# Kaggle Playground Season 3 Episode 5 - Wine Quality Data Competition

# Part 1 - Data Exploration, Preparation and Model Spot-Checking

The Kaggle Playground competitions provide monthly opportunities to practice skills on realistic, real world type data sets.

This is my first try. The challenge is to predict wine quality ratings (between 3 and 8), based on wine chemistry data. This version was done in R.

## **Load Packages**

```
In [1]:
```

```
#load packages

package_names <- c("tidyverse", "caret", "Amelia", "UBL", "corrplot")

check_install_load_packages <- function(package_names){
    for (i in package_names) {
        # if(!i %in% installed.packages()){
        # install.packages(i, dependencies = c("Depends", "Suggests")))
        #
        if(!i %in% (.packages())){
            library(i, character.only = TRUE)
            }
    }
}

check_install_load_packages(package_names)
(.packages())</pre>
```

```
— Attaching packages ————
                                                    —— tidyverse
1.3.2 —
√ ggplot2 3.4.0 √ purrr 1.0.1
✓ tibble 3.1.8 ✓ dplyr 1.0.10
√ tidyr 1.2.1
                   ✓ stringr 1.5.0
√ readr 2.1.3 √ forcats 0.5.2
— Conflicts —
                                                — tidyverse_confl
icts() —
x dplyr::filter() masks stats::filter()
x dplyr::lag() masks stats::lag()
Loading required package: lattice
Attaching package: 'caret'
The following object is masked from 'package:purrr':
   lift
The following object is masked from 'package:httr':
   progress
Loading required package: Rcpp
##
## Amelia II: Multiple Imputation
## (Version 1.8.1, built: 2022-11-18)
## Copyright (C) 2005-2023 James Honaker, Gary King and Matthew Bla
ckwell
## Refer to http://gking.harvard.edu/amelia/ for more information
##
Loading required package: MBA
Loading required package: gstat
Loading required package: automap
Loading required package: sp
```

```
Loading required package: randomForest
  randomForest 4.6-14
  Type rfNews() to see new features/changes/bug fixes.
 Attaching package: 'randomForest'
 The following object is masked from 'package:dplyr':
       combine
 The following object is masked from 'package:ggplot2':
       margin
 corrplot 0.92 loaded
\hbox{'corrplot'}\cdot \hbox{ 'UBL'}\cdot \hbox{ 'randomForest'}\cdot \hbox{ 'automap'}\cdot \hbox{ 'sp'}\cdot \hbox{ 'gstat'}\cdot \hbox{ 'MBA'}\cdot \hbox{ 'Amelia'}\cdot
'Rcpp' · 'caret' · 'lattice' · 'forcats' · 'stringr' · 'dplyr' · 'purrr' · 'readr' · 'tidyr' ·
\hbox{'tibble'} \cdot \hbox{'ggplot2'} \cdot \hbox{'tidyverse'} \cdot \hbox{'stats'} \cdot \hbox{'graphics'} \cdot \hbox{'grDevices'} \cdot \hbox{'utils'} \cdot
'datasets' · 'bigrquery' · 'httr' · 'methods' · 'base'
```

## **Import Data**

```
In [2]:
```

```
#import data
train <- read.csv(file = "/kaggle/input/playground-series-season-3-episode-5/tra
in.csv")
test <- read.csv(file = "/kaggle/input/playground-series-season-3-episode-5/tes
t.csv")
head(train, 3)
dim(train)
table(train$quality)
dim(test)
head(test, 3)</pre>
```

## A data.frame: 3 × 13

	Id	fixed.acidity	volatile.acidity	citric.acid	residual.sugar	chlorides	free.sulfur.dioxid
	<int></int>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
1	0	8.0	0.50	0.39	2.2	0.073	30
2	1	9.3	0.30	0.73	2.3	0.092	30
3	2	7.1	0.51	0.03	2.1	0.059	3
4							<b>→</b>

