Choose Your Own Project: Wine Quality

HarvardX PH125.9x Data Science: Capstone

Shunsuke Kobayashi

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Contents

1 Introduction

The goal of this project is to use wine quality data sets for classification.

In the previous MovieLens project, we did machine learning using 10 million data, and we see this as an application problem in BtoC business such like Netflix, Amazon etc. In this CYO project, we set it up as a way to apply it to BtoB business, especially with small data sets in the field of product manufacturing and technology development. The red wine quality data set is a set of about 1,600 tabular tables, consisting of information such as alcohol and acid content, pH, and density, in addition to the target quality (This is similar to the structure of information in the chemical industry to which I belong).

In addition, the goal was to learn and compare not only learned methods but also newly algorithms developed and apply new technologies. In addition to the gradient boosting method, we also worked on the deep learning library **torch**, whose R version will be implemented in September 2020, and the classification in **Tabnet** that utilizes it, and created 10 models. In the new technology, we also worked on using the **GPU** with Google Colaboratory and succeeded in reducing the computation time from 53 minutes when using the CPU to 35 minutes when using the GPU.

2 Data Preprocessing and Explanatory Data Analysis

In the UCI repository, there are two datasets related to the Portuguese wine Vinho Verde, red and white. Due to privacy and logistical issues, only physicochemical (input) and sensory (output) variables are available.

The red wine quality data set is a set of about 1,600 tabular tables, consisting of information such as alcohol and acid content, pH, and density, in addition to the target quality (This is similar to the structure of information in the chemical industry to which I belong).

A similar dataset is the Water portability dataset from Kaggle, but we chose this one because it requires sign-in for automatic download and the red wine dataset has less data.

2.1 Initial Data Preprocessing

It was confirmed that the 1599 rows of data consisted of only numerical data and that there was no missing data.

```r
# Wine Quality Data Set
# https://archive.ics.uci.edu/ml/datasets/Wine+Quality
# https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv

url <- c("https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequality-red.csv")
wine <- read_delim(url,delim = ";")

# modify the column name

colnames(wine) <- c("fixed_acidity", "volatile_acidity","citric_acid",
                    "residual_sugar","chlorides","free_sulfur_dioxide",
                    "total_sulfur_dioxide","density","pH",
                    "sulphates","alcohol","quality")

### Check the data -----

# whole the data

head(wine)
```

```
## # A tibble: 6 x 12
##   fixed_acidity volatile_acidity citric_acid residual_sugar chlorides
##           <dbl>            <dbl>       <dbl>          <dbl>     <dbl>
## 1           7.4             0.7         0               1.9     0.076
## 2           7.8             0.88        0               2.6     0.098
## 3           7.8             0.76        0.04            2.3     0.092
## 4          11.2             0.28        0.56            1.9     0.075
## 5           7.4             0.7         0               1.9     0.076
## 6           7.4             0.66        0               1.8     0.075
## # ... with 7 more variables: free_sulfur_dioxide <dbl>,
## #   total_sulfur_dioxide <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,
## #   alcohol <dbl>, quality <dbl>
```

```
wine %>% summary()
```

```
##  fixed_acidity   volatile_acidity  citric_acid    residual_sugar
##  Min.   : 4.60   Min.   :0.1200   Min.   :0.000   Min.   : 0.900
##  1st Qu.: 7.10   1st Qu.:0.3900   1st Qu.:0.090   1st Qu.: 1.900
##  Median : 7.90   Median :0.5200   Median :0.260   Median : 2.200
##  Mean   : 8.32   Mean   :0.5278   Mean   :0.271   Mean   : 2.539
##  3rd Qu.: 9.20   3rd Qu.:0.6400   3rd Qu.:0.420   3rd Qu.: 2.600
##  Max.   :15.90   Max.   :1.5800   Max.   :1.000   Max.   :15.500
##    chlorides       free_sulfur_dioxide total_sulfur_dioxide    density
##  Min.   :0.01200   Min.   : 1.00       Min.   :  6.00       Min.   :0.9901
##  1st Qu.:0.07000   1st Qu.: 7.00       1st Qu.: 22.00       1st Qu.:0.9956
##  Median :0.07900   Median :14.00       Median : 38.00       Median :0.9968
##  Mean   :0.08747   Mean   :15.87       Mean   : 46.47       Mean   :0.9967
##  3rd Qu.:0.09000   3rd Qu.:21.00       3rd Qu.: 62.00       3rd Qu.:0.9978
##  Max.   :0.61100   Max.   :72.00       Max.   :289.00       Max.   :1.0037
##        pH          sulphates         alcohol         quality
##  Min.   :2.740   Min.   :0.3300   Min.   : 8.40   Min.   :3.000
##  1st Qu.:3.210   1st Qu.:0.5500   1st Qu.: 9.50   1st Qu.:5.000
##  Median :3.310   Median :0.6200   Median :10.20   Median :6.000
##  Mean   :3.311   Mean   :0.6581   Mean   :10.42   Mean   :5.636
##  3rd Qu.:3.400   3rd Qu.:0.7300   3rd Qu.:11.10   3rd Qu.:6.000
##  Max.   :4.010   Max.   :2.0000   Max.   :14.90   Max.   :8.000
```

```
sum(is.na(wine))
```

```
## [1] 0
```

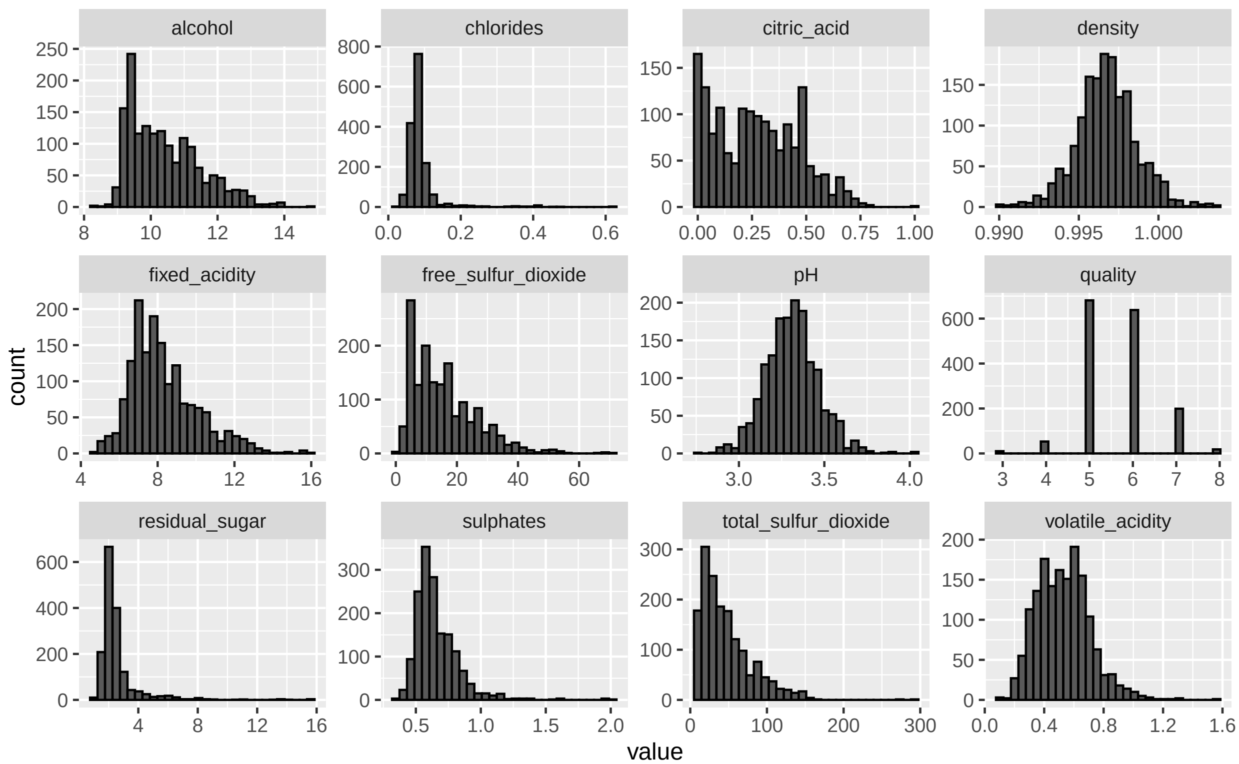
2.2 Explanatory Data Analysis (EDA)

The relationship between the quality data and each Attribution, which is the target for classification, was confirmed. The relationship with quality and the correlation between each were confirmed. It can be seen that while alcohol and volatile acidity are likely to have an effect on quality, residual sugar has a small relationship not only with quality but also with other Attributions.

