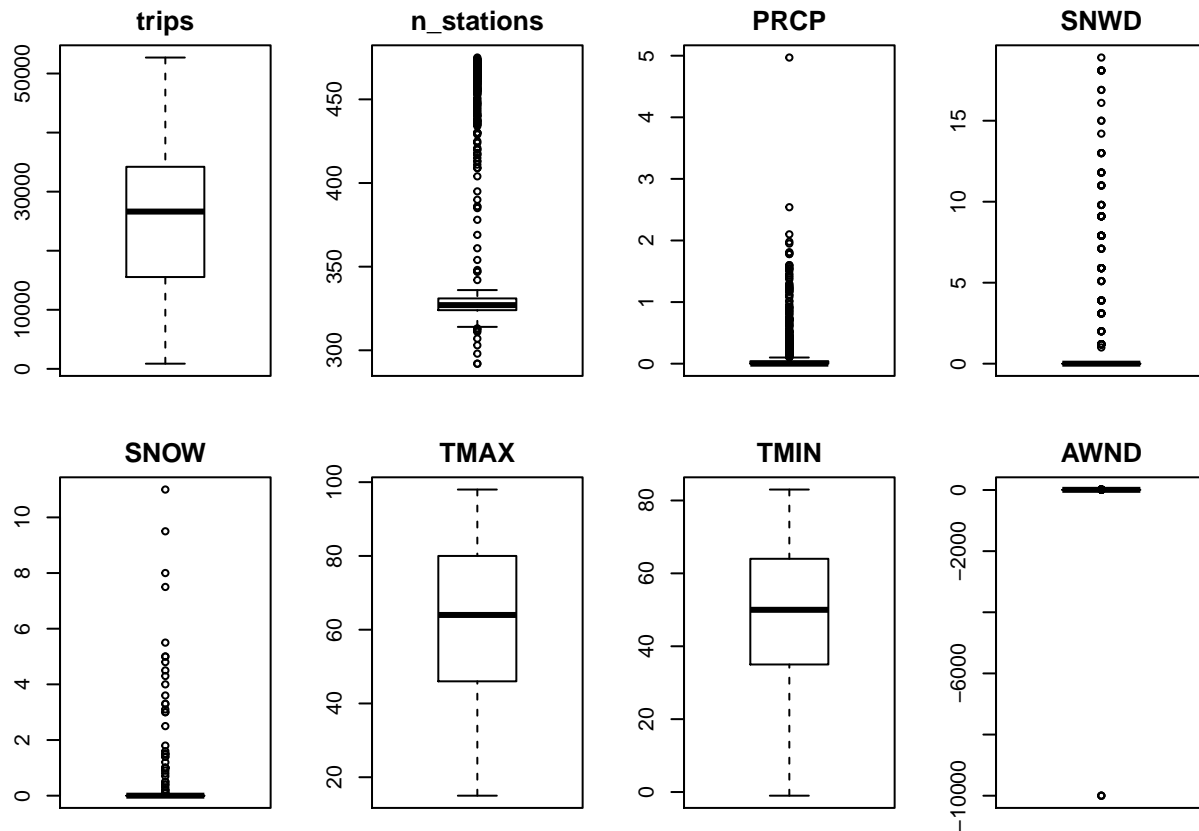


```
par(mfrow = c(2,4))
par(mar = c(2, 2, 2, 2))
list_numeric = c(1:2,6:11)
for(i in list_numeric){
```

```

boxplot(citi_train[,i],main=(names(citi_train)[i]))
}

```



```

#test whether the data is reasonable
#return 0
#dim(citi_train%>%filter(TMAX<=TMIN))[1]

#remove the unreasonable wind speed
citi_train <- citi_train%>%
  filter(AWND>=0 & AWND<=11.2 & SNWD<18.9)%>%group_by(month,yr)%>%
  mutate(PRCP = case_when(
    (PRCP<=2) ~ PRCP,
    (PRCP>2) ~ median(PRCP)
  ),
  SNOW = case_when(
    (SNOW<=8) ~ SNOW,
    (SNOW>8) ~ median(SNOW))

```

```

)%>%ungroup()%>%dplyr::select(-yr)

citi_test <-citi_test)%>%mutate(AWND = case_when(
  AWND>=0 ~ AWND,
  TRUE ~ median(AWND)
))

```

## Problem 2 Part b.

below is the model with all the possible variables

```

#model with all the variables
fit <- lm(trips~.,data = citi_train)
summary(fit)