2056 · 13

3 4 5 6 7 8 12 55 839 778 333 39

1372 · 12

## A data.frame: 3 × 12

	1.1	f	1	. 16. 2		a la La ad al a a	C
	ld	fixed.acidity	volatile.acidity	citric.acid	residual.sugar	chlorides	free.sulfur.dioxid
	<int></int>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
1	2056	7.2	0.510	0.01	2	0.077	31
2	2057	7.2	0.755	0.15	2	0.102	14
3	2058	8.4	0.460	0.40	2	0.065	21
4							<b>•</b>

We can see that the data is fairly unbalanced between the different quality categories.

```
In [3]:
```

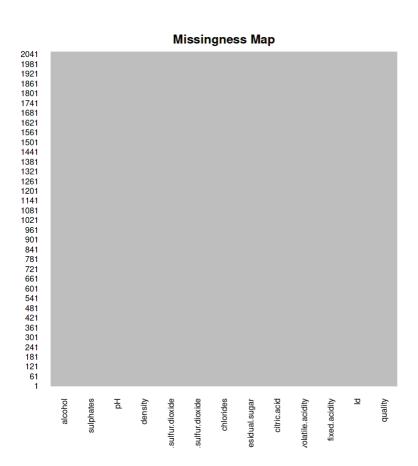
```
#change some variable classes, rearrrange columns and check for missing values
train$quality <- factor(train$quality)
str(train$quality)
train <- train %>%
    relocate(quality)

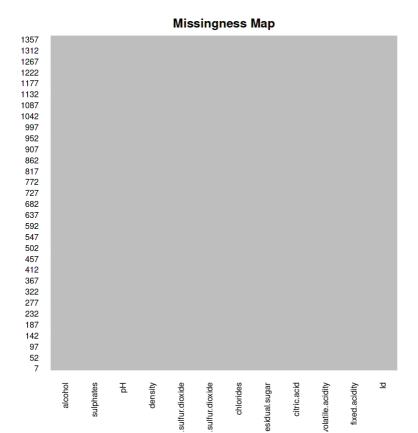
#check for duplicates
clean <- unique(train)
dim(train) - dim(clean)
clean <- unique(test)
dim(test) - dim(clean)

#check for missing values
missmap(train, col=c("black", "grey"), legend=FALSE)
missmap(test, col=c("black", "grey"), legend=FALSE)</pre>
```

0 · 0

0 · 0



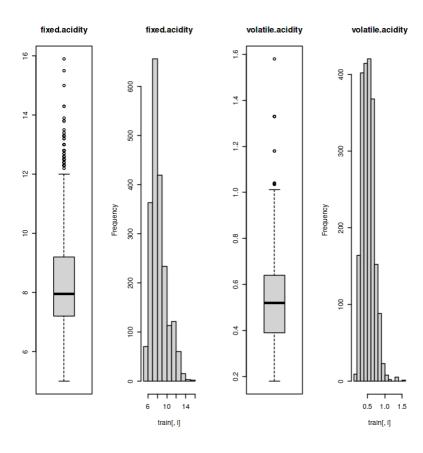


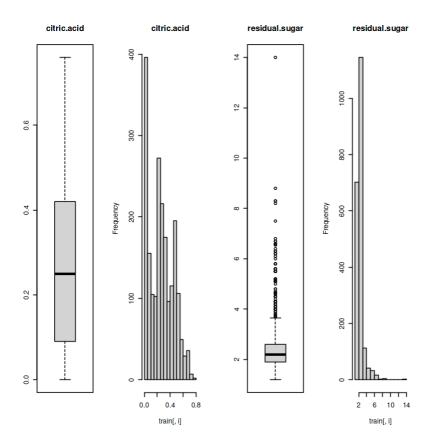
No duplicates. No missing values.

