STAT 6340 Statistical and Machin Learning

Project 4

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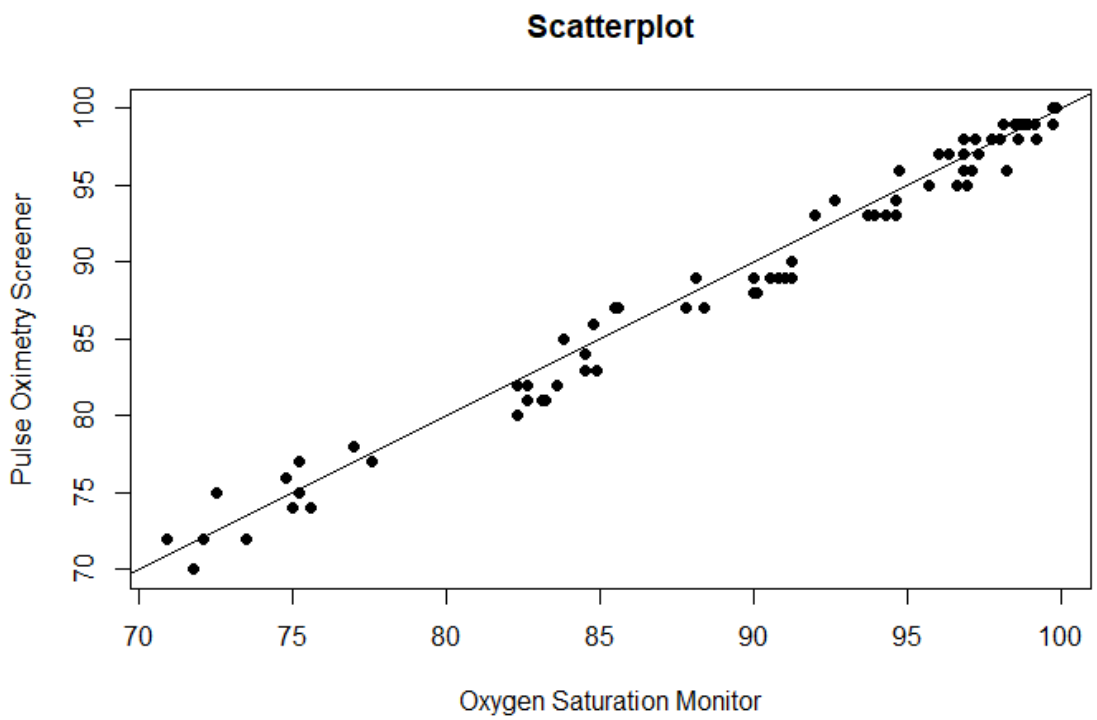
Section 1

Problem 1

a)



b) Two populations are in perfect agreement, when they are identical. Then $\mu_1 = \mu_2$ and $\sigma_1 = \sigma_2$ and vice versa. From the Pearson's correlation coefficient, we have

$$\rho = \frac{cov(X_1, X_2)}{\sigma_1 \sigma_2}$$

where $cov(X_1, X_2) = \sigma_1^2$ when X_1 and X_2 are identical. Thus $\rho = 1$.

c)

i. Since $(\sigma_1 - \sigma_2)^2 \geq 0 \;\Rightarrow\; \sigma_1^2 + \sigma_2^2 \geq 2\sigma_1\sigma_2$ and $(\mu_1 - \mu_2)^2 \geq 0$

Thus

$$\frac{2\sigma_1\sigma_2}{(\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2} \leq 1$$

Therefore

$$|\theta| = |\rho| \left| \frac{2\sigma_1\sigma_2}{(\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2} \right| \leq |\rho|$$

We know that the correlation between two population satisfy $0 \leq |\rho| \leq 1$

Hence we have $0 \leq |\theta| \leq |\rho| \leq 1$

ii. Assume $\theta = 1$. Then

$$\rho \frac{2\sigma_1\sigma_2}{(\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2} = 1$$

$$2\rho\sigma_1\sigma_2 = (\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2$$

$$(\mu_1 - \mu_2)^2 + \sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2 = 0$$

$$(\mu_1 - \mu_2)^2 + (\sigma_1 - \sigma_2)^2 + 2\sigma_1\sigma_2 - 2\rho\sigma_1\sigma_2 = 0$$

$$(\mu_1 - \mu_2)^2 + (\sigma_1 - \sigma_2)^2 + 2(1 - \rho)\sigma_1\sigma_2 = 0$$