```

```

##
## Call:
## lm(formula = trips ~ ., data = citi_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -18001.1  -2199.1    238.5   2476.9  15191.5
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -14232.299   1462.055   -9.734 < 2e-16 ***
## n_stations      71.668     2.804   25.557 < 2e-16 ***
## holidayTRUE  -10878.750    782.048  -13.911 < 2e-16 ***
## monthAug       4545.484    783.689    5.800 9.02e-09 ***
## monthDec      -2788.993    738.798   -3.775 0.000170 ***
## monthFeb      -4963.121    903.479   -5.493 5.07e-08 ***
## monthJan      -4976.984    815.816   -6.101 1.54e-09 ***
## monthJul       3057.235    811.453    3.768 0.000175 ***
## monthJun       4901.322    807.152    6.072 1.82e-09 ***

```

```

## monthMar      -2979.466    740.735   -4.022  6.22e-05 ***
## monthMay      3985.920    762.057    5.230  2.08e-07 ***
## monthNov      2337.717    711.269    3.287  0.001051 **
## monthOct      7113.183    694.104   10.248 < 2e-16 ***
## monthSep      7002.524    736.992    9.501 < 2e-16 ***
## dayofweekMon  -763.630    478.297   -1.597  0.110697
## dayofweekSat -5096.812    477.994  -10.663 < 2e-16 ***
## dayofweekSun -6574.046    481.302  -13.659 < 2e-16 ***
## dayofweekThurs  528.091    475.128    1.111  0.266648
## dayofweekTues -421.366    477.103   -0.883  0.377366
## dayofweekWed   522.199    476.202    1.097  0.273098
## PRCP          -9753.592    462.889  -21.071 < 2e-16 ***
## SNWD          -241.946     63.355   -3.819  0.000143 ***
## SNOW           202.115    240.878    0.839  0.401637
## TMAX           335.410     29.090   11.530 < 2e-16 ***
## TMIN          -71.273     31.817   -2.240  0.025317 *
## AWND          -329.082     73.329   -4.488  8.08e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3967 on 949 degrees of freedom
## Multiple R-squared:  0.8817, Adjusted R-squared:  0.8786
## F-statistic: 283 on 25 and 949 DF, p-value: < 2.2e-16

```

**Model Selection: use AIC to decide the best model and make sure check the multicollinearity**

### Steps

1. for  $p = 1, 2, 3, 4, 5$  iterate all the possible combinations
2. when a model with lower AIC comes up, update the best model for the  $p$
3. control multicollinearity by eliminating the model with any parameters  $VIF > 4$
4. test whether the situations without intercept would have better performance

```

#model selection
best <- list()

#q = 1
fit0 = lm(trips~1,data = citi_train)
best[[1]]<-list(fit0,NULL)

#consider the conditions that has intercept
for (i in 1:4){
  AIC <- 10^10
  for (iter in 1:dim(combn(10, i))[2]){
    df <- data.frame(citi_train[,c(1,combn(10, i)[,iter]+1)])
    fit_temp <- lm(trips~.,data = df)
    #if(i>2){print(car::vif(fit_temp))}
    if(i >1&& any(car::vif(fit_temp)>4)){next}
    if (AIC >AIC(fit_temp)){
      best[[i+1]]<- list(fit_temp,names(citi_train)[combn(10, i)[,iter]+1])
    }
  }
}

#consider the conditions that no intercept
for (i in 1:5){
  AIC <- AIC(best[[i]][[1]])
  for (iter in 1:dim(combn(10, i))[2]){
    df <- data.frame(citi_train[,c(1,combn(10, i)[,iter]+1)])
    fit_temp <- lm(trips~.-1,data = df)
    #if(i>2){print(car::vif(fit_temp))}
    if(i >1&& any(car::vif(fit_temp)>4)){next}
    if (AIC >AIC(fit_temp)){
      best[[i]]<- list(fit_temp,names(citi_train)[combn(10, i)[,iter]+1])
    }
  }
}

```



```

mse <- function(sm)
  mean(sm$residuals^2)
rsq <- function (preds, actual,y) {
  rss <- sum((preds - (actual))^ 2) ## residual sum of squares
  ess <- sum((preds - mean(actual))^ 2)
  tss <- sum((actual - mean(y))^ 2) ## total sum of squares
  rsq <- 1-rss/tss}
modelperf <- data.frame()
model <- NULL
for (i in 1:5){
  sm <- summary(best[[i]][[1]])
  y_test <- citi_test$trips
  new_data <- citi_test%>%dplyr::select(best[[i]][[2]])
  y_pred <- predict(best[[i]][[1]],new_data)
  mse_test <- mean(y_pred-y_test)^2
  model[i]<-paste(best[[i]][[2]], collapse = ',')
  modelperf <- rbind(modelperf,
                     c(i,mse(sm),sm$r.squared,mse_test,rsq(y_pred, y_test,citi_train$trips) ))
}
modelperf <- cbind(modelperf,model)
names(modelperf)<-c('q','mse','rsq','mse_test','rsq_test','model parameter')
kable(modelperf)