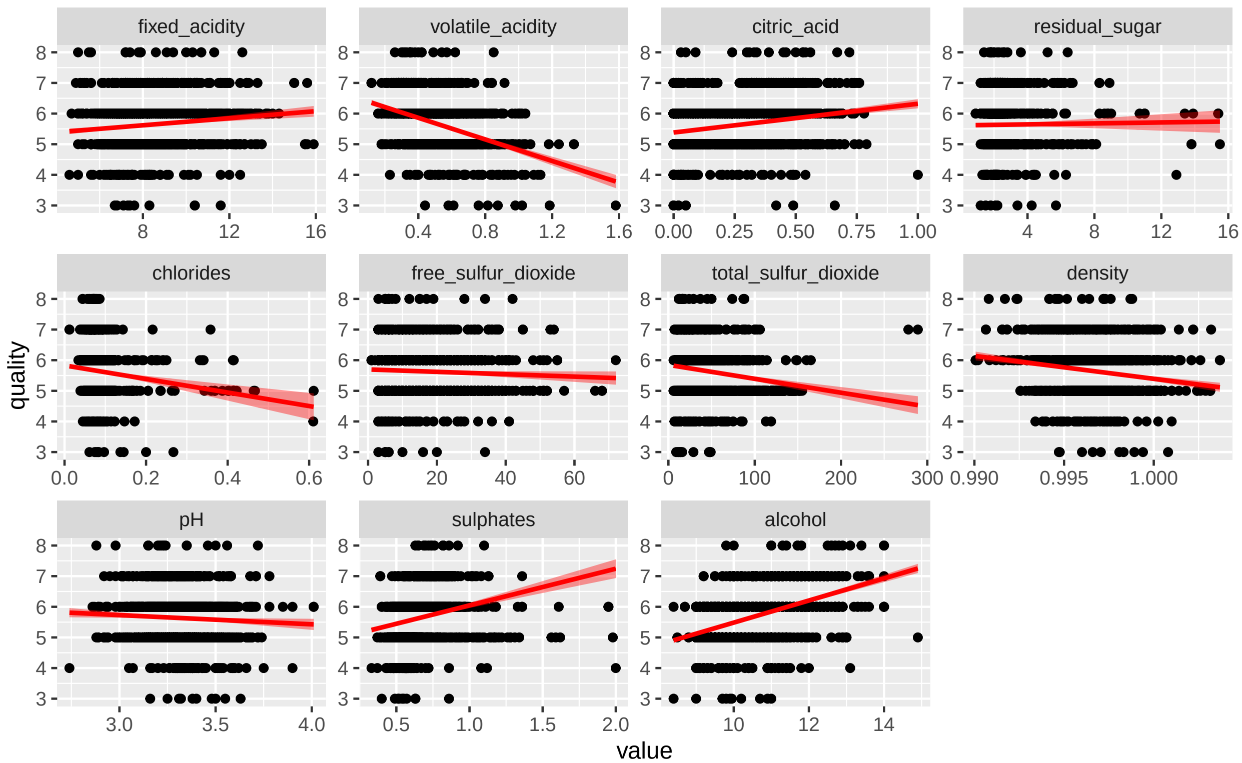
```
# Target: quality

table(wine$quality)
```

```
##
##    3   4   5   6   7   8
##   10  53 681 638 199  18
```

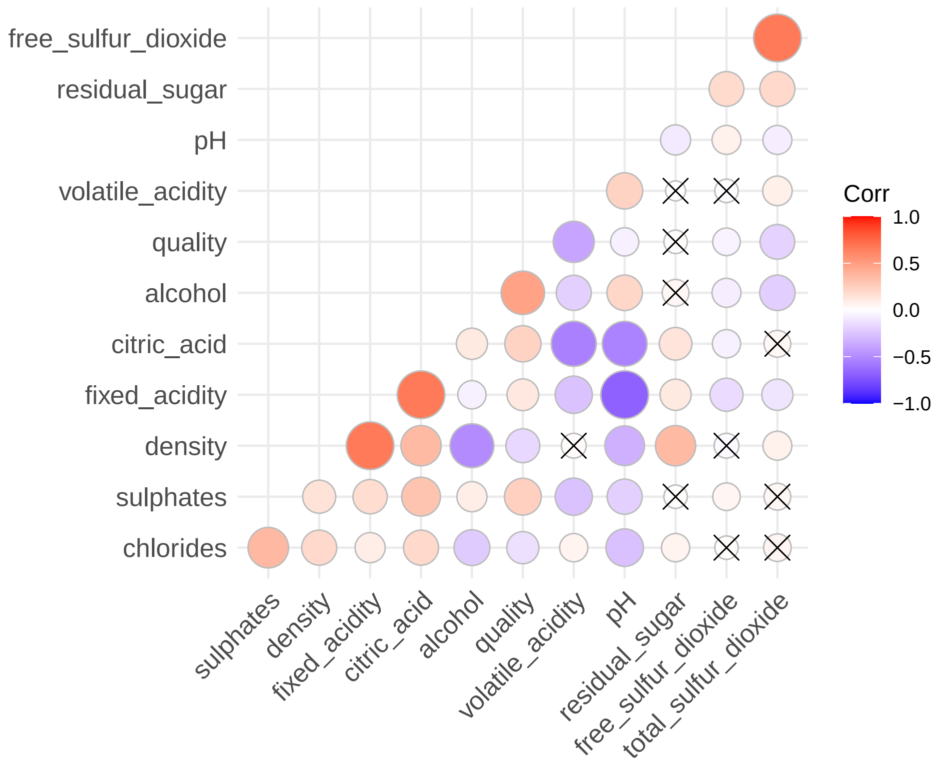
```r
# Distribution of each value

wine %>% gather() %>%
  ggplot(aes(value)) +
  geom_histogram(col="black") +
  facet_wrap(~key, scales = "free")
```




```r
# Check the relations between each attribute and quality (target)

wine  %>% reshape2::melt(.,"quality") %>%
  ggplot(aes(value, quality)) +
  geom_point() +
  geom_smooth(method = lm, col = "red", fill = "red") +
  facet_wrap(~variable, scales = "free")
```




```r
# Check the correlation
## Compute a matrix of correlation p-values

p.mat <- cor_pmat(wine)

# X means no significant coefficient

round(cor(wine),2) %>%
ggcorrplot(., method = "circle",  hc.order = TRUE, type = "lower", p.mat = p.mat)
```



