Homework 3

Yuki Joyama

2024-04-03

```
# data prep
df = read_csv("auto.csv")
```

First, I will split the dataset into two parts: training data (70%) and test data (30%)

```
set.seed(1995)
data_split = initial_split(df, prop = .70)

# training data
df_train = training(data_split)

# test data
df_test = testing(data_split)

# set up 10-fold CV
ctrl <- trainControl(
  method = "cv",
  number = 10,
  summaryFunction = twoClassSummary,
  classProbs = TRUE
)
```

(a)

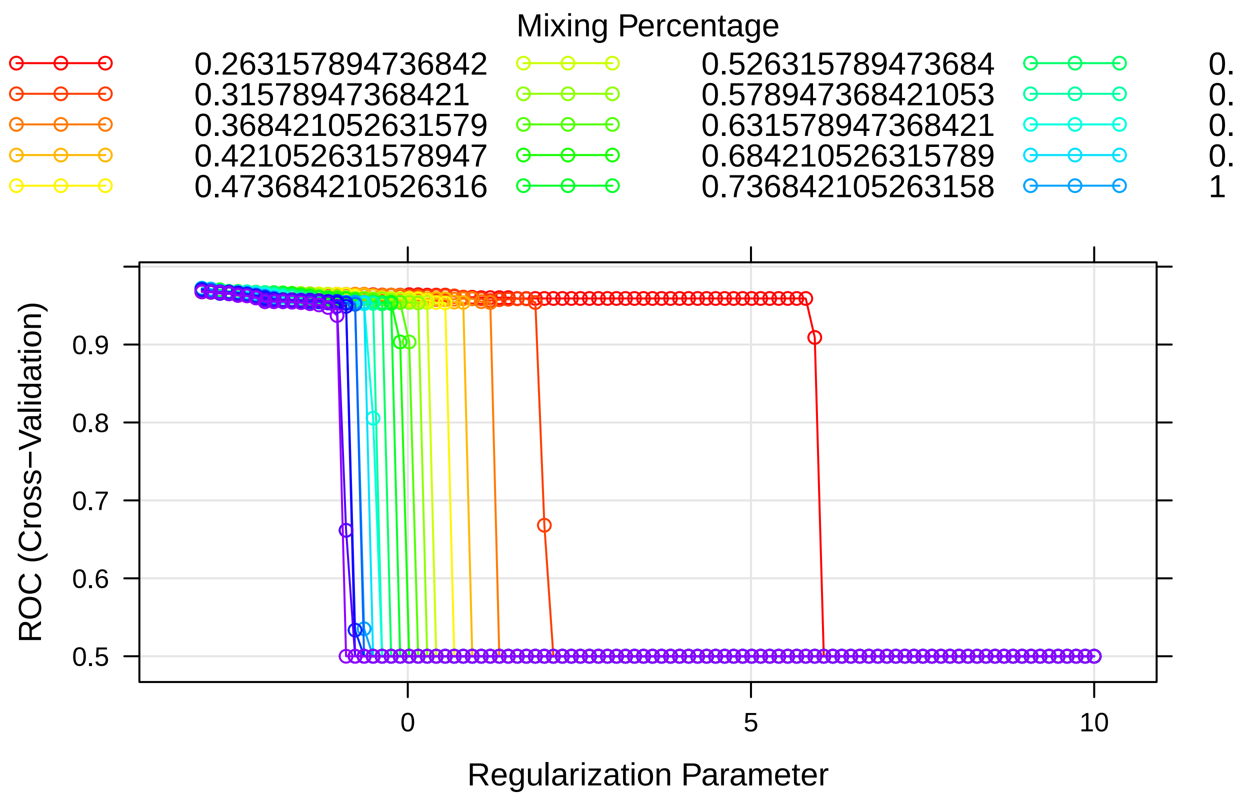
In this section, I will fit an elastic net model as a penalized logistic regression.

```
set.seed(1995)

# find tuning parameter by CV
enet.fit <-
  train(
    x = df_train[1:7],
    y = df_train$mpg_cat,
    data = df_train,
    method = "glmnet",
    metric = "ROC",
    tuneGrid = expand.grid(
      alpha = seq(0, 1, length = 20),
      lambda = exp(seq(-3, 10, length = 100))
    ),
```

```r
    trControl = ctrl
  )

# check the best tuning parameter
enet.fit$bestTune
```

```
##          alpha     lambda
## 1201 0.6315789 0.04978707
```

```r
# plot RMSE, lambda and alpha
myCol <- rainbow(25)
myPar <- list(
  superpose.symbol = list(col = myCol),
  superpose.line = list(col = myCol)
)

plot(enet.fit, par.settings = myPar, xTrans = log)
```




```r
# coefficients in the final model
coef(enet.fit$finalModel, s = enet.fit$bestTune$lambda)
```

```
## 8 x 1 sparse Matrix of class "dgCMatrix"
##                         s1
## (Intercept)   3.686115761
```

```
## cylinders     0.310176287
## displacement  0.005605687
## horsepower    0.008097918
## weight        0.001260020
## acceleration  .
## year         -0.140885415
## origin       -0.002635188
```