```

q	mse	rsq	mse_test	rsq_test	model parameter
1	62156100	0.9197630	179395619	0.4704363	TMIN
2	62142631	0.9197804	180258264	0.4684775	TMIN,AWND
3	54594133	0.9295247	175467386	0.4993307	SNOW,TMAX,AWND
4	52541373	0.9321746	172741726	0.5031978	SNWD,SNOW,TMAX,AWND
5	51190546	0.9339184	177835683	0.5012867	PRCP,SNWD,SNOW,TMIN,AWND

the second model gives the better result with least mse and largest rsq.

## Problem 2 Part c.

The process of knn is showed as below, we can compare the test and train set, then pick the  $k = 5$  since when  $k = 5$  the test results are getting stable and reached the lowest error rate, wouldn't cause a overfitting or underfitting problem

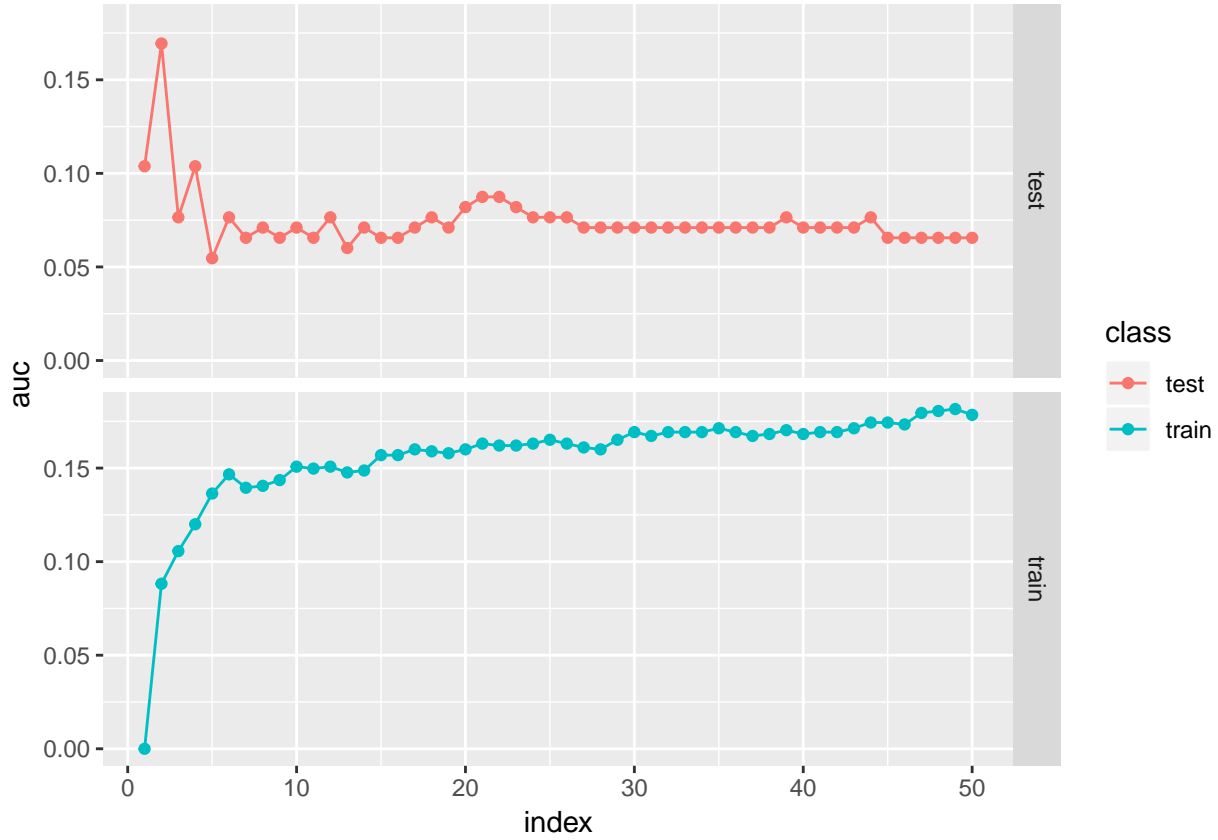
```
citi_train$train <- 1
citi_test$train <- 0
citi_train_new <- rbind(citi_train,citi_test)%>%
  mutate(class = ifelse(trips>median(trips),1,0))%>%
  dplyr::select(-c(trips,holiday,month,dayofweek))

y_train = (citi_train_new%>%filter(train ==1))$class
X_train = (citi_train_new%>%filter(train ==1))[, -c(8,9)]
y_test = (citi_train_new%>%filter(train ==0))$class
X_test = (citi_train_new%>%filter(train ==0))[, -c(8,9)]

X_train = scale(X_train)
X_test = scale(X_test, center=attr(X_train, "scaled:center"),
               scale=attr(X_train, "scaled:scale"))

test_auc <- c()
train_auc <- c()
for (i in 1:50){
  train_auc <-c(train_auc,
               sum(as.numeric(knn(X_train, X_train, y_train, k = i))-1!=y_train)/length(y_train))
  test_auc <-c(test_auc,
               sum(as.numeric(knn(X_train, X_test, y_train, k = i))-1!=y_test)/length(y_test))
}
result <- data.frame(index = rep(1:50,2),
                    class = rep(c("train","test"),each=50),auc = c(train_auc,test_auc))
ggplot(data=result,
      aes(x = index, y = auc,group = class,color = class))+
```

```
geom_line()+facet_grid(class~.)+geom_point()
```