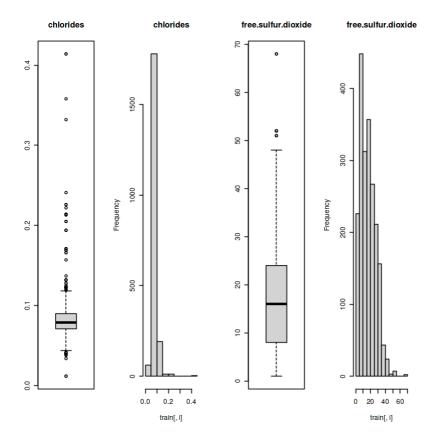
# **Data Visualisation**

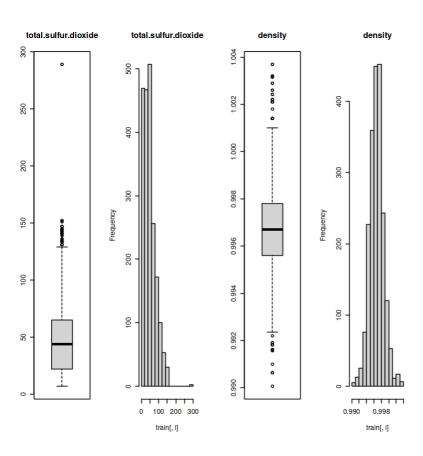
```
In [4]:
```

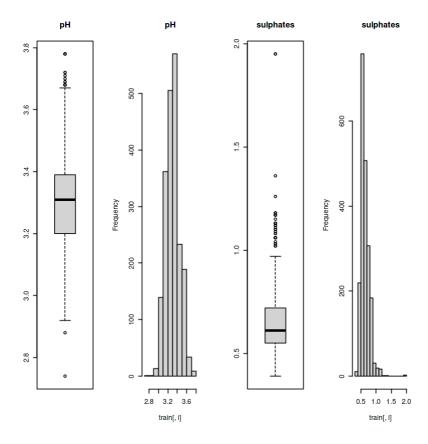
```
#Boxplot and density plot of each attribute
col_first_var <- 3</pre>
col_last_var <- dim(train)[2]</pre>
nrows<- 1
ncols<- 4
num_plotsets <- ceiling((col_last_var - col_first_var)/(nrows*ncols))</pre>
num_plotsets
first <- col_first_var</pre>
last <- first + nrows*ncols - 1</pre>
for (j in 1:num_plotsets) {
        par(mfrow=c(nrows, ncols))
        for(i in first:last) {
                 boxplot(train[,i], main=names(train)[i])
             #densityplot(train[,i], main=names(train)[i])
             hist(train[,i], main=names(train)[i])
        }
        first <- last+1
        last <- first + nrows*ncols - 1</pre>
        if (last > dim(train)[2]) \{ last = dim(train)[2] \}
}
# correlation plot
par(mfrow=c(1,1))
correlations <- cor(train[,col_first_var:col_last_var])</pre>
corrplot(correlations, method="number", tl.cex = 0.5)
```

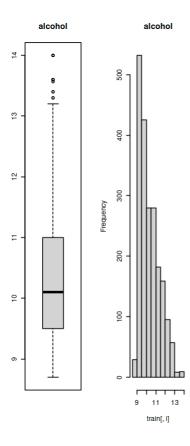


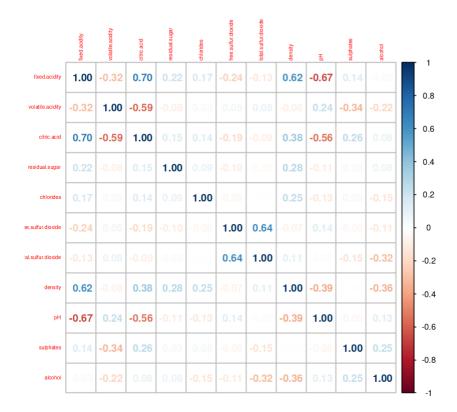












We note quite a lot of outliers on many of the variables.

Let's split off some validation data and build some classification models. We'll compare test and compare the balanced and imbalanced data.