10-fold cross validation is implemented to select the optimal tuning parameters ($\alpha = 0.63$, $\lambda = 0.05$). The model includes five predictors. `acceleration` was found to be redundant in this model.

(b)

Setting a probability threshold to 0.5 and determine the class labels. If $Pr(Y = \text{low}|X) < 0.5$, we will classify this as `low`, otherwise `high`.

```r
test.pred.prob <- predict(enet.fit, newdata = df_test, type = "prob")
test.pred <- rep("high", nrow(df_test))
test.pred[test.pred.prob[1] < 0.5] <- "low"
```

The confusion matrix using the test data is as follows.

```r
confusionMatrix(
  data = as.factor(test.pred),
  reference = as.factor(df_test$mpg_cat)
)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction high low
##       high   50   9
##       low     2  57
##
##                Accuracy : 0.9068
##                  95% CI : (0.8393, 0.9525)
##     No Information Rate : 0.5593
##     P-Value [Acc > NIR] : < 2e-16
##
##                   Kappa : 0.8136
##
##  Mcnemar's Test P-Value : 0.07044
##
##             Sensitivity : 0.9615
##             Specificity : 0.8636
##          Pos Pred Value : 0.8475
##          Neg Pred Value : 0.9661
##              Prevalence : 0.4407
##          Detection Rate : 0.4237
##    Detection Prevalence : 0.5000
##       Balanced Accuracy : 0.9126
```

```
##
##        'Positive' Class : high
##
```

Given the confusion matrix with `high` being the `Positive Class`, we can see that:
True Positive (TP) = 50
True Negative (TN) = 57
False Positive (FP) = 9
False Negative (FN) = 2

The metric Accuracy ($\frac{TP+TN}{TP+FP+TN+FN}$) signifies that 90.68% of the samples were correctly classified out of all the samples. Sensitivity ($\frac{TP}{TP+FN}$) indicates that out of all actual Positive Class instances, 96.15% were correctly predicted as `high`. On the other hand, Specificity ($\frac{TN}{FP+TN}$), which is 86.36%, represents the proportion of actual Negative Class instances correctly predicted as `low`.

(c)

Here, I will train a MARS model using the training data.

```r
set.seed(1995)

# fit mars model
mars.fit <- train(
  x = df_train[1:7],
  y = df_train$mpg_cat,
  method = "earth",
  tuneGrid = expand.grid(degree = 1:5, nprune = 2:20),
  metric = "ROC",
  trControl = ctrl
)

summary(mars.fit$finalModel)
```