Since all these parts are positive, each of them should equal to zero separately.
This implies $\mu_1 = \mu_2, \sigma_1 = \sigma_2$ and $\rho = 1$

Now assume $\mu_1 = \mu_2, \sigma_1 = \sigma_2$ and $\rho = 1$. Then by substituting, we get $\theta = 1$
From part b) this imply perfect agreement.

d)

$$\hat{\theta} = \frac{2\hat{\sigma}_{12}}{(\hat{\mu}_1 - \hat{\mu}_2)^2 + \hat{\sigma}_1^2 + \hat{\sigma}_2^2}$$

Where $\hat{\mu}_1, \hat{\mu}_2$ are population means, $\hat{\sigma}_1, \hat{\sigma}_2$ are population standard deviations and $\hat{\sigma}_{12}$ is covariance of the two populations.
With this function `CCC = 0.9892748`

e) With my bootstrap function, following results were obtained.

```
   CCC_original    CCC_my          bias    std_error
      0.9892748 0.9889337 -0.0003411283 0.0002304046
```

Confident Interval computed using Standard Error.

```
   lower_bound_SE upper_bound_SE
        0.9887033      0.9891641
```

Confident Interval computed using percentile method.

```
       lower_bound_Perc
 47.5%        0.9889895

       upper_bound_Perc
 52.5%        0.9892421
```

f) With the boot package, results are

```
Bootstrap Statistics :
     original        bias    std. error
t1* 0.9892748 -0.0003717729 0.002032808
```

and the Confident Interval using percentile method,

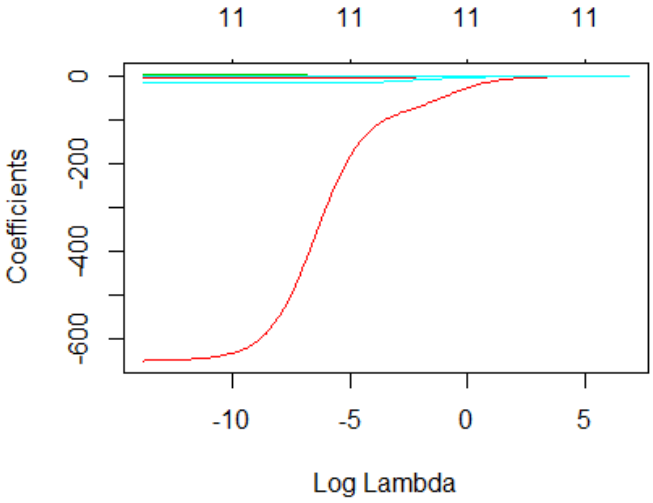
```
Intervals :
Level     Percentile
95%   ( 0.9841,  0.9923 )
Calculations and Intervals on Original Scale
```

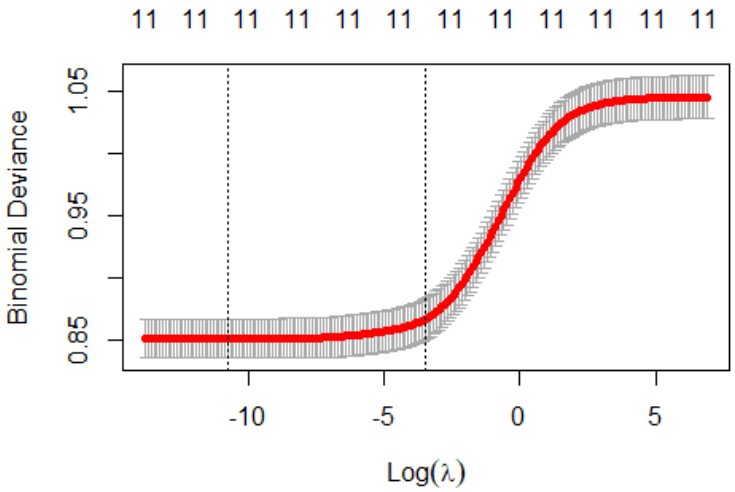
	Bias	Standard Error	Lower bound for CI
My code	-0.0003411283	0.0002304046	0.9889895
bootstrap	-0.0003717729	0.002032808	0.9841

g) Results shows the two methods gives nearly the same Bias and CI except for the standard Error. Thus both these methods can be used interchangeably in practice but with the low standard error, my code gives slightly better results.