# Split Data into Training and Validation Sets

```
#split data into training and validation sets
set.seed(100)
part <- createDataPartition(train$quality, p = 3/4, list = FALSE)
training <- train[part, ]
validate <- train[-part, ]
table(training$quality)
table(validate$quality)</pre>
```

```
3 4 5 6 7 8
9 42 630 584 250 30
3 4 5 6 7 8
3 13 209 194 83 9
```

# **Identify and Remove Outliers**

```
In [6]:
```

```
out_ind <- 0
missing <- 0
train_no_outliers <- training</pre>
for (i in col_first_var:col_last_var) {
        below <- quantile(train_no_outliers[, i], 0.01) #remove bottom 2%
        above <- quantile(train_no_outliers[, i], 0.99) #remove top 2%
        out_ind <- which(train_no_outliers[, i] < below | train_no_outliers[, i]</pre>
> above)
        train_no_outliers[out_ind, i] = NA
        missing[i-1] = sum(is.na(train_no_outliers[, i])) #count the amount of N
A's for that variable
        #replace values by KNN imputation
        #imp <- preProcess(train_no_outliers, method = "knnImpute", k = 8)</pre>
        #train_no_outliers <- predict(imp, train_no_outliers)</pre>
        #replace values with averages by group (courtesy of)[https://stackoverflo
w.com/questions/55345593/impute-missing-data-with-mean-by-group]
        train_no_outliers[i] <- ave(train_no_outliers[, i],</pre>
                                     #train_no_outliers$user_name, train_no_outlier
s$classe,
                                     FUN = function(x) ifelse(is.na(x), mean(x,n))
a.rm=TRUE), x))
}
print("Amount of values that were identified as outliers, removed, and imputed -
per variable:")
missing
print("Check if any NA's are left after imputation command:")
ouliers_remaining <- sapply(train_no_outliers, function(x) sum(is.na(x)))</pre>
ouliers_remaining[ouliers_remaining>0]
```

```
[1] "Amount of values that were identified as outliers, removed, an d imputed - per variable:"
```

$$0 \cdot 31 \cdot 23 \cdot 8 \cdot 16 \cdot 30 \cdot 16 \cdot 20 \cdot 31 \cdot 29 \cdot 28 \cdot 15$$

[1] "Check if any NA's are left after imputation command:"

# **Model Training - Imbalanced Data**

For ideas of available models in CARET, see: [https://topepo.github.io/caret/available-models.html]

In [7]:

```
x <- training
#train models
tcont <- trainControl(method = "repeatedcv", number=5, repeats=3)</pre>
#CART model
set.seed(100)
grid <- expand.grid(.cp=c(0.01, 0.05, 0.1))
model_cart <- train(quality ~ ., method="rpart", data = subset(x, select = -c( I</pre>
d)), tuneGrid=grid,
                     preProcess = c("center", "scale"), trControl=tcont)
#print(model_cart)
library(randomForest)
#use tuneRF() function from the randomForest package to find the optimal value for
mtry
tune_mtry <- tuneRF(subset(x, select = -c(quality, Id)), x$quality,
                     mtryStart = 2, stepFactor=1.5, ntreeTry = 100, improve = 0.0
1)
#print(tune_mtry)
#set mtry to value corresponding to minimum OOBerror
tunegrid <- expand.grid(.mtry = subset(tune_mtry, tune_mtry[,2] == min(tune_mtry</pre>
[,2], na.rm=TRUE))[1])
#manual iterations were performed to find the lowest value for ntree without havin
g a noticeable effect on the resulting accuracy.
set.seed(100)
rf_{tuned} \leftarrow train(quality \sim ., method = "rf", data = subset(x, select = -c(Id)),
ntree = 20.
                   tuneGrid = tunegrid, preProcess = c("center", "scale"), trCont
rol = tcont )
#print(rf_tuned)
# Linear Discriminant Analysis
set.seed(100)
model_lda \leftarrow train(quality \sim ., method = "lda", data = subset(x, select = -c(I))
d)), metric = "Accuracy",
                    preProcess = c("center", "scale"), trControl = tcont)
```

mtry = 2 00B error = 44.01%
Searching left ...
Searching right ...
mtry = 3 00B error = 42.85%
0.02647059 0.01
mtry = 4 00B error = 43.43%
-0.01359517 0.01

Time difference of 2.827233 secs

#### Call:

summary.resamples(object = results)