2.3 Prepare the train / test data set

In order to build a model as a classification problem for quality, we divided the data. Since the number of data is small (1600), we decided to split the data 80:20. In order to make it a classification problem, a binomial classification was made for quality, with 1 being above 6 and 0 being below 6. In order to check the magnitude of the effect of each Attribution, the numbers were centered and standardized. The **recipe** library was used for the conversion. By using this library, it is easy to complete missing values and to make dummy variables for categorical variables (although we did not use this library, we commented it out in the code).

```
### Data preparation: Split the data set ----
# Preparation test and train data set for model selection
# Due to the small amount of data, 20% was used as test data.

set.seed(1, sample.kind="Rounding")
test_index <- createDataPartition(y = wine$quality, times = 1, p = 0.2, list = FALSE)
train_set <- wine[-test_index,]
test_set <- wine[test_index,]

# To build each model, centralization and standardization are done with recipe.

rec_pre <- recipe(train_set, quality~.) %>%
  step_center(all_numeric(),-quality) %>% # Centralization
  step_scale(all_numeric(), -quality) %>%  # Standardization
  # step_knnimpute(all_predictors(),K=5)  # There is no NA
  # step_dummy(all_predictors(), -all_numeric()) # There is no categorical data
  prep()
```

```r
# apply the recipe

train <- bake(rec_pre, new_data = train_set)
test <-  bake(rec_pre, new_data = test_set)

# check the data

head(train)
```

```
## # A tibble: 6 x 12
##   fixed_acidity volatile_acidity citric_acid residual_sugar chlorides
##           <dbl>            <dbl>       <dbl>          <dbl>     <dbl>
## 1        -0.521            0.934       -1.39         -0.445    -0.246
## 2        -0.283            1.93        -1.39          0.0476    0.210
## 3        -0.283            1.26        -1.18         -0.163     0.0859
## 4         1.74            -1.38         1.50         -0.445    -0.266
## 5        -0.521            0.934       -1.39         -0.445    -0.246
## 6        -0.521            0.713       -1.39         -0.515    -0.266
## # ... with 7 more variables: free_sulfur_dioxide <dbl>,
## #   total_sulfur_dioxide <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,
## #   alcohol <dbl>, quality <dbl>
```

```r
head(test)
```

```
## # A tibble: 6 x 12
##   fixed_acidity volatile_acidity citric_acid residual_sugar chlorides
##           <dbl>            <dbl>       <dbl>          <dbl>     <dbl>
## 1        -0.461           -0.168       0.471          2.51     -0.349
## 2        -1.59             0.465      -1.39          -0.656     0.0238
## 3        -0.223           -0.554      -0.303         -0.656     0.376
## 4        -0.699            0.989      -1.39          -0.445    -0.163
## 5        -0.342            0.493      -1.18           0.892    -0.0798
## 6        -0.640            1.07       -1.13           1.49     -0.0384
## # ... with 7 more variables: free_sulfur_dioxide <dbl>,
## #   total_sulfur_dioxide <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,
## #   alcohol <dbl>, quality <dbl>
```

```r
# Transform "quality" into binary

train$quality[train$quality < 6] <- 0
test$quality[test$quality < 6] <- 0
train$quality[train$quality > 0] <- 1
test$quality[test$quality > 0] <- 1

train$quality <- as.factor(train$quality)
test$quality <- as.factor(test$quality)


# summary

summary(train)
```

```
##  fixed_acidity     volatile_acidity   citric_acid       residual_sugar
##  Min.   :-2.1872   Min.   :-2.2623   Min.   :-1.38758   Min.   :-1.14804
##  1st Qu.:-0.6993   1st Qu.:-0.7194   1st Qu.:-0.92290   1st Qu.:-0.44474
##  Median :-0.2232   Median :-0.0581   Median :-0.07098   Median :-0.23375
##  Mean   : 0.0000   Mean   : 0.0000   Mean   : 0.00000   Mean   : 0.00000
##  3rd Qu.: 0.5357   3rd Qu.: 0.6032   3rd Qu.: 0.78094   3rd Qu.: 0.04757
##  Max.   : 4.5382   Max.   : 5.7830   Max.   : 3.77556   Max.   : 9.12018
##    chlorides        free_sulfur_dioxide total_sulfur_dioxide
##  Min.   :-1.57164   Min.   :-1.4219     Min.   :-1.2264
##  1st Qu.:-0.36992   1st Qu.:-0.8527     1st Qu.:-0.7441
##  Median :-0.18344   Median :-0.1885     Median :-0.2618
##  Mean   : 0.00000   Mean   : 0.0000     Mean   : 0.0000
##  3rd Qu.: 0.04447   3rd Qu.: 0.4757     3rd Qu.: 0.4919
##  Max.   :10.83929   Max.   : 5.3145     Max.   : 7.3048
##     density               pH              sulphates          alcohol
##  Min.   :-3.605932   Min.   :-3.71497   Min.   :-1.9078   Min.   :-1.8854
##  1st Qu.:-0.603029   1st Qu.:-0.66652   1st Qu.:-0.6301   1st Qu.:-0.8651
##  Median : 0.004086   Median :-0.01792   Median :-0.2236   Median :-0.2158
##  Mean   : 0.000000   Mean   : 0.00000   Mean   : 0.0000   Mean   : 0.0000
##  3rd Qu.: 0.603033   3rd Qu.: 0.56583   3rd Qu.: 0.4152   3rd Qu.: 0.6190
##  Max.   : 3.810123   Max.   : 4.52232   Max.   : 7.7907   Max.   : 4.1438
##  quality
##  0:595
##  1:683
##
##
##
##
```

```
summary(test)
```

```
##  fixed_acidity     volatile_acidity    citric_acid       residual_sugar
##  Min.   :-1.9492   Min.   :-1.93166   Min.   :-1.38758   Min.   :-1.14804
##  1st Qu.:-0.6993   1st Qu.:-0.82956   1st Qu.:-0.87127   1st Qu.:-0.44474
##  Median :-0.1636   Median :-0.05810   Median :-0.04517   Median :-0.23375
##  Mean   : 0.1325   Mean   :-0.07475   Mean   : 0.05729   Mean   : 0.02260
##  3rd Qu.: 0.7886   3rd Qu.: 0.46539   3rd Qu.: 0.93583   3rd Qu.: 0.04757
##  Max.   : 4.3596   Max.   : 2.80734   Max.   : 2.53640   Max.   : 9.04985
##    chlorides        free_sulfur_dioxide total_sulfur_dioxide    density
##  Min.   :-1.57164   Min.   :-1.42193    Min.   :-1.22645     Min.   :-3.6059
##  1st Qu.:-0.34920   1st Qu.:-0.85266    1st Qu.:-0.71397     1st Qu.:-0.5023
##  Median :-0.18344   Median :-0.28338    Median :-0.26178     Median : 0.1239
##  Mean   :-0.03996   Mean   :-0.05283    Mean   :-0.03245     Mean   : 0.1470
##  3rd Qu.: 0.04447   3rd Qu.: 0.47566    3rd Qu.: 0.37128     3rd Qu.: 0.8045
##  Max.   : 7.85569   Max.   : 3.70157    Max.   : 3.02411     Max.   : 3.8101
##        pH              sulphates           alcohol         quality
##  Min.   :-2.74206   Min.   :-1.67548   Min.   :-1.60715   0:149
##  1st Qu.:-0.66652   1st Qu.:-0.63014   1st Qu.:-0.86509   1:172
##  Median :-0.01792   Median :-0.22362   Median :-0.30854
##  Mean   :-0.05328   Mean   :-0.01032   Mean   :-0.04457
##  3rd Qu.: 0.56583   3rd Qu.: 0.47328   3rd Qu.: 0.52628
##  Max.   : 3.80886   Max.   : 4.07390   Max.   : 3.30902
```

3 Methods and Analysis

We made the following models for the classification problem. The evaluation was done by using Accuracy. Accuracy was calculated by comparing the predictions made by each model using the test data set with the actual quality.

The importance of each item was extracted and graphed if it could be extracted. As mentioned in the introduction, the model is intended to be used in actual business, and it is important to understand how the target changes by changing the value of each item.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

$$where TP = True\ positive;\ FP = False\ positive;\ TN = True\ negative;\ FN = False\ negative$$

In the analysis of each model using the library **caret**, we decided to use cross validation and made 10 divisions. Automatic parameter tuning was used for tuning.

```
#################
# MODEL Analysis
#################

# set the Cross Validation for caret package

trControl = trainControl(method = "cv", number = 10)
```

3.1 Logistic Regression

Logistic regression analysis is a type of "multivariate analysis" in which analysis is performed from multiple variables to predict qualitative probabilities.

$$p = \frac{1}{1 + e^{-(a_1x_1 + a_2x_2 + \ldots + a_nx_x + b)}}$$

3.2 CART (Classification and Regression Tree)

CART is a machine learning method that makes predictions based on "Yes or No" conditions for feature values. We selected it as one of the models because it is characterized by easy understanding and interpretation of learning results.