Problem 2

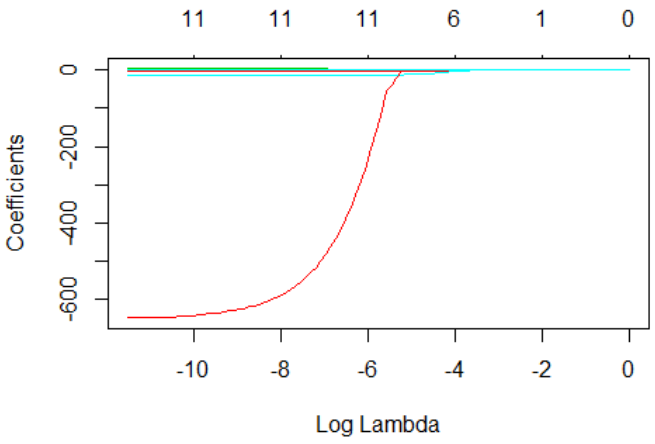
a) Test error rate = 0.2000789
b) Test error rate = 0.1990572
c) Test error rate = 0.1990572
d) Test error rate = 0.1994666
e)

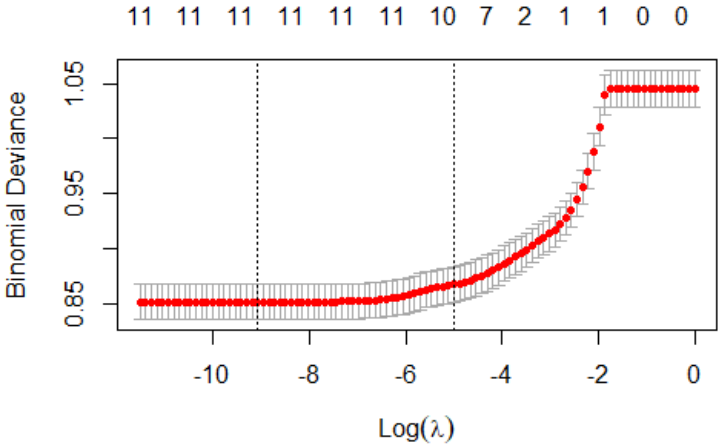




Best λ = 2.049075e-05
Test error rate = 0.1976317

f)





Best λ = 0.0001149757
Test error rate = 0.1978359

g)

	Full	Best Subset	Backward	Forward	Ridge	Lasso
X.Intercept.	6.361576e+02	7.443217e+02	7.443217e+02	641.2029336	6.195350e+02	6.066693e+02
fixed.acidity	5.521067e-01	6.301870e-01	6.301870e-01	0.5546123	5.391177e-01	5.262977e-01
volatile.acidity	-3.784880e+00	-3.686958e+00	-3.686958e+00	-3.8031154	-3.781939e+00	-3.767113e+00
citric.acid	-7.377814e-01	-6.927095e-01	-6.927095e-01	-0.7431531	-7.391644e-01	-7.252818e-01
residual.sugar	2.951950e-01	3.324403e-01	3.324403e-01	0.2967673	2.889508e-01	2.837514e-01
chlorides	-1.263994e+01	-1.238154e+01	-1.238154e+01	-12.6752942	-1.276662e+01	-1.273346e+01
free.sulfur.dioxide	8.644758e-03	8.176799e-03	8.176799e-03	0.0083011	8.748570e-03	8.690595e-03
total.sulfur.dioxide	-2.696022e-04	NA	NA	NA	-3.514132e-04	-3.507052e-04
density	-6.590763e+02	-7.683960e+02	-7.683960e+02	-664.1842221	-6.422076e+02	-6.290951e+02
pH	3.342979e+00	3.682339e+00	3.682339e+00	3.3514899	3.286873e+00	3.231570e+00
sulphates	2.167765e+00	2.306562e+00	2.306562e+00	2.1707966	2.144495e+00	2.118287e+00
alcohol	1.423452e-01	NA	NA	0.1384844	1.602747e-01	1.732598e-01
AIC	4.167223e+03	4.164778e+03	4.164778e+03	4165.2553390	NA	NA
Test.Error	2.000789e-01	1.990572e-01	1.990572e-01	0.1994666	1.976317e-01	1.978359e-01

From reduced models, Best subset selection method and Backward method gives the same model and their Test error rates are low compared to the full model. Out of all the models compared, Ridge regression method gives the lowest Test error rate. Thus the preferred model is with the Ridge regression.