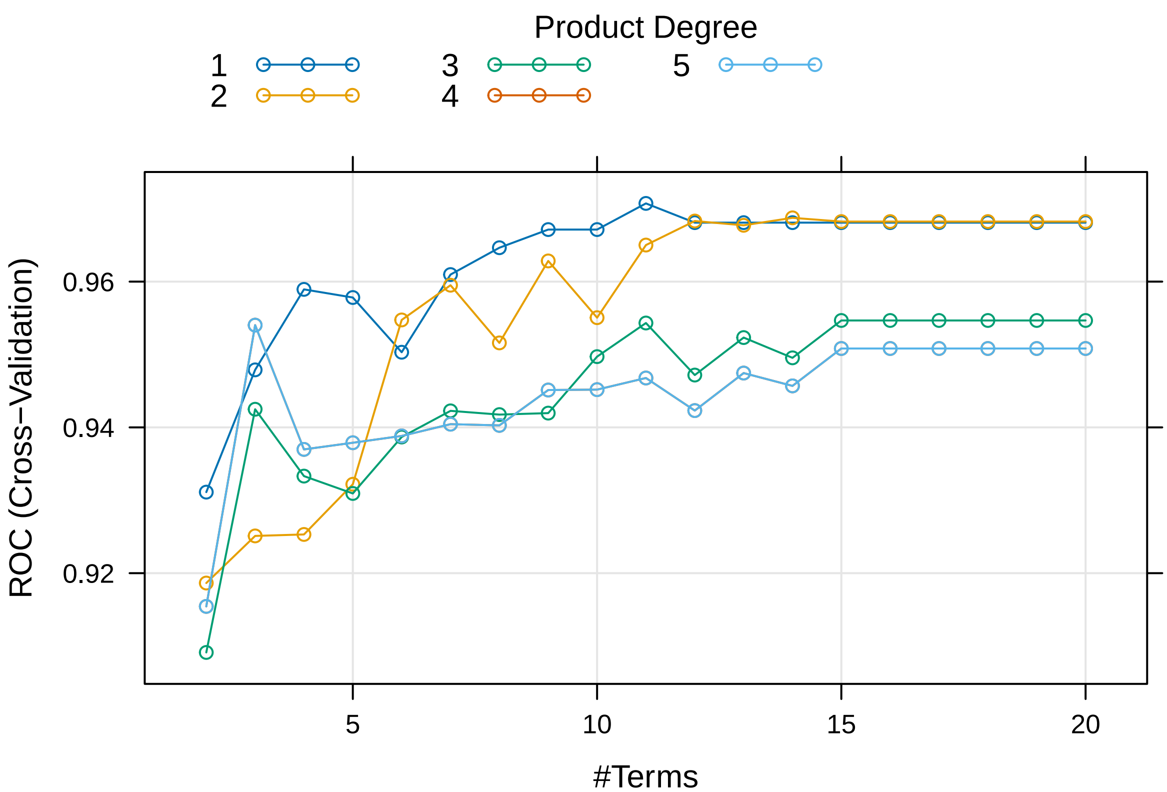
```
## Call: earth(x=tbl_df[274,7], y=factor.object, keepxy=TRUE,
##             glm=list(family=function.object, maxit=100), degree=1, nprune=11)
##
## GLM coefficients
##                              low
## (Intercept)            1.2345750
## h(4-cylinders)         3.2372865
## h(displacement-151)    0.0666967
## h(displacement-232)   -0.2391780
## h(displacement-262)    0.1598567
## h(horsepower-72)      -0.3494185
## h(horsepower-75)       0.4166781
## h(horsepower-133)      6.7119843
## h(3459-weight)        -0.0042551
## h(78-year)             0.3123450
## h(year-78)            -1.1279091
##
## GLM (family binomial, link logit):
##  nulldev  df       dev  df   devratio     AIC iters converged
```

```
##  379.129 273   76.2609 263      0.799   98.26    23         1
##
## Earth selected 11 of 16 terms, and 5 of 7 predictors (nprune=11)
## Termination condition: Reached nk 21
## Importance: displacement, year, weight, horsepower, cylinders, ...
## Number of terms at each degree of interaction: 1 10 (additive model)
## Earth GCV 0.0644561    RSS 15.05756    GRSq 0.7433841    RSq 0.7796063
```