Models: CART, RF, LDA, TEST Number of resamples: 15

## Accuracy

Min. 1st Qu. Median Mean 3rd Qu. Max. N
A's

CART 0.5419355 0.5593511 0.5649351 0.5730283 0.5896649 0.605178 0

RF 0.5096774 0.5444201 0.5548387 0.5588146 0.5672729 0.631068 0

LDA 0.4903226 0.5582530 0.5714286 0.5670076 0.5799718 0.605178 0

TEST 0.4903226 0.5582530 0.5714286 0.5670076 0.5799718 0.605178 0

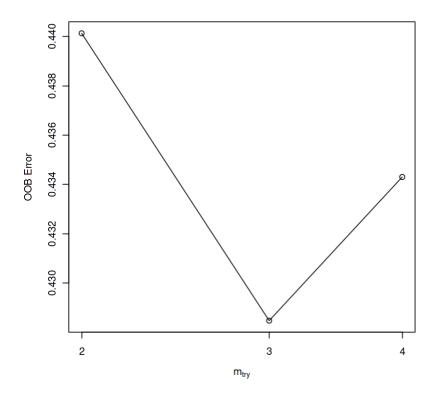
#### Kappa

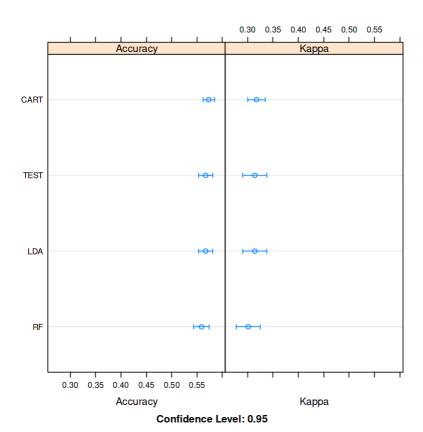
Min. 1st Qu. Median Mean 3rd Qu. Max. N
A's

CART 0.2649367 0.2916379 0.3159072 0.3176116 0.3398006 0.3630911
0

RF 0.2306436 0.2833575 0.2983326 0.3013348 0.3144233 0.4145296
0
LDA 0.1904534 0.2968883 0.3267196 0.3142422 0.3365145 0.3788331
0

TEST 0.1904534 0.2968883 0.3268076 0.3143233 0.3365145 0.3788331





The results look poor, considering that a 50% accuracy would be just as good as a flip of a coin and we are sitting around 57 with all of the models.

Let's see how predicting on our validation set goes.

# Model Validation - Trained on Imbalanced Data

```
In [8]:
```

```
set.seed(100)
print("Results on test set prediction for CART: single decision tree")
predQ1 <- predict(object = model_cart, newdata = subset(validate, select = -c(qu</pre>
ality)))
result1 <- confusionMatrix(validate$quality, predQ1)</pre>
result1$table
set.seed(100)
print("Results on test set prediction for rf_tuned: tuned random forest with out
liers included")
predQ2 <- predict(object = rf_tuned, newdata = subset(validate, select = -c(qual</pre>
result2 <- confusionMatrix(validate$quality, predQ2)</pre>
result2$table
set.seed(100)
print("Results on test set prediction for model_lda: linear discriminant analyis
model")
predQ3 <- predict(object = model_lda, newdata = subset(validate, select = -c(qua</pre>
lity)))
result3 <- confusionMatrix(validate$quality, predQ3)</pre>
result3$table
set.seed(100)
print("Results on test set prediction for model_lda: TEST model")
predQ4 <- predict(object = model_test, newdata = subset(validate, select = -c(qu</pre>
ality)))
result4 <- confusionMatrix(validate$quality, predQ4)</pre>
result4$table
compare_validation_result <- data.frame(Model = c("CART", "RF", "LDA", "TEST"),</pre>
                                          Accuracy = c(result1$overall[1], result2
$overall[1],
                                                        result3$overall[1], result4
$overall[1] ))
print("Out of sample accuracies compared:")
compare_validation_result
```

[1] "Results on test set prediction for CART: single decision tree"

## Reference

Prediction 0 12 0 158 51 0 0 64 118 12 0 14 57 

[1] "Results on test set prediction for rf\_tuned: tuned random fore st with outliers included"

## Reference

Prediction 0 11 1 148 54 0 56 113 25 0 12 44 

[1] "Results on test set prediction for model\_lda: linear discrimin ant analyis model"