All the models build in the previous project for wine data set have larger test error rates. Thus the best model is still with the Ridge regression.

Section 1

```
# problem 1

library(boot) # for bootstrap
library(gdata) # for resample
data_set <- read.delim("oxygen_saturation.txt")
attach(data_set)
n <- dim(data_set)[1]

# problem 1 a)

plot(osm, pos, main="Scatterplot",
     xlab="Oxygen Saturation Monitor",
     ylab="Pulse Oximetry Screener", pch=19)
abline(0, 1)


# problem 1 d)

# function to compute concordance correlation coefficient (CCC)
CCC.fn <- function(data, indices) {
  x <- data[indices,1]
  y <- data[indices,2]
  mu1 <- mean(x)
  mu2 <- mean(y)
  sigma1 <- var(x)
  sigma2 <- var(y)
  sigma12 <- cov(x, y)
  result <- 2*sigma12/((mu1-mu2)^2+sigma1+sigma2)
  return(result)
}

CCC.fn(data_set, 1:n) # original CCC
# [1] 0.9892748



# my own code for the bootstrap method
my_boot.fn <- function(data, n, B) {
  para <- c()
  i = 1
  while(i<=B) {
    sample <- data[resample(1:n, n, replace = TRUE, prob = NULL),]
    para[i] <- CCC.fn(sample, 1:n) # CCC of the sample
    i <- i+1
  }
  CCC_original <- CCC.fn(data_set, 1:n) # original CCC
  CCC_my <- mean(para) # mean of the CCC from samples
  bias <- CCC_my - CCC_original

  #computation of the CI from standard error
  std_error<-sd(para)/sqrt(n) # standard error
  lower_bound_SE <- mean(para)-std_error
  upper_bound_SE <- mean(para)+std_error

  #computation of the 95% CI of the mean
  perc <- quantile(para, probs = c(0.475, 0.525))
```

```
  lower_bound_Perc <- perc[1]
  upper_bound_Perc <- perc[2]
  return(list(data.frame(CCC_original, CCC_my, bias, std_error),
              "Standerd Error CI" = data.frame(lower_bound_SE, upper_bound_SE),
              "Percentile method CI" = data.frame(lower_bound_Perc),
              "Percentile method CI" = data.frame(upper_bound_Perc)))
}

set.seed(1)
my_boot.fn(data_set, n, 1000)
#   CCC_original    CCC_my          bias    std_error
# 1    0.9892748 0.9889337 -0.0003411283 0.0002304046
#
# $`Standerd Error CI`
#   lower_bound_SE upper_bound_SE
# 1      0.9887033      0.9891641
#
# $`Percentile method CI`
#       lower_bound_Perc
# 47.5%        0.9889895
#
# $`Percentile method CI`
#       upper_bound_Perc
# 52.5%        0.9892421



# problem 1 f)

set.seed(1)
CCC.boot <- boot(data_set, CCC.fn, R = 1000) # bootstrap estimates of bias and standard
error for CCC
# ORDINARY NONPARAMETRIC BOOTSTRAP
#
#
# Call:
#   boot(data = data_set, statistic = CCC.fn, R = 1000)
#
#
# Bootstrap Statistics :
#      original        bias    std. error
# t1* 0.9892748 -0.0003717729 0.002032808


boot.ci(CCC.boot, conf = 0.95, type = "perc") # 95% lower confidence bound for CCC
# BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
# Based on 1000 bootstrap replicates
#
# CALL :
# boot.ci(boot.out = CCC.boot, type = "perc")
#
# Intervals :
# Level     Percentile
# 95%   ( 0.9841,  0.9923 )
# Calculations and Intervals on Original Scale
```

```
# problem 2

library(caret) # for cross-validation
library(leaps) # for best-subset selection
# library(bestglm) # for
# library(MASS)
library(glmnet) # for Ridge and lasso Regression

wine <- read.csv("winequality-white.csv", header = T, sep=';')
wine$quality <- ifelse(wine$quality >= 7, 1, 0)
wine$quality <- as.factor(wine$quality)
attach(wine)

str(wine)

# problem 2 a)

# Using caret package to fit glm and calculate test error rate with 10-fold cross-
validation
set.seed(1234)
fit.full.GLM.CARET <- train(quality ~ . ,
                            data = wine,
                            method ="glm",
                            trControl = trainControl(method = "cv", number = 10))

summary(fit.full.GLM.CARET)