3.3 Random Forest

Since the learning results are easy to understand and interpret, we choose Random Forest as one of the models and train it using multiple decision trees. Random forests are trained using multiple decision trees, which are generated by randomly selecting data from the original training data. Then, when actually evaluating the unknown data, the conclusions of the individual decision trees are combined into an overall conclusion by majority voting.

Decision trees are a very straightforward algorithm, but they are known to fail to generate the desired tree structure depending on the data, and are prone to overlearning. Random forests, on the other hand, have the advantage that the effect of overlearning is much smaller than that of decision trees because the correlation between individual decision trees is low.

3.4 SVM (Support-vector machine)

SVM is a machine learning model that can be applied to problems such as classification and regression. It is a method of determining which hyperplane (or straight line in the case of 2D) separating two classes of data is the farthest from each data. Compared to other methods, it has advantages such as being able to obtain a highly accurate model even with a small amount of data, easily maintaining discrimination accuracy even when the number of dimensions (number of features) increases, and making it easy to adjust parameters. On the other hand, the amount of computation increases rapidly when the amount of training data increases, and the principle is two-class classification, so it is difficult to apply to multi-class classification.

3.5 Neural Net

A neural network is a model of how the human brain works and is applied to computers. Deep learning is a method of applying neural networks, also known as deep neural networks. The basic model structure of a neural network consists of an **input layer**, a **hidden layer**, and an **output layer**.

3.6 Gradient Boosting

Gradient boosting is a machine learning method for tasks such as regression and classification that generates a predictive model in the form of an ensemble of weak prediction models (usually decision trees).

In addition to XGBoost's Linear and Tree, which were also used in the MovieLens project, modeling is also done using a method called DART. In gradient boosting, there was a problem that the gradient was generally applied to fit the data in the more extreme locations towards the end of the step. In order to prevent overlearning, MART (Multiple Additive Regression Trees) is improved by introducing the concept of Drop Out, which is called DART (Dropouts meet Multiple Additive Regression Trees).

3.7 Deep Learning

Deep learning, or deep learning, is a machine learning method that uses a neural network that reproduces the mechanism of human neurons, and is characterized by the use of a multilayer neural network. Deep learning is a machine learning method that uses neural networks that replicate the mechanism of human neurons, and is characterized by the use of multi-layered neural networks. It is currently producing significant results in various fields such as image recognition, speech recognition, and translation.

It has been possible to use the library **keras** to build deep learning models in R for some time. However, it requires a **python** environment for installation and is not suitable for automatic installation of projects. The library **torch** has been implemented in R version in September 2020. In this project, we used torch to build a model for deep learning.

We also worked on building a model with tabnet, which is available by installing torch; it is a deep learning for data tables announced by Google Cloud in 2020. Unlike deep learning, which works like a black box, in the case of TabNet the model can interpret the features it chooses.

4 Results

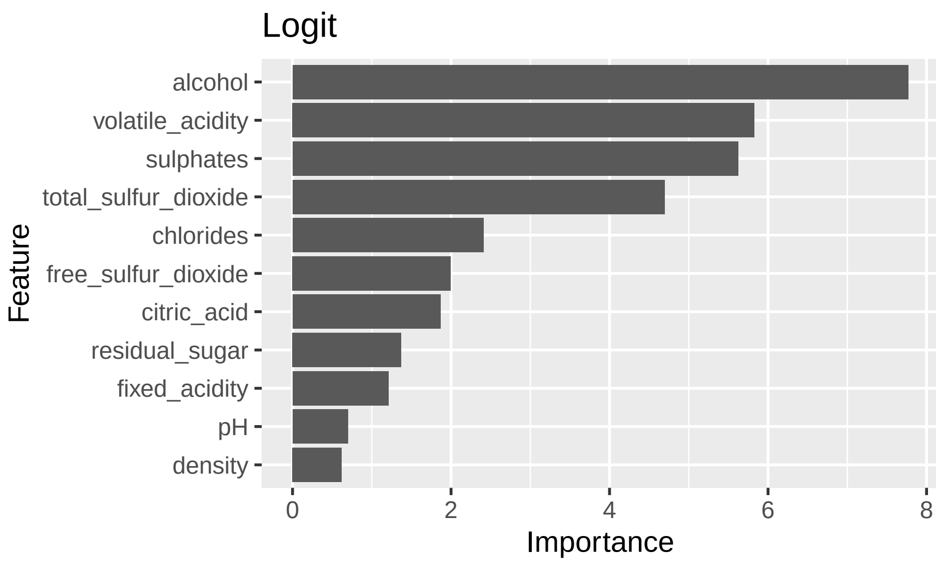
4.1 Each model

4.1.1 logit

```r
# logistic ------

set.seed(1, sample.kind="Rounding")

# train the model

wine_logit <- train(
  quality ~ .,
  data = train,
  method = "glm",
  family = binomial(),
  trControl = trControl
)

# Check the model

summary(wine_logit)
```

```
##
## Call:
## NULL
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -3.5361  -0.8221   0.2879   0.7995   2.3193
##
## Coefficients:
##                      Estimate Std. Error z value Pr(>|z|)
## (Intercept)           0.25808    0.07050   3.660 0.000252 ***
## fixed_acidity         0.22858    0.18891   1.210 0.226269
## volatile_acidity     -0.58151    0.09980  -5.827 5.65e-09 ***
## citric_acid          -0.23073    0.12360  -1.867 0.061938 .
## residual_sugar        0.11745    0.08566   1.371 0.170373
## chlorides            -0.20340    0.08437  -2.411 0.015918 *
## free_sulfur_dioxide   0.19234    0.09640   1.995 0.046024 *
## total_sulfur_dioxide -0.49020    0.10438  -4.696 2.65e-06 ***
## density              -0.10475    0.16926  -0.619 0.536022
## pH                   -0.08697    0.12414  -0.701 0.483587
## sulphates             0.49160    0.08742   5.624 1.87e-08 ***
## alcohol               0.98504    0.12682   7.767 8.02e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 1765.6  on 1277  degrees of freedom
## Residual deviance: 1303.5  on 1266  degrees of freedom
## AIC: 1327.5
##
## Number of Fisher Scoring iterations: 4
```

```r
p_logit <- varImp(wine_logit,scale = F) %>%
  ggplot() + ggtitle("Logit")
p_logit
```




```r
# Evaluate

confusionMatrix(predict(wine_logit, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 106  45
##          1  43 127
##
##                Accuracy : 0.7259
##                  95% CI : (0.6736, 0.7739)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : 2.246e-12
##
##                   Kappa : 0.4494
##
##  Mcnemar's Test P-Value : 0.9151
##
##             Sensitivity : 0.7114
##             Specificity : 0.7384
##          Pos Pred Value : 0.7020
##          Neg Pred Value : 0.7471
##              Prevalence : 0.4642
##          Detection Rate : 0.3302
##    Detection Prevalence : 0.4704
##       Balanced Accuracy : 0.7249
##
```

```
##        'Positive' Class : 0
##
```

```
logit_acc <- confusionMatrix(predict(wine_logit, test), test$quality)$overall["Accuracy"]
logit_acc
```

```
##  Accuracy
## 0.7258567
```