#### Reference

Prediction 0 152 49 0 57 120 

[1] "Results on test set prediction for model\_lda: TEST model"

## Reference

Prediction	3	4	5	6	7	8
3	0	0	3	0	0	0
4	0	0	9	4	0	0
5	2	0	152	49	6	0
6	0	0	57	119	18	0
7	0	0	9	48	25	1
8	0	0	1	6	2	0

[1] "Out of sample accuracies compared:"

A data.frame: 4 × 2

Model	Accuracy
<chr></chr>	<dbl></dbl>
CART	0.5636008
RF	0.5616438
LDA	0.5812133
TEST	0.5792564

The results are equally unimpressive. Let's look at the variable importance.

```
In [9]:
```

## [1] "Variable Imporantance for RF"

A data.frame: 11 × 1

	Overall
	<dbl></dbl>
sulphates	100.00000000
alcohol	83.72262306
total.sulfur.dioxide	39.23826040
density	33.15882276
volatile.acidity	17.79559890
fixed.acidity	16.84326368
chlorides	10.70318153
citric.acid	6.65155401
рН	4.98328101
residual.sugar	0.05447381
free.sulfur.dioxide	0.00000000

## [1] "Variable Imporantance for CART model"

A data.frame: 11 × 1

	Overall
	<dbl></dbl>
sulphates	100.000000
alcohol	78.4020582
total.sulfur.dioxide	43.6273108
volatile.acidity	39.0899918
citric.acid	26.0223489
fixed.acidity	11.5924071
residual.sugar	4.9987303
density	1.8073669
free.sulfur.dioxide	1.0284015
рН	0.6706679
chlorides	0.0000000

# **Model Training on Balanced Data**

## Balancing Data for multi-class problem

We'll try to rebalance the data with SMOTE.

(I found help here)[https://stackoverflow.com/questions/48215299/any-package-in-r-which-can-do-multi-class-oversampling-under-sampling-both-and]

Create a second training set with balanced data:

```
#rebalance data - use synthetic balancing from te UBL package

#?AdasynClassif
#?RandOverClassif
set.seed(100)
training.balanced <- AdasynClassif(quality ~ ., dat = training)
#training.balanced <- RandOverClassif(quality ~ ., dat = training) #This one does
even worse
table(training.balanced$quality)</pre>
```

```
3 4 5 6 7 8
629 628 630 584 674 632
```

In [11]:

```
#train models
tcont <- trainControl(method = "repeatedcv", number=5, repeats=3)</pre>
#CART model
set.seed(100)
start.time1 <- Sys.time()</pre>
grid <- expand.grid(.cp=c(0.01,0.05,0.1))
model_cart.balanced <- train(quality ~ ., method="rpart", data = training.balanc</pre>
ed, tuneGrid=grid, trControl=tcont)
end.time1 <- Sys.time()</pre>
time.taken1 <- end.time1 - start.time1</pre>
time.taken1
print(model_cart.balanced)
library(randomForest)
#use tuneRF() function from the randomForest package to find the optimal value for
tune_mtry <- tuneRF(subset(training.balanced, select = -quality), training.balan
ced$quality,
                     mtryStart = 2, stepFactor=1.5, ntreeTry = 100, improve = 0.0
1)
print(tune_mtry)
#set mtry to value corresponding to minimum OOBerror
tunegrid <- expand.grid(.mtry = subset(tune_mtry, tune_mtry[,2] == min(tune_mtry
[,2], na.rm=TRUE))[1])
#manual iterations were performed to find the lowest value for ntree without havin
g a noticeable effect on the resulting accuracy.
set.seed(100)
start.time2 <- Sys.time()</pre>
rf_tuned.balanced <- train(quality ~ ., method = "rf", data = training.balanced,
ntree = 100,
                   tuneGrid = tunegrid, preProcess = c("center", "scale"),trContr
ol = tcont)
end.time2 <- Sys.time()</pre>
time.taken2 <- end.time2 - start.time2</pre>
time.taken2
print(rf_tuned.balanced)
```

```
# Linear Discriminant Analysis
set.seed(100)
start.time3 <- Sys.time()

model_lda.balanced <- train(quality ~ ., method = "lda", data = training.balance
d, metric="Accuracy", trControl=tcont)

end.time3 <- Sys.time()
time.taken3 <- end.time3 - start.time3

time.taken3
print(model_lda.balanced)

#show model comparison based on resampling accuracy results:
results.balanced <- resamples(list(CART = model_cart.balanced, RF=rf_tuned.balanced, LDA = model_lda.balanced))
summary(results.balanced)
dotplot(results.balanced)</pre>
```

```
CART
```

```
3777 samples
  12 predictor
  6 classes: '3', '4', '5', '6', '7', '8'
No pre-processing
Resampling: Cross-Validated (5 fold, repeated 3 times)
Summary of sample sizes: 3021, 3021, 3023, 3022, 3021, 3022, ...
Resampling results across tuning parameters:
       Accuracy Kappa
  ср
  0.01 0.4609456 0.3525591
  0.05 0.3636929 0.2345431
  0.10 0.3108272 0.1729886
Accuracy was used to select the optimal model using the largest val
ue.
The final value used for the model was cp = 0.01.
mtry = 2 00B error = 25.68%
Searching left ...
Searching right ...
mtry = 3
               00B error = 26.34\%
-0.0257732 0.01
     mtry OOBError
2.00B 2 0.2568176
3.00B 3 0.2634366
```