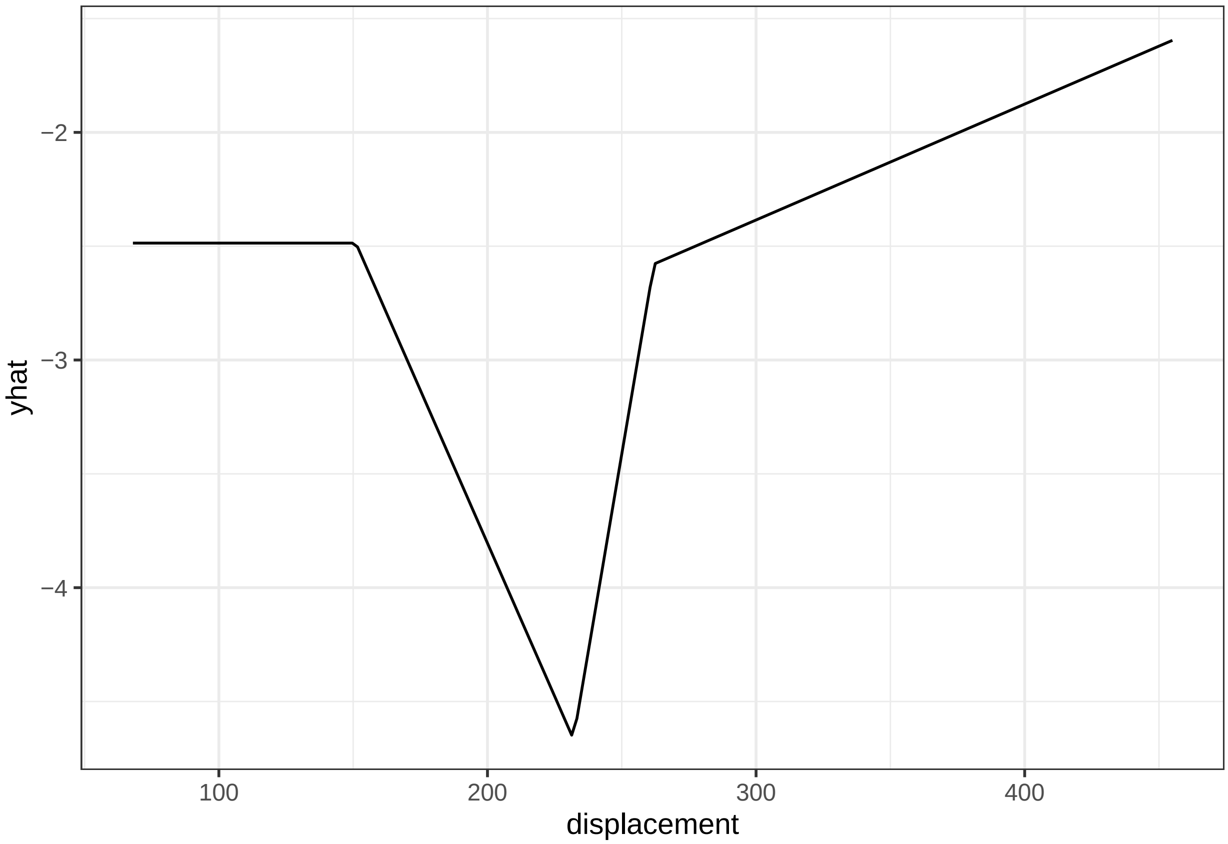
```r
# best tuning parameters
mars.fit$bestTune
```

```
##    nprune degree
## 10     11      1
```

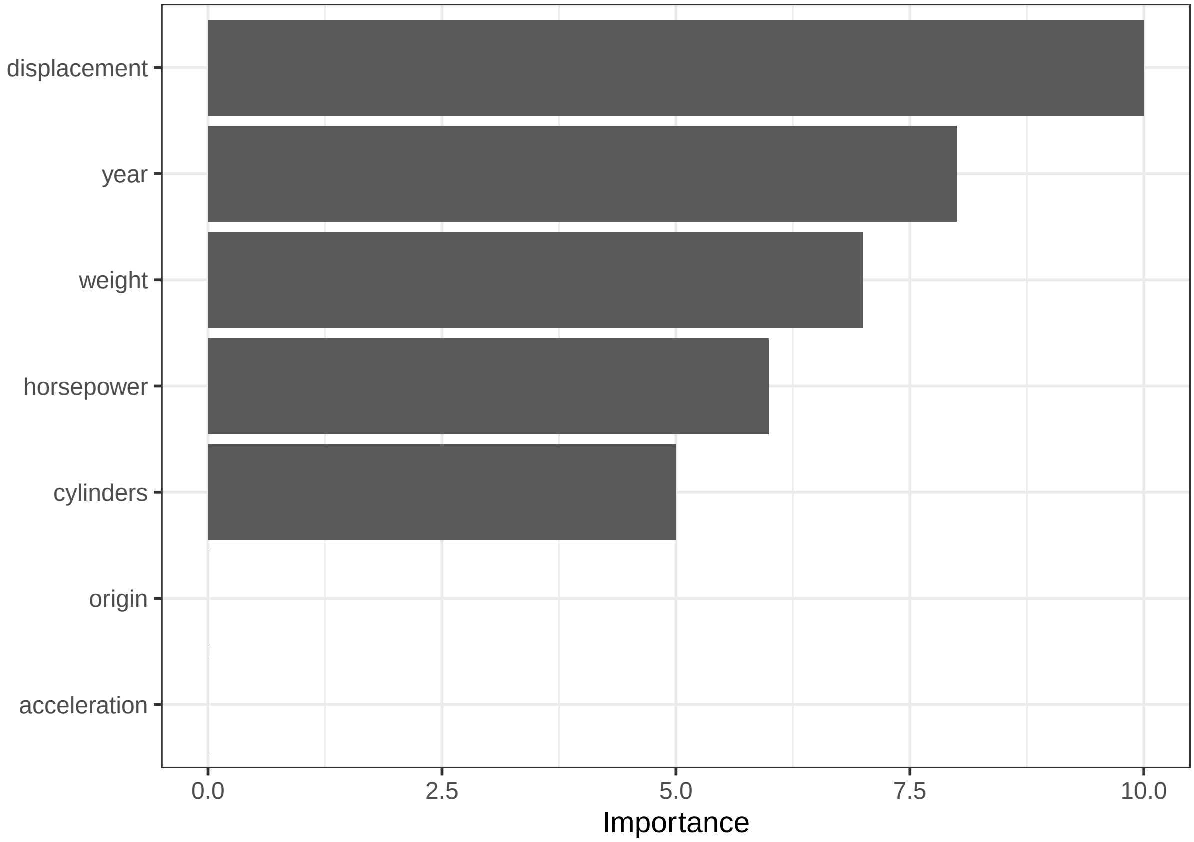
```r
# plot
plot(mars.fit)
```




```r
# pdp
pdp::partial(mars.fit, pred.var = "displacement", grid.resolution = 200) |> autoplot()
```




```r
# relative variable importance
vip(mars.fit$finalModel, type = "nsubsets")
```