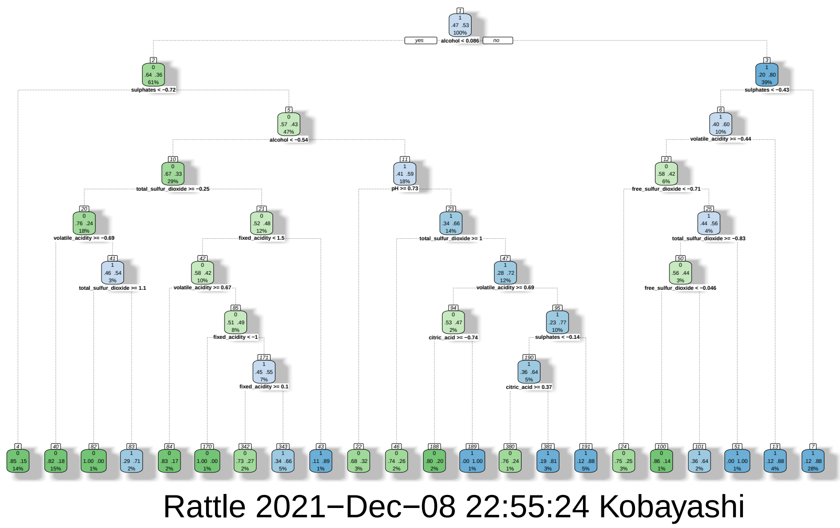
4.1.2 rpart

```
### Rpart -------

set.seed(1, sample.kind="Rounding")

# train the model

wine_rpart <- train(
  quality ~ .,
  data = train,
  method = "rpart",
  trControl = trControl,
  tuneLength = 10
)

# Check the model

wine_rpart
```

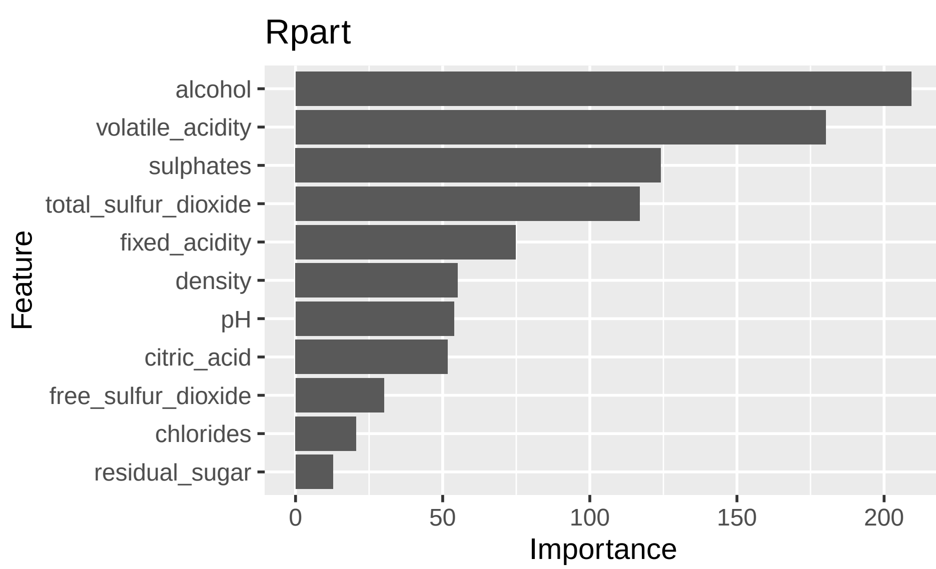
```
## CART
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   cp           Accuracy   Kappa
##   0.006722689  0.7316243  0.4608685
##   0.007563025  0.7221574  0.4398870
##   0.008403361  0.7237323  0.4434475
##   0.010084034  0.7198688  0.4363828
##   0.010924370  0.7198688  0.4363828
##   0.011764706  0.7191303  0.4340019
##   0.018487395  0.7121112  0.4204372
##   0.026890756  0.7081805  0.4142043
##   0.034453782  0.6894418  0.3808617
##   0.357983193  0.6579027  0.3040603
```

```
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was cp = 0.006722689.
```

```
fancyRpartPlot(wine_rpart$finalModel)
```




```
p_rpart <- varImp(wine_rpart,scale = F) %>%
  ggplot() + ggtitle("Rpart")
p_rpart
```




```
# Evaluate

confusionMatrix(predict(wine_rpart, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 106  38
##          1  43 134
##
##                Accuracy : 0.7477
##                  95% CI : (0.6964, 0.7943)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : 4.333e-15
##
##                   Kappa : 0.4916
##
##  Mcnemar's Test P-Value : 0.6567
##
##             Sensitivity : 0.7114
##             Specificity : 0.7791
##          Pos Pred Value : 0.7361
##          Neg Pred Value : 0.7571
##              Prevalence : 0.4642
##          Detection Rate : 0.3302
##    Detection Prevalence : 0.4486
##       Balanced Accuracy : 0.7452
##
##        'Positive' Class : 0
##
```

```
rpart_acc <- confusionMatrix(predict(wine_rpart, test), test$quality)$overall["Accuracy"]
rpart_acc
```

```
##  Accuracy
## 0.7476636
```

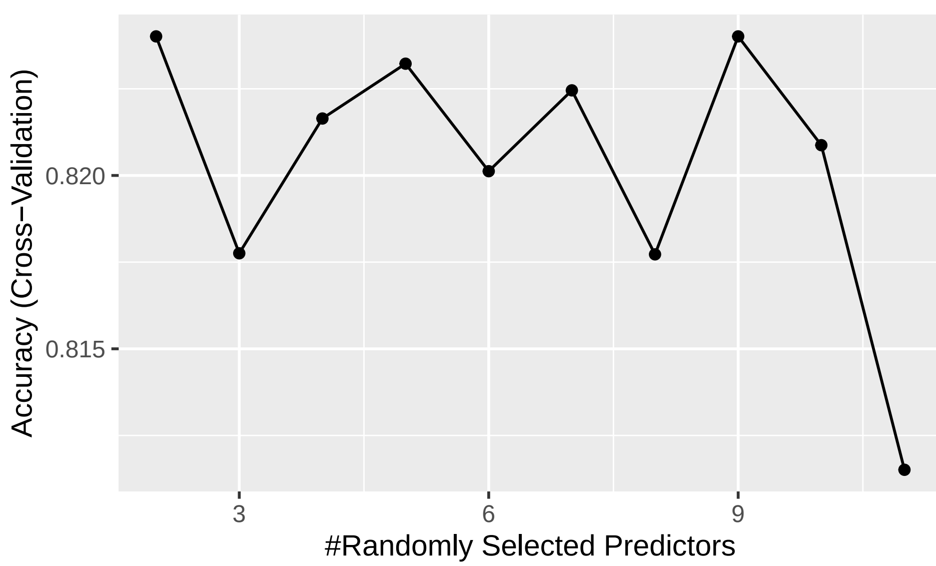
4.1.3 rf

```
### Random forest ------

set.seed(1, sample.kind="Rounding")

# train the model

wine_rf <- train(
  quality ~ .,
  data = train,
  method = "rf",
  trControl = trControl,
  tuneLength = 10
)

# Check the model
```