Time difference of 10.7838 secs

```
3777 samples
 12 predictor
   6 classes: '3', '4', '5', '6', '7', '8'
Pre-processing: centered (12), scaled (12)
Resampling: Cross-Validated (5 fold, repeated 3 times)
Summary of sample sizes: 3021, 3021, 3023, 3022, 3021, 3022, ...
Resampling results:
  Accuracy
            Kappa
  0.7332908 0.6799054
Tuning parameter 'mtry' was held constant at a value of 2
Time difference of 0.8569205 secs
Linear Discriminant Analysis
3777 samples
 12 predictor
   6 classes: '3', '4', '5', '6', '7', '8'
No pre-processing
Resampling: Cross-Validated (5 fold, repeated 3 times)
Summary of sample sizes: 3021, 3021, 3023, 3022, 3021, 3022, ...
Resampling results:
  Accuracy
             Kappa
  0.2696162 0.1231001
```

#### Call:

summary.resamples(object = results.balanced)

Models: CART, RF, LDA Number of resamples: 15

## Accuracy

Min. 1st Qu. Median Mean 3rd Qu. Max. N A's CART 0.4291391 0.4510582 0.4668435 0.4609456 0.4765050 0.4854497

RF 0.7086093 0.7225166 0.7320955 0.7332908 0.7456967 0.7582563 0

LDA 0.2370861 0.2624256 0.2701987 0.2696162 0.2794672 0.2993377 0

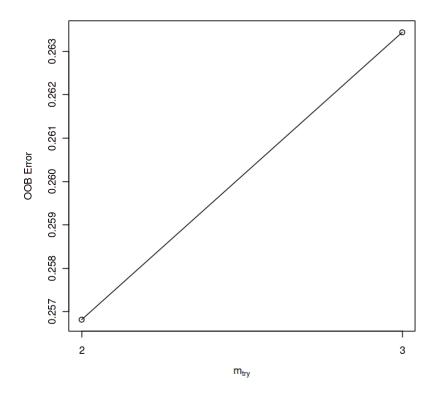
## Kappa

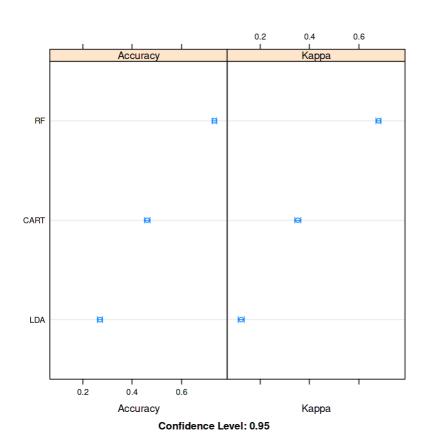
 $\mbox{Min.} \quad \mbox{1st Qu.} \qquad \mbox{Median} \qquad \mbox{Mean} \quad \mbox{3rd Qu.} \qquad \mbox{Max.} \ \mbox{N} \\ \mbox{A's} \qquad \mbox{} \qquad \mbox{}$ 