The best tuning parameters selected from the cross validation is nprune (the upper bound of the number of terms) = 11 and degree = 1.

The final model can be expressed as the following:
$\hat{y}$ = 1.235 - 0.239 $\times$ h(displacement-232) - 1.128 $\times$ h(year-78) + 0.312 $\times$ h(78-year) - 0.004 $\times$ h(3459-weight) + 0.067 $\times$ h(displacement-151) + 0.417 $\times$ h(horsepower-75) + 6.712 $\times$ h(horsepower-133) + 0.16 $\times$ h(displacement-262) - 0.349 $\times$ h(horsepower-72) + 3.237 $\times$ h(4-cylinders)
where $h(.)$ is hinge function.

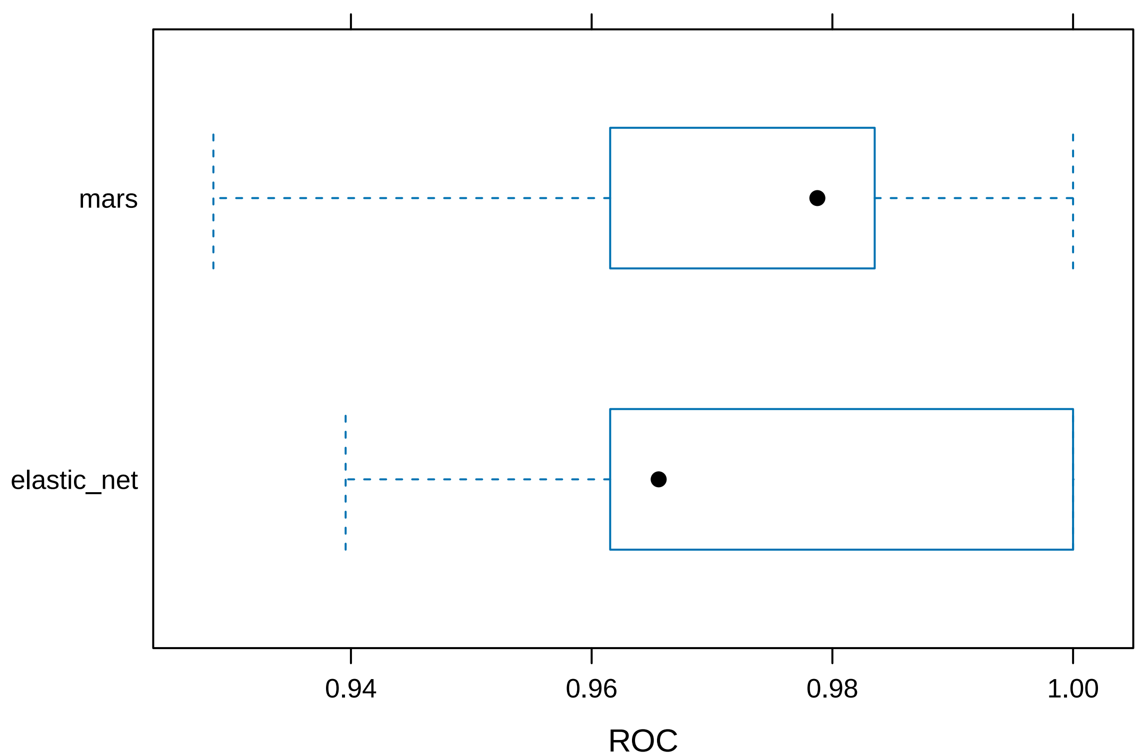
Now, let's compare the two models.

```
res <- resamples(
  list(
    elastic_net = enet.fit,
    mars = mars.fit
  )
)

summary(res)
```

```
##
## Call:
## summary.resamples(object = res)
##
## Models: elastic_net, mars
## Number of resamples: 10
##
```

```
## ROC
##                  Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## elastic_net 0.9395604 0.9621795 0.9655678 0.9724542 0.9923077    1    0
## mars        0.9285714 0.9634615 0.9787546 0.9707326 0.9825092    1    0
##
## Sens
##                  Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## elastic_net 0.8666667 0.9500000 1.0000000 0.9728571 1.0000000    1    0
## mars        0.7333333 0.8666667 0.9285714 0.9119048 0.9821429    1    0
##
## Spec
##                  Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## elastic_net 0.6923077 0.8461538 0.8846154 0.8538462 0.9230769 0.9230769    0
## mars        0.7692308 0.8461538 0.9230769 0.8923077 0.9230769 1.0000000    0
```

```
bwplot(res, metric = "ROC")
```