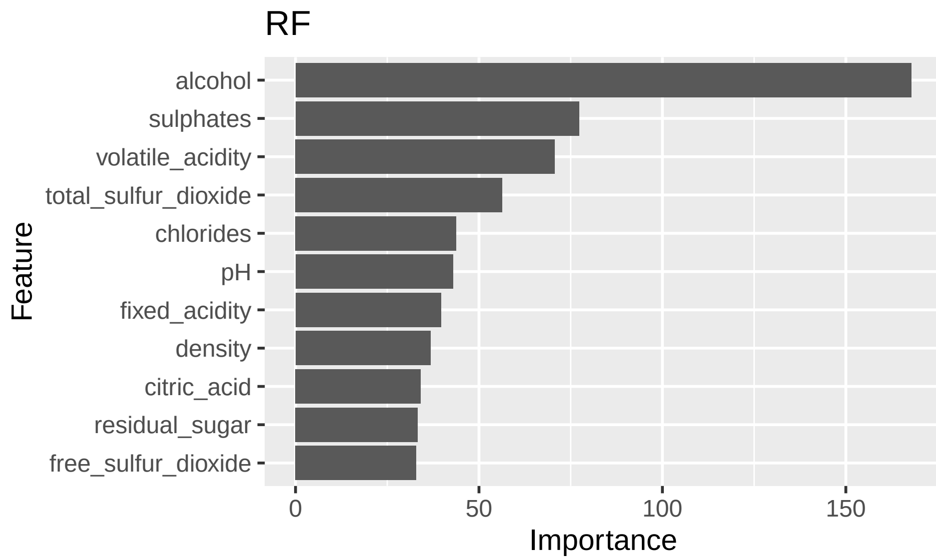
```r
wine_rf
```

```
## Random Forest
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   mtry  Accuracy   Kappa
##    2    0.8240111  0.6462582
##    3    0.8177548  0.6333618
##    4    0.8216428  0.6417497
##    5    0.8232236  0.6449335
##    6    0.8201232  0.6385645
##    7    0.8224546  0.6432484
##    8    0.8177244  0.6336485
##    9    0.8240112  0.6464435
##   10    0.8208738  0.6400483
##   11    0.8115108  0.6213133
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 9.
```

```r
ggplot(wine_rf)
```




```r
p_rf <- varImp(wine_rf,scale = F) %>%
  ggplot() + ggtitle("RF")
p_rf
```




```r
# Evaluate

confusionMatrix(predict(wine_rf, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 115  33
##          1  34 139
##
##                Accuracy : 0.7913
##                  95% CI : (0.7427, 0.8344)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.5802
##
##  Mcnemar's Test P-Value : 1
##
##             Sensitivity : 0.7718
##             Specificity : 0.8081
##          Pos Pred Value : 0.7770
##          Neg Pred Value : 0.8035
##              Prevalence : 0.4642
##          Detection Rate : 0.3583
##    Detection Prevalence : 0.4611
##       Balanced Accuracy : 0.7900
##
##        'Positive' Class : 0
##
```

```
rf_acc <- confusionMatrix(predict(wine_rf, test), test$quality)$overall["Accuracy"]
rf_acc
```

```
##  Accuracy
## 0.7912773
```

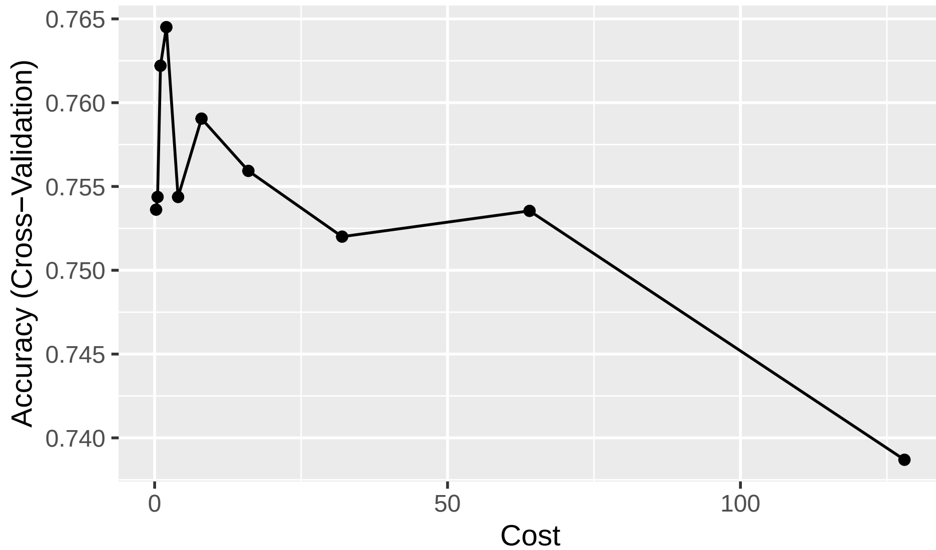
4.1.4 svm

```
### SVM ------


set.seed(1, sample.kind="Rounding")

# train the model

wine_svm <- train(
  quality ~ .,
  data = train,
  method = "svmRadial",
  trControl = trControl,
  tuneLength = 10
)

# Check the model

wine_svm
```

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   C       Accuracy   Kappa
##     0.25  0.7536164  0.5074271
##     0.50  0.7543732  0.5084859
##     1.00  0.7622040  0.5235872
##     2.00  0.7645052  0.5281345
##     4.00  0.7543731  0.5078602
##     8.00  0.7590486  0.5171078
##    16.00  0.7559298  0.5109009
##    32.00  0.7520054  0.5029998
##    64.00  0.7535435  0.5063640
##   128.00  0.7386931  0.4753174
##
## Tuning parameter 'sigma' was held constant at a value of 0.09316274
```

```
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were sigma = 0.09316274 and C = 2.
```

```r
ggplot(wine_svm)
```




```r
# Evaluate

confusionMatrix(predict(wine_svm, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 108  40
##          1  41 132
##
##                Accuracy : 0.7477
##                  95% CI : (0.6964, 0.7943)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : 4.333e-15
##
##                   Kappa : 0.4925
##
##  Mcnemar's Test P-Value : 1
##
##             Sensitivity : 0.7248
##             Specificity : 0.7674
##          Pos Pred Value : 0.7297
##          Neg Pred Value : 0.7630
##              Prevalence : 0.4642
##          Detection Rate : 0.3364
##    Detection Prevalence : 0.4611
##       Balanced Accuracy : 0.7461
##
```

```
##        'Positive' Class : 0
##
```

```
svm_acc <- confusionMatrix(predict(wine_svm, test), test$quality)$overall["Accuracy"]
svm_acc
```

```
##  Accuracy
## 0.7476636
```

4.1.5 nnet

```
### Neural Net ------

set.seed(1, sample.kind="Rounding")

# train the model

wine_nnet <- train(
  quality ~ .,
  data = train,
  method = "nnet",
  trControl = trControl,
  tuneLength = 10,
  trace = FALSE
)

# Check the model

wine_nnet
```

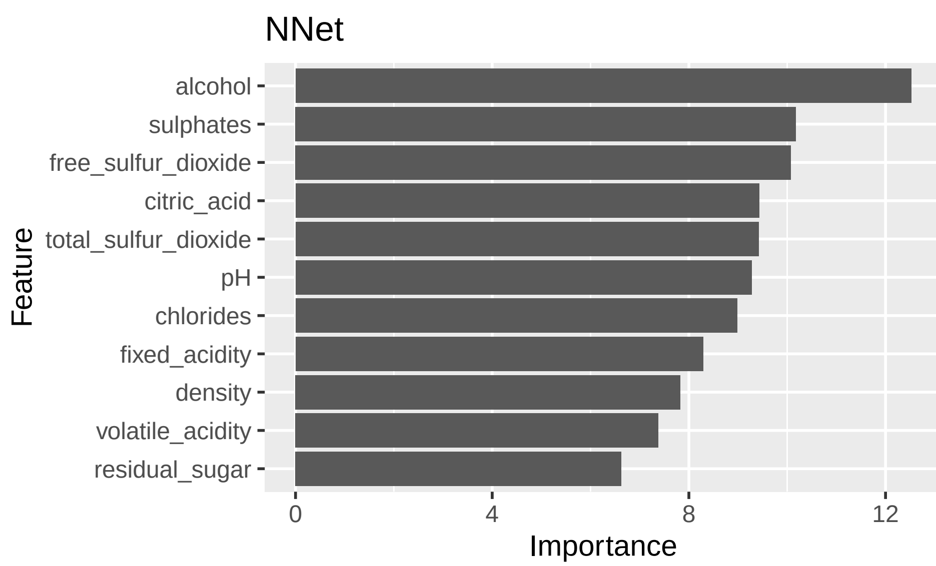
```
## Neural Network
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   size  decay         Accuracy   Kappa
##    1    0.0000000000  0.7411282  0.4823255
##    1    0.0001000000  0.7411282  0.4823255
##    1    0.0002371374  0.7380032  0.4753936
##    1    0.0005623413  0.7403349  0.4811305
##    1    0.0013335214  0.7411282  0.4823255
##    1    0.0031622777  0.7411282  0.4823255
##    1    0.0074989421  0.7395596  0.4792031
##    1    0.0177827941  0.7387722  0.4776884
##    1    0.0421696503  0.7387722  0.4776884
```