# Call:
#   NULL
#
# Deviance Residuals:
#   Min       1Q   Median       3Q      Max
# -2.1436  -0.6725  -0.4114  -0.1798   2.8331
#
# Coefficients:
#                           Estimate Std. Error z value Pr(>|z|)
#   (Intercept)           6.362e+02  9.412e+01   6.759 1.39e-11 ***
#   fixed.acidity         5.521e-01  9.053e-02   6.099 1.07e-09 ***
#   volatile.acidity     -3.785e+00  4.885e-01  -7.749 9.28e-15 ***
#   citric.acid          -7.378e-01  4.010e-01  -1.840 0.065776 .
#   residual.sugar        2.952e-01  3.564e-02   8.283  < 2e-16 ***
#   chlorides            -1.264e+01  3.816e+00  -3.312 0.000926 ***
#   free.sulfur.dioxide   8.645e-03  3.130e-03   2.762 0.005749 **
#   total.sulfur.dioxide -2.696e-04  1.506e-03  -0.179 0.857936
#   density              -6.591e+02  9.540e+01  -6.909 4.89e-12 ***
#   pH                    3.343e+00  4.268e-01   7.832 4.81e-15 ***
#   sulphates             2.168e+00  3.475e-01   6.238 4.42e-10 ***
#   alcohol               1.423e-01  1.139e-01   1.250 0.211334
# ---
#   Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
#
# (Dispersion parameter for binomial family taken to be 1)
#
# Null deviance: 5116.8  on 4897  degrees of freedom
# Residual deviance: 4143.2  on 4886  degrees of freedom
# AIC: 4167.2
#
# Number of Fisher Scoring iterations: 6
```

```
summary(fit.full.GLM.CARET)$coefficients[,1]
#    (Intercept)        fixed.acidity     volatile.acidity          citric.acid
#   6.361576e+02         5.521067e-01        -3.784880e+00        -7.377814e-01
# residual.sugar            chlorides  free.sulfur.dioxide total.sulfur.dioxide
#   2.951950e-01        -1.263994e+01         8.644758e-03        -2.696022e-04
#        density                   pH            sulphates              alcohol
#  -6.590763e+02         3.342979e+00         2.167765e+00         1.423452e-01


Test.full <- 1 - fit.full.GLM.CARET$results$Accuracy # Test error rate
# [1] 0.2000789

pred <- predict(fit.full.GLM.CARET, wine, type = 'raw')
mean(quality != pred) # training error rate
# [1] 0.1976317



# problem 2 b)


X <- wine[,1:11]
y <- wine[,12]
Xy <- cbind(as.data.frame(X), y)

res.best.logistic <- bestglm(Xy, family = binomial, # binomial family for logistic
                             IC = "AIC",            # Information criteria
                             method = "exhaustive")


## Show top 5 models
res.best.logistic$BestModels
#   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides free.sulfur.dioxide
# 1          TRUE             TRUE        TRUE           TRUE      TRUE                TRUE
# 2          TRUE             TRUE        TRUE           TRUE      TRUE                TRUE
# 3          TRUE             TRUE       FALSE           TRUE      TRUE                TRUE
# 4          TRUE             TRUE        TRUE           TRUE      TRUE                TRUE
# 5          TRUE             TRUE       FALSE           TRUE      TRUE                TRUE
#   total.sulfur.dioxide density   pH sulphates alcohol Criterion
# 1                FALSE    TRUE TRUE      TRUE   FALSE  4162.778
# 2                FALSE    TRUE TRUE      TRUE    TRUE  4163.255
# 3                FALSE    TRUE TRUE      TRUE   FALSE  4163.877
# 4                 TRUE    TRUE TRUE      TRUE   FALSE  4164.774
# 5                FALSE    TRUE TRUE      TRUE    TRUE  4164.778


## Show result for the best model: Same model was chosen
summary(res.best.logistic$BestModel)
# Call:
#   glm(formula = y ~ ., family = family, data = Xi, weights = weights)
#
# Deviance Residuals:
#     Min       1Q   Median       3Q      Max
# -2.3552  -0.6766  -0.4103  -0.1794   2.8148
#
# Coefficients:
#   Estimate Std. Error z value Pr(>|z|)
#   (Intercept)          7.443e+02  3.464e+01  21.490  < 2e-16 ***
#   fixed.acidity        6.302e-01  6.587e-02   9.567  < 2e-16 ***
```

```