Based on the results, the MARS model exhibits a larger median ROC, suggesting improved prediction performance compared to logistic regression.

(d)

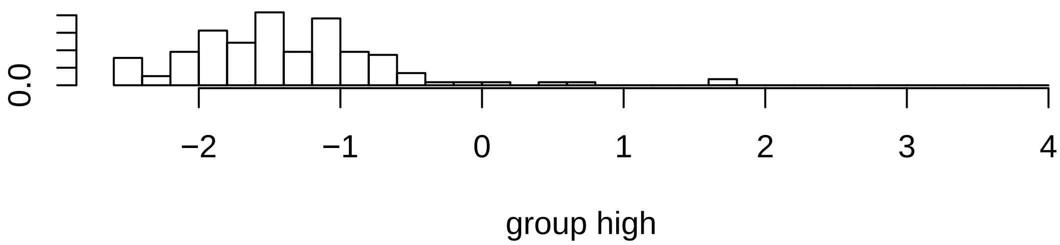
In this section, I will perform linear discriminant analysis using the training data.

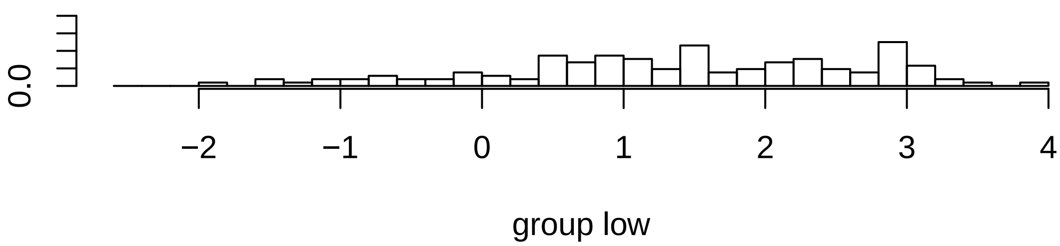
```r
lda.fit1 <- lda(mpg_cat ~., data = df_train)
lda.fit1
```

```
## Call:
## lda(mpg_cat ~ ., data = df_train)
##
## Prior probabilities of groups:
##      high       low
## 0.5255474 0.4744526
##
## Group means:
##      cylinders displacement horsepower   weight acceleration     year   origin
## high  4.166667     115.6979   78.84722 2337.493     16.52708 77.59028 1.909722
## low   6.700000     267.0615  128.19231 3606.038     15.03154 74.69231 1.153846
##
## Coefficients of linear discriminants:
##                        LD1
## cylinders     0.4427082930
## displacement  0.0004154543
## horsepower   -0.0092609288
## weight        0.0012859297
## acceleration  0.0160904075
## year         -0.1260946087
## origin       -0.1076052271
```

The group means represent the average values of each predictor within each `mpg_cat` group. For example, we can see that in `high` group, the mean number of cylinders is 4.17 whereas in `low` group, it's 6.70. The linear discriminant variables are plotted below:

```r
plot(lda.fit1, col = as.numeric(df_train$mpg_cat))
```