CART 0.31671902 0.3397053 0.3593802 0.3525591 0.3708770 0.3835531

RF 0.65040558 0.6669986 0.6784349 0.6799054 0.6948283 0.7098487

LDA 0.08288379 0.1140860 0.1235856 0.1231001 0.1353144 0.1586122 0





The results from the cross validation suggest that the random forest model gained a significant jump in accuracy from 56% to just over 69%. The LDA model, by contrast, lost about 20% of accuracy. Let's have a look at predictions on the validation set.

# Model Validation after training on Balanced Data

```
In [12]:
```

```
set.seed(100)
print("Results on test set prediction for CART: single decision tree")
predQ1.balanced <- predict(object = model_cart.balanced, newdata = subset(valida</pre>
te, select = -c(quality))
result1.balanced <- confusionMatrix(validate$quality, predQ1.balanced)</pre>
result1.balanced$table
set.seed(100)
print("Results on test set prediction for rf_tuned: tuned random forest with out
liers included")
predQ2.balanced <- predict(object = rf_tuned.balanced, newdata = subset(validat</pre>
e, select = -c(quality))
result2.balanced <- confusionMatrix(validate$quality, predQ2.balanced)</pre>
result2.balanced$table
set.seed(100)
print("Results on test set prediction for model_lda: linear discriminant analyis
model")
predQ3.balanced <- predict(object = model_lda.balanced, newdata = subset(validat</pre>
e, select = -c(quality))
result3.balanced <- confusionMatrix(validate$quality, predQ3.balanced)</pre>
result3.balanced$table
compare_validation_result.balanced <- data.frame(Model = c("CART", "RF", "LDA"),</pre>
                                         Accuracy = c(result1.balanced$overall
[1], result2.balanced$overall[1],
                                                       result3.balanced$overall
[1]))
print("Out of sample accuracies compared:")
compare_validation_result.balanced
```

[1] "Results on test set prediction for CART: single decision tree"

#### Reference

Prediction 0 6 0 123 49 32 0 0 28 91 0 4 25 53 

[1] "Results on test set prediction for rf\_tuned: tuned random fore st with outliers included"

## Reference

Prediction 2 1 0 10 2 4 0 144 54 1 0 56 107 29 0 0 14 34 

[1] "Results on test set prediction for model\_lda: linear discrimin ant analyis model"

#### Reference

Prediction 3 4 5 6 7 8 3 0 0 3 0 0 0 4 2 3 5 1 2 0 5 35 21 94 47 12 0 6 47 18 62 53 14 0 7 18 3 25 26 11 0 8 3 2 1 0 3 0

[1] "Out of sample accuracies compared:"

#### A data.frame: 3 × 2

Model	Accuracy
<chr></chr>	<dbl></dbl>
CART	0.5244618
RF	0.5577299
LDA	0.3150685

## Conclusion on Balancing Data

In this case, the out of sample accuracy is worse on all counts compared to using the imbalanced data.

## **Conclusion on Removing Outliers**

We tried removing outliers ranging from 10% to 1% on the top and bottom end of the data and imputing by KNN or means and it didn't do much good!

## Conclusion on model selection

The LDA proved to be the best model to use and the data will be output as a prediction on the test set

```
In [13]:
```

```
print("Results on test set prediction for model_lda: linear discriminant analyis
model")
pred_final <- predict(object = model_lda, newdata = test)
df_final <- data.frame(Id = test$Id, quality = pred_final)
head(df_final, 10)
write.csv(df_final, "/kaggle/working/submission.csv", row.names=FALSE)</pre>
```

[1] "Results on test set prediction for model\_lda: linear discrimin ant analyis model"

A data.frame: 10 × 2

	ld	quality
	<int></int>	<fct></fct>
1	2056	5
2	2057	5
3	2058	5
4	2059	6
5	2060	6
6	2061	6
7	2062	6
8	2063	6
9	2064	7
10	2065	5