#   volatile.acidity    -3.687e+00  4.671e-01  -7.893 2.95e-15 ***
#   citric.acid         -6.927e-01  3.972e-01  -1.744 0.081151 .
#   residual.sugar       3.324e-01  1.932e-02  17.205  < 2e-16 ***
#   chlorides           -1.238e+01  3.800e+00  -3.259 0.001119 **
#   free.sulfur.dioxide  8.177e-03  2.470e-03   3.310 0.000932 ***
#   density             -7.684e+02  3.574e+01 -21.501  < 2e-16 ***
#   pH                   3.682e+00  3.313e-01  11.115  < 2e-16 ***
#   sulphates            2.307e+00  3.296e-01   6.999 2.58e-12 ***
#   ---
#   Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#
# (Dispersion parameter for binomial family taken to be 1)
#
#     Null deviance: 5116.8  on 4897  degrees of freedom
# Residual deviance: 4144.8  on 4888  degrees of freedom
# AIC: 4164.8
#
# Number of Fisher Scoring iterations: 6

res.best.logistic$BestModel$coefficients
#    (Intercept)       fixed.acidity    volatile.acidity         citric.acid
#   7.443217e+02        6.301870e-01       -3.686958e+00       -6.927095e-01
# residual.sugar           chlorides free.sulfur.dioxide             density
#   3.324403e-01       -1.238154e+01        8.176799e-03       -7.683960e+02
#             pH           sulphates
#   3.682339e+00        2.306562e+00

res.best.logistic$BestModel$aic
# [1] 4164.778

set.seed(1234)
fit.bestset.GLM.CARET <- train(quality ~ . - total.sulfur.dioxide - alcohol,
                           data = wine,
                           method ="glm",
                           trControl = trainControl(method = "cv", number = 10))

summary(fit.bestset.GLM.CARET)

Test.best <- 1 - fit.bestset.GLM.CARET$results$Accuracy # Test error rate
# [1] 0.1990572


pred <- round(predict(res.best.logistic$BestModel, newdata=X, type='response'))
mean(quality != pred) # Traning error rate
# [1] 0.1984483



# problem 2 c)

full <- glm(quality ~ ., family = binomial, data = wine)
backwards <- step(full)
# Step: AIC=4164.78

# b<-stepAIC(full)
# formula(b)
# # Step: AIC=4164.78
```

```
backwards$coefficients
#    (Intercept)       fixed.acidity    volatile.acidity         citric.acid
#   7.443217e+02        6.301870e-01       -3.686958e+00       -6.927095e-01
# residual.sugar           chlorides free.sulfur.dioxide             density
#   3.324403e-01       -1.238154e+01        8.176799e-03       -7.683960e+02
#             pH           sulphates
#   3.682339e+00        2.306562e+00


set.seed(1234)
# 10 fold crossvalidation
fit.backward.GLM.CARET <- train(formula(backwards),
                                data = wine,
                                method ="glm",
                                trControl = trainControl(method = "cv", number = 10))

Test.backward <- 1 - fit.backward.GLM.CARET$results$Accuracy # Test error rate
# [1] 0.1990572

pred <- predict(fit.backward.GLM.CARET, wine, type='raw')
mean(quality != pred) # training error rate
# [1] 0.1984483


# problem 2 d)

null.model <- glm(quality ~ 1, family = binomial, data = wine)

forwards <- step(null.model,scope=list(lower=formula(null.model),upper=formula(full)),
                 direction="forward")
# Step:  AIC=4165.26


f <- stepAIC(null.model,scope=list(lower=formula(null.model),upper=formula(full)),
             direction="forward")
formula(f)
# Step:  AIC=4165.26

forwards$coefficients
#    (Intercept)             alcohol    volatile.acidity           chlorides
#    641.2029336           0.1384844         -3.8031154         -12.6752942
# residual.sugar                  pH             density           sulphates
#      0.2967673           3.3514899        -664.1842221           2.1707966
#  fixed.acidity free.sulfur.dioxide         citric.acid
#     0.5546123           0.0083011          -0.7431531


set.seed(1234)
# 10 fold crossvalidation
fit.forward.GLM.CARET <- train(formula(forwards),