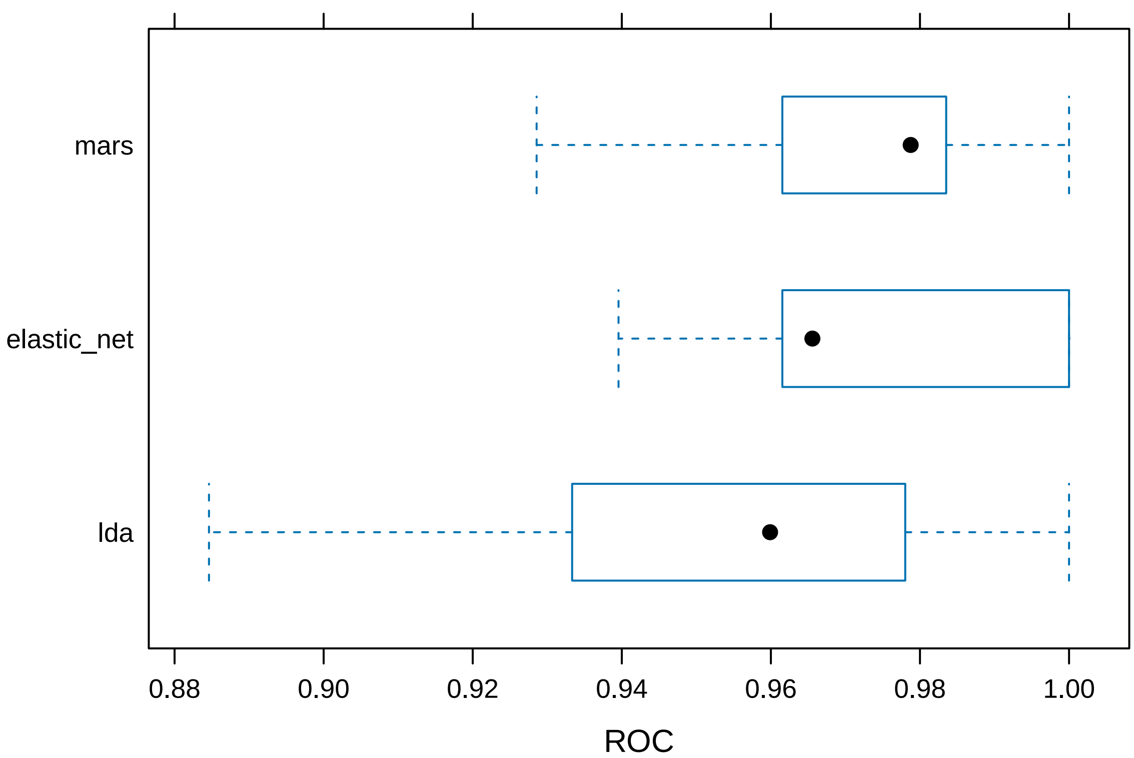
(e)

```
set.seed(1995)

lda.fit <- train(
  x = df_train[1:7],
  y = df_train$mpg_cat,
  method = "lda",
  metric = "ROC",
  trControl = ctrl
)

res <- resamples(
  list(
    elastic_net = enet.fit,
    mars = mars.fit,
    lda = lda.fit
  )
)

summary(res)
```