```
##    1    0.1000000000  0.7379848  0.4760318
##    3    0.0000000000  0.7411651  0.4784584
##    3    0.0001000000  0.7309347  0.4617602
##    3    0.0002371374  0.7355797  0.4707178
##    3    0.0005623413  0.7433558  0.4853736
##    3    0.0013335214  0.7441918  0.4878423
##    3    0.0031622777  0.7363916  0.4725871
##    3    0.0074989421  0.7418546  0.4829034
##    3    0.0177827941  0.7442165  0.4870011
##    3    0.0421696503  0.7449734  0.4871806
##    3    0.1000000000  0.7465662  0.4906912
##    5    0.0000000000  0.7426478  0.4850420
##    5    0.0001000000  0.7392907  0.4752348
##    5    0.0002371374  0.7371484  0.4721912
##    5    0.0005623413  0.7418607  0.4833875
##    5    0.0013335214  0.7387909  0.4763028
##    5    0.0031622777  0.7277672  0.4550144
##    5    0.0074989421  0.7473543  0.4940767
##    5    0.0177827941  0.7434230  0.4856350
##    5    0.0421696503  0.7363855  0.4717189
##    5    0.1000000000  0.7387597  0.4753341
##    7    0.0000000000  0.7364894  0.4707394
##    7    0.0001000000  0.7300495  0.4584486
##    7    0.0002371374  0.7278283  0.4545386
##    7    0.0005623413  0.7277854  0.4528632
##    7    0.0013335214  0.7285785  0.4564756
##    7    0.0031622777  0.7402670  0.4806715
##    7    0.0074989421  0.7229201  0.4418487
##    7    0.0177827941  0.7166457  0.4287281
##    7    0.0421696503  0.7286517  0.4554615
##    7    0.1000000000  0.7489099  0.4970318
##    9    0.0000000000  0.7246781  0.4487092
##    9    0.0001000000  0.7324483  0.4633832
##    9    0.0002371374  0.7222611  0.4414049
##    9    0.0005623413  0.7239212  0.4458059
##    9    0.0013335214  0.7254474  0.4500294
##    9    0.0031622777  0.7270097  0.4504285
##    9    0.0074989421  0.7324978  0.4641461
##    9    0.0177827941  0.7316917  0.4606521
##    9    0.0421696503  0.7395038  0.4774235
##    9    0.1000000000  0.7426174  0.4839751
##   11    0.0000000000  0.7309041  0.4597021
##   11    0.0001000000  0.7488858  0.4957492
##   11    0.0002371374  0.7143204  0.4255914
##   11    0.0005623413  0.7325031  0.4634055
##   11    0.0013335214  0.7193439  0.4373631
##   11    0.0031622777  0.7339806  0.4661220
##   11    0.0074989421  0.7300807  0.4575253
##   11    0.0177827941  0.7356343  0.4693615
##   11    0.0421696503  0.7324427  0.4627939
##   11    0.1000000000  0.7426422  0.4828828
##   13    0.0000000000  0.7106647  0.4184417
##   13    0.0001000000  0.7347250  0.4673072
##   13    0.0002371374  0.7293114  0.4565664
```

```
##    13    0.0005623413  0.7206922  0.4388827
##    13    0.0013335214  0.7293720  0.4555830
##    13    0.0031622777  0.7394984  0.4767887
##    13    0.0074989421  0.7270160  0.4514281
##    13    0.0177827941  0.7348292  0.4671441
##    13    0.0421696503  0.7550565  0.5086654
##    13    0.1000000000  0.7465237  0.4915275
##    15    0.0000000000  0.7409996  0.4780454
##    15    0.0001000000  0.7394805  0.4756444
##    15    0.0002371374  0.7254419  0.4472550
##    15    0.0005623413  0.7239164  0.4450928
##    15    0.0013335214  0.7308858  0.4599140
##    15    0.0031622777  0.7411100  0.4810926
##    15    0.0074989421  0.7136859  0.4237930
##    15    0.0177827941  0.7582729  0.5135487
##    15    0.0421696503  0.7575229  0.5117582
##    15    0.1000000000  0.7535003  0.5045235
##    17    0.0000000000  0.7521331  0.5006737
##    17    0.0001000000  0.7315996  0.4599450
##    17    0.0002371374  0.7332608  0.4634188
##    17    0.0005623413  0.7418539  0.4819537
##    17    0.0013335214  0.7346884  0.4671634
##    17    0.0031622777  0.7346575  0.4657347
##    17    0.0074989421  0.7387969  0.4755462
##    17    0.0177827941  0.7183128  0.4350593
##    17    0.0421696503  0.7394313  0.4770899
##    17    0.1000000000  0.7472869  0.4928088
##    19    0.0000000000  0.7364280  0.4702842
##    19    0.0001000000  0.7426296  0.4836545
##    19    0.0002371374  0.7268818  0.4511408
##    19    0.0005623413  0.7527925  0.5029529
##    19    0.0013335214  0.7558563  0.5086475
##    19    0.0031622777  0.7590302  0.5151016
##    19    0.0074989421  0.7386987  0.4738227
##    19    0.0177827941  0.7536167  0.5051497
##    19    0.0421696503  0.7481231  0.4940005
##    19    0.1000000000  0.7637485  0.5260543
##
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were size = 19 and decay = 0.1.
```

```
ggplot(wine_nnet)
```


```r
p_nnet <- varImp(wine_nnet,scale = F) %>%
  ggplot() + ggtitle("NNet")
p_nnet
```




```r
# Evaluate

confusionMatrix(predict(wine_nnet, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 116  37
##          1  33 135
```

```
##
##                Accuracy : 0.7819
##                  95% CI : (0.7327, 0.8259)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.5624
##
##  Mcnemar's Test P-Value : 0.7199
##
##             Sensitivity : 0.7785
##             Specificity : 0.7849
##          Pos Pred Value : 0.7582
##          Neg Pred Value : 0.8036
##              Prevalence : 0.4642
##          Detection Rate : 0.3614
##    Detection Prevalence : 0.4766
##       Balanced Accuracy : 0.7817
##
##        'Positive' Class : 0
##
```

```
nnet_acc <- confusionMatrix(predict(wine_nnet, test), test$quality)$overall["Accuracy"]
nnet_acc
```

```
##  Accuracy
## 0.7819315
```

4.1.6 xgbLinear

```
### XGBoost: xgbLinear----

set.seed(1, sample.kind="Rounding")

# train the model

wine_xgbl <- train(
  quality ~ .,
  data = train,
  method = "xgbLinear",
  trControl = trControl,
  tuneLength = 5
)
```

```
# Check the model

wine_xgbl
```

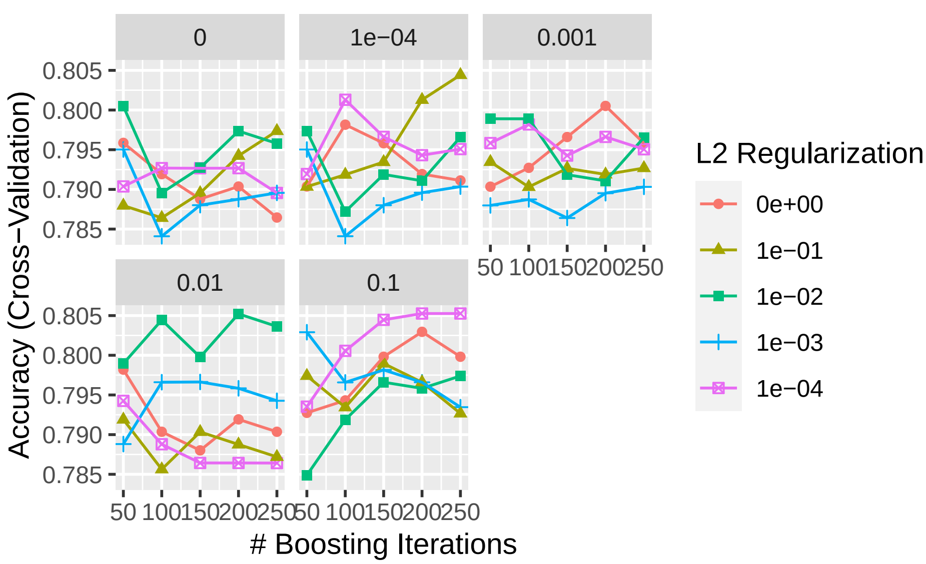
```
## eXtreme Gradient Boosting
##
## 1278 samples
```