                               data = wine,
                               method ="glm",
                               trControl = trainControl(method = "cv", number = 10))

Test.forward <- 1 - fit.forward.GLM.CARET$results$Accuracy # Test error rate
# [1] 0.1994666

pred <- predict(fit.forward.GLM.CARET, wine, type='raw')
```

```
mean(quality != pred) # Training error rate
# [1] 0.1982442



# problem 2 e)

# Create response vector and the design matrix (without the first column of 1s)
y <- as.numeric(levels(quality))[quality]
x <- model.matrix(quality ~ ., wine)[, -1]

grid <- 10^seq(3, -6, length = 200)

# Fit ridge regression for each lambda on the grid -->

out <- glmnet(x, y, alpha = 0, lambda = grid, family = "binomial")
plot(out, xvar = "lambda")

# 10 fold cross-validation
set.seed(1)
cv.out <- cv.glmnet(x, y, alpha = 0, lambda = grid, family = "binomial")
plot(cv.out)

# Find the best value of lambda
bestlam <- cv.out$lambda.min
# [1] 2.049075e-05
# log(bestlam) = -10.79554


coef.ridge <- predict(out, type = "coefficients", s = bestlam)[1:12, ]
#   (Intercept)        fixed.acidity     volatile.acidity         citric.acid       residual.sugar
#  6.195350e+02         5.391177e-01        -3.781939e+00        -7.391644e-01         2.889508e-01
#     chlorides  free.sulfur.dioxide total.sulfur.dioxide              density                   pH
# -1.276662e+01         8.748570e-03        -3.514132e-04        -6.422076e+02         3.286873e+00
#     sulphates              alcohol
#  2.144495e+00         1.602747e-01



ridge.pred <- round(predict(out, s = bestlam, newx = x, type='response'))
Test.ridge <- mean((ridge.pred - y)^2)
# [1] 0.1976317

# problem 2 f)


grid <- 10^seq(0, -5, length = 100)

# Fit lasso regression for each lambda on the grid -->

out <- glmnet(x, y, alpha = 1, lambda = grid, family = "binomial")
plot(out, xvar = "lambda")

# 10 fold cross-validation
set.seed(1)
cv.out <- cv.glmnet(x, y, alpha = 1, lambda = grid, family = "binomial")
plot(cv.out)

# Find the best value of lambda
```

```
bestlam <- cv.out$lambda.min
# [1] 0.0001149757
# log(bestlam) = -9.07079

coef.lasso <- predict(out, type = "coefficients", s = bestlam)[1:12, ]
#   (Intercept)        fixed.acidity     volatile.acidity          citric.acid       residual.sugar
#  6.066693e+02         5.262977e-01        -3.767113e+00        -7.252818e-01         2.837514e-01
#     chlorides  free.sulfur.dioxide total.sulfur.dioxide              density                    pH
# -1.273346e+01         8.690595e-03        -3.507052e-04        -6.290951e+02         3.231570e+00
#     sulphates              alcohol
#  2.118287e+00         1.732598e-01


lasso.pred <- round(predict(out, s = bestlam, newx = x, type='response'))
Test.lasso <- mean((lasso.pred - y)^2)
# [1] 0.1978359

# problem 2 g)

table <-
data.frame(t(rbind.fill(data.frame(t(summary(fit.full.GLM.CARET)$coefficients[,1]),
                                           "AIC"=summary(fit.full.GLM.CARET)$aic, "Test
Error"=Test.full),
                                data.frame(t(res.best.logistic$BestModel$coefficients),
                                           "AIC"=res.best.logistic$BestModel$aic, "Test
Error"=Test.best),
                                data.frame(t(backwards$coefficients),
                                           "AIC"=backwards$aic, "Test
Error"=Test.backward),
                                data.frame(t(forwards$coefficients),
                                           "AIC"=forwards$aic, "Test
Error"=Test.forward),
                                data.frame(t(coef.ridge), "Test Error"=Test.ridge),
                                data.frame(t(coef.lasso), "Test Error"=Test.lasso))))
colnames(table) <- c("Full", "Best Subset", "Backward", "Forward", "Ridge", "Lasso")
table
```