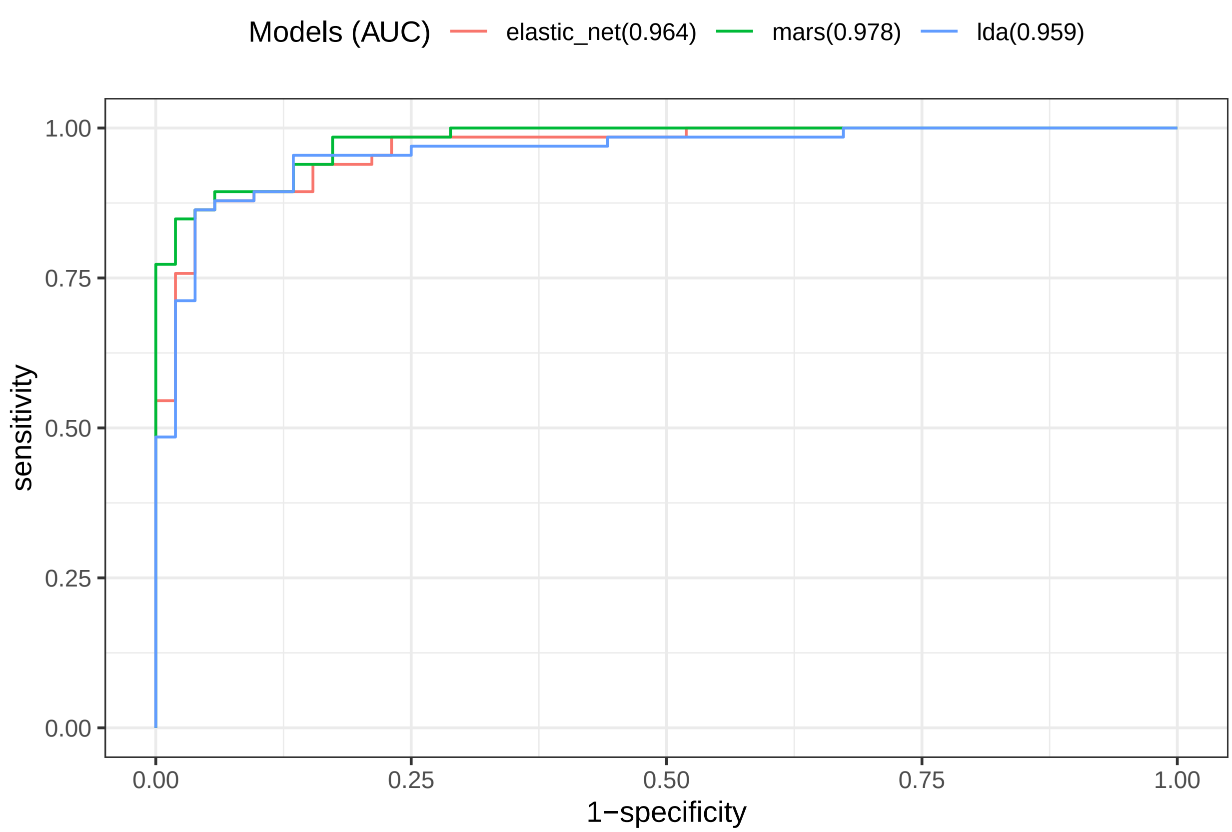
```
##
```

```
## Call:
## summary.resamples(object = res)
##
## Models: elastic_net, mars, lda
## Number of resamples: 10
##
## ROC
##                  Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## elastic_net 0.9395604 0.9621795 0.9655678 0.9724542 0.9923077    1    0
## mars        0.9285714 0.9634615 0.9787546 0.9707326 0.9825092    1    0
## lda         0.8846154 0.9346154 0.9598901 0.9554945 0.9766484    1    0
##
## Sens
##                  Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## elastic_net 0.8666667 0.9500000 1.0000000 0.9728571 1.0000000    1    0
## mars        0.7333333 0.8666667 0.9285714 0.9119048 0.9821429    1    0
## lda         0.8666667 0.9464286 1.0000000 0.9661905 1.0000000    1    0
##
## Spec
##                  Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## elastic_net 0.6923077 0.8461538 0.8846154 0.8538462 0.9230769 0.9230769    0
## mars        0.7692308 0.8461538 0.9230769 0.8923077 0.9230769 1.0000000    0
## lda         0.6153846 0.7884615 0.8461538 0.8307692 0.9038462 0.9230769    0
```

```r
bwplot(res, metric = "ROC")
```



```r
# test data performance
enet.pred <- predict(enet.fit, newdata = df_test, type = "prob")[,2]
mars.pred <- predict(mars.fit, newdata = df_test, type = "prob")[,2]
lda.pred <- predict(lda.fit, newdata = df_test, type = "prob")[,2]

roc.enet <- roc(df_test$mpg_cat, enet.pred)
roc.mars <- roc(df_test$mpg_cat, mars.pred)
roc.lda <- roc(df_test$mpg_cat, lda.pred)

auc <- c(roc.enet$auc[1], roc.mars$auc[1], roc.lda$auc[1])

modelNames <- c("elastic_net", "mars", "lda")

ggroc(list(roc.enet, roc.mars, roc.lda), legacy.axes = TRUE) +
  scale_color_discrete(labels = paste0(modelNames, "(", round(auc, 3), ")"), name = "Models (AUC)")
```



The resampling results shows that the MARS model has the largest median ROC among the three models. Thus, I would prefer to utilize the MARS model for predicting the response variable. Next, I will generate ROC curves for all three models using the test data.
We can see that the MARS model has the largest AUC of 0.978.

```r
test.pred.prob <- predict(mars.fit, newdata = df_test, type = "raw")

confusionMatrix(
  data = test.pred.prob,
```

```
  reference = as.factor(df_test$mpg_cat)
)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction high low
##       high   48   7
##       low     4  59
##
##                Accuracy : 0.9068
##                  95% CI : (0.8393, 0.9525)
##     No Information Rate : 0.5593
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.812
##
##  Mcnemar's Test P-Value : 0.5465
##
##             Sensitivity : 0.9231
##             Specificity : 0.8939
##          Pos Pred Value : 0.8727
##          Neg Pred Value : 0.9365
##              Prevalence : 0.4407
##          Detection Rate : 0.4068
##    Detection Prevalence : 0.4661
##       Balanced Accuracy : 0.9085
##
##        'Positive' Class : high
##
```

The misclassification error rate can be obtained by
1 - accuracy = 1 - 0.9068 = **0.0932**