### Problem 3: Classification for a Gaussian Mixture (25 points)

#### Problem 3 Part a.

For loss function  $\mathbf{1}\{f(X) \neq Y\}$ ,

$$E(\mathbf{1}\{f(X) \neq Y\}) = P(f(X) \neq Y)$$

is exactly the bayes risk, which can be minimized by the bayes rule where the decision boundary is  $P(Y = 1 | X = x) > \frac{1}{2}$

$$\begin{aligned} P(Y = 1 | X = x) &= \frac{P(X | Y = 1)P(Y = 1)}{P(X | Y = 0)P(Y = 0) + P(X | Y = 1)P(Y = 1)} \\ &= \frac{P(X | Y = 1)}{P(X | Y = 0) + P(X | Y = 1)} = \frac{f_0(x)}{f_0(x) + f_1(x)} \geq \frac{1}{2} \end{aligned}$$

we simplify it as

$$f(X) = \begin{cases} 1 & \text{if } f_1(X) > f_0(X) \\ 0 & \text{else} \end{cases}$$

$$f_0(x) = f_1(x) \text{ when } x^2 = (x-3)^2 \Rightarrow x = \frac{3}{2}$$

Thus, we have

$$f(X) = \begin{cases} 1 & \text{if } X > \frac{3}{2} \\ 0 & \text{else} \end{cases}$$

$$\begin{aligned} \text{Bayes Error Rate} &= P(Y=0)P(f(\hat{X})=1 \text{ while } f(X)=0 \mid Y=0) + P(Y=1)P(f(\hat{X})=0 \text{ while } f(X)=1 \mid Y=1) \\ &= \frac{1}{2}(0.0668072 + 0.0668072) = 0.0668072 \end{aligned}$$

### Problem 3 Part b.

when the variances of two Gaussians are different, the expected loss will still be minimized by the bayes classifiers, but with the different decision boundary which is the root  $a$  of the following equation

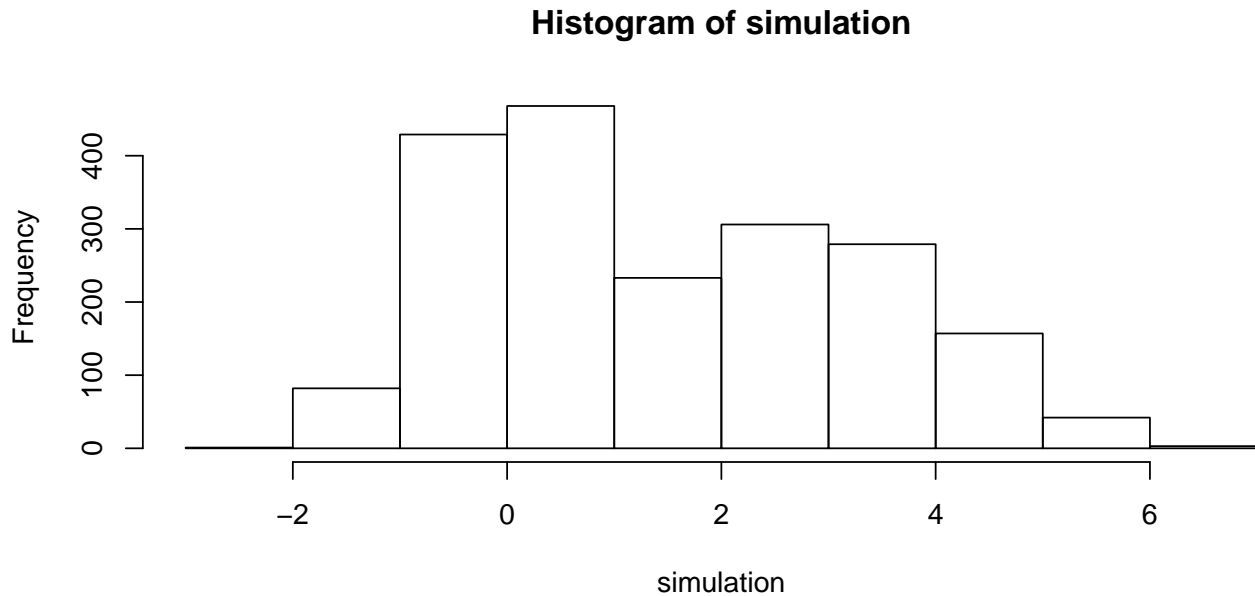
$$f_0(x) = f_1(x) \text{ when } \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{x^2}{2\sigma_0^2}} = \frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{(x-3)^2}{2\sigma_1^2}}$$

Thus, we have

$$f(X) = \begin{cases} 1 & \text{if } X > a \\ 0 & \text{else} \end{cases}$$

### Problem 3 Part c.

```
set.seed(22)
n = 2000
Y1 <- rbinom(n,1,1/2)
mixture <- function(x){if(x==1) return(rnorm(1,3,sqrt(1.5))) else return(rnorm(1,0,sqrt(0.5)))}
simulation<- sapply(Y1, mixture)
sim_df <- data.frame(label = Y1,simulation = simulation)
hist(simulation)
```



```
test<- sample(n,n/5)
sim_df_test <- sim_df[test,]
sim_df_train <- sim_df[-test,]
sim_df_train_mean <- sim_df_train%>%group_by(label)%>%summarise(mean = mean(simulation))
```

the decision boundary is decided by  $\frac{\hat{\mu}_0 + \hat{\mu}_1}{2} = 1.2520827$

$$f(X) = \begin{cases} 1 & \text{if } X > 1.252083 \text{ i.e. } f_1(x) > f_0(x) \\ 0 & \text{else} \end{cases}$$

```
therhold <- solve(polynomial(c(-3-(1/2)*log(3),2,2/3)))[2]
sim_df_test <- sim_df_test%>%
  mutate(yhat =
    ifelse(simulation>therhold,1,0))%>%
  mutate(y_diff = (yhat ==label))
estimator<-1-sum(sim_df_test$y_diff)/length(sim_df_test$y_diff)# the error rate
```

The predict error rate is 0.0525

### Problem 3 Part d.

The variance of the error rates are overall stable when  $n$  is increasing, we can see from the plot below, since when  $n$  is large enough the estimation values  $\mu_1$ ,  $\mu_0$  are

```

seq.n <- seq(from = 2000, to = 20000, by = 10)
estimator <- c()
for(n in seq.n){
  Y1 <- rbinom(n,1,1/2)
  mixture <- function(x){if(x==1) return(rnorm(1,3,sqrt(1.5))) else return(rnorm(1,0,sqrt(0.5)))}
  simulation<- sapply(Y1, mixture)
  sim_df <- data.frame(label = Y1,simulation = simulation)
  sim_df_train_mean <- sim_df%>%group_by(label)%>%
    summarise(mean = mean(simulation))%>%arrange(label)
  mu0<- sim_df_train_mean[1,2]
  mu1<- sim_df_train_mean[2,2]
  #print(paste(mu0,mu1))
  Y1_test <- rbinom(10000,1,1/2)
  simulation_test<- sapply(Y1_test, mixture)
  sim_df <- data.frame(label = Y1_test,simulation = simulation_test)

  #print(solve(polynomial(c(mu0^2 -(1/3)*mu1^2 -(1/2)*log(3), (2/3)*mu1-2*mu0,2/3)))[2])
  sim_df <- sim_df%>%
    mutate(yhat = ifelse(simulation>
      solve(polynomial(c(mu0^2 -(1/3)*mu1^2 -
        (1/2)*log(3), (2/3)*mu1-2*mu0,2/3)))[2],1,0))%>%
    mutate(y_diff = (yhat ==label))
  estimator<-c(estimator,1-sum(sim_df$y_diff)/length(sim_df$y_diff))
}
sim <- data.frame(n = seq.n, errorate = estimator)

ggplot(data = sim, aes(x = n, y=errorate))+geom_point()+ylab("error rate")+
  xlab("number of simulation")

```