```
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   lambda  alpha  nrounds  Accuracy   Kappa
##   0e+00   0e+00   50      0.7958608  0.5901153
##   0e+00   0e+00  100      0.7919239  0.5819415
##   0e+00   0e+00  150      0.7887863  0.5758016
##   0e+00   0e+00  200      0.7903611  0.5789057
##   0e+00   0e+00  250      0.7864547  0.5711173
##   0e+00   1e-04   50      0.7903736  0.5793526
##   0e+00   1e-04  100      0.7981557  0.5949843
##   0e+00   1e-04  150      0.7958178  0.5899729
##   0e+00   1e-04  200      0.7919299  0.5823010
##   0e+00   1e-04  250      0.7911241  0.5807874
##   0e+00   1e-03   50      0.7903431  0.5793143
##   0e+00   1e-03  100      0.7927174  0.5841713
##   0e+00   1e-03  150      0.7965993  0.5920801
##   0e+00   1e-03  200      0.8005179  0.6001858
##   0e+00   1e-03  250      0.7958119  0.5905590
##   0e+00   1e-02   50      0.7981923  0.5945793
##   0e+00   1e-02  100      0.7903611  0.5789104
##   0e+00   1e-02  150      0.7880173  0.5742684
##   0e+00   1e-02  200      0.7919235  0.5819371
##   0e+00   1e-02  250      0.7903609  0.5790912
##   0e+00   1e-01   50      0.7927477  0.5838754
##   0e+00   1e-01  100      0.7943101  0.5870522
##   0e+00   1e-01  150      0.7998158  0.5983935
##   0e+00   1e-01  200      0.8029531  0.6042649
##   0e+00   1e-01  250      0.7998158  0.5980556
##   1e-04   0e+00   50      0.7903736  0.5791694
##   1e-04   0e+00  100      0.7926808  0.5837737
##   1e-04   0e+00  150      0.7926623  0.5835631
##   1e-04   0e+00  200      0.7926745  0.5836261
##   1e-04   0e+00  250      0.7895555  0.5775625
##   1e-04   1e-04   50      0.7919361  0.5823667
##   1e-04   1e-04  100      0.8012930  0.6013778
##   1e-04   1e-04  150      0.7966175  0.5916675
##   1e-04   1e-04  200      0.7943104  0.5871763
##   1e-04   1e-04  250      0.7950794  0.5887282
##   1e-04   1e-03   50      0.7958365  0.5905345
##   1e-04   1e-03  100      0.7981864  0.5949388
##   1e-04   1e-03  150      0.7942616  0.5870887
##   1e-04   1e-03  200      0.7966175  0.5920263
##   1e-04   1e-03  250      0.7950549  0.5888721
##   1e-04   1e-02   50      0.7942553  0.5867674
##   1e-04   1e-02  100      0.7887863  0.5759726
##   1e-04   1e-02  150      0.7864302  0.5712484
##   1e-04   1e-02  200      0.7864302  0.5710535
##   1e-04   1e-02  250      0.7864179  0.5712193
```

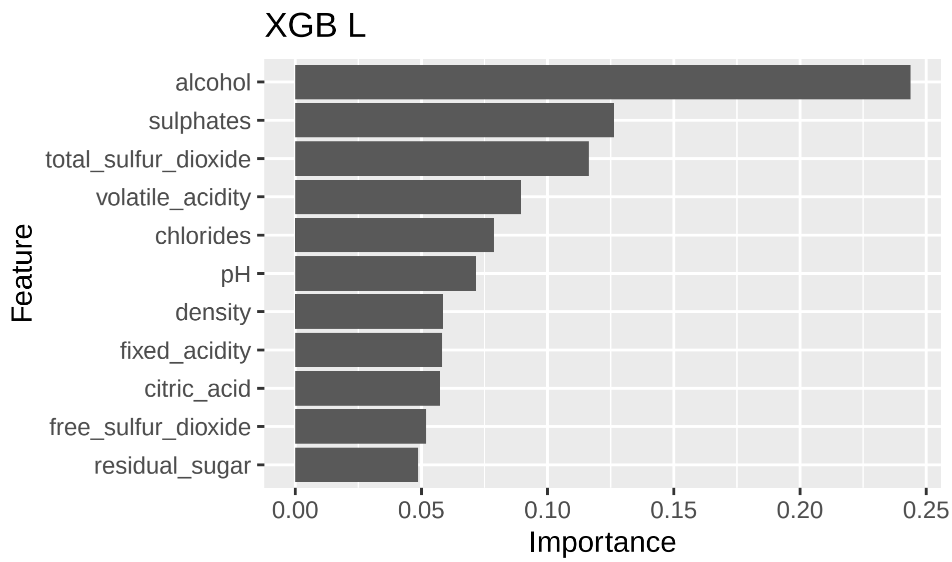
```
##    1e-04   1e-01   50       0.7935229  0.5855653
##    1e-04   1e-01  100       0.8005604  0.5995975
##    1e-04   1e-01  150       0.8044668  0.6073136
##    1e-04   1e-01  200       0.8052602  0.6087793
##    1e-04   1e-01  250       0.8052603  0.6086133
##    1e-03   0e+00   50       0.7950245  0.5883815
##    1e-03   0e+00  100       0.7840928  0.5662288
##    1e-03   0e+00  150       0.7880114  0.5739719
##    1e-03   0e+00  200       0.7887620  0.5751140
##    1e-03   0e+00  250       0.7895618  0.5770784
##    1e-03   1e-04   50       0.7950245  0.5885734
##    1e-03   1e-04  100       0.7840990  0.5666732
##    1e-03   1e-04  150       0.7880053  0.5744831
##    1e-03   1e-04  200       0.7895862  0.5776089
##    1e-03   1e-04  250       0.7903492  0.5790568
##    1e-03   1e-03   50       0.7879808  0.5742439
##    1e-03   1e-03  100       0.7887377  0.5756211
##    1e-03   1e-03  150       0.7863938  0.5711292
##    1e-03   1e-03  200       0.7895189  0.5774744
##    1e-03   1e-03  250       0.7903186  0.5791545
##    1e-03   1e-02   50       0.7888109  0.5757457
##    1e-03   1e-02  100       0.7966052  0.5914658
##    1e-03   1e-02  150       0.7966357  0.5918528
##    1e-03   1e-02  200       0.7958361  0.5900723
##    1e-03   1e-02  250       0.7942674  0.5867986
##    1e-03   1e-01   50       0.8029043  0.6046522
##    1e-03   1e-01  100       0.7965806  0.5914601
##    1e-03   1e-01  150       0.7981555  0.5949643
##    1e-03   1e-01  200       0.7965929  0.5917418
##    1e-03   1e-01  250       0.7934618  0.5853906
##    1e-02   0e+00   50       0.8004750  0.5995516
##    1e-02   0e+00  100       0.7895615  0.5778349
##    1e-02   0e+00  150       0.7927231  0.5840040
##    1e-02   0e+00  200       0.7973497  0.5934654
##    1e-02   0e+00  250       0.7957931  0.5901931
##    1e-02   1e-04   50       0.7973254  0.5930882
##    1e-02   1e-04  100       0.7871993  0.5732167
##    1e-02   1e-04  150       0.7918869  0.5822658
##    1e-02   1e-04  200       0.7910874  0.5806455
##    1e-02   1e-04  250       0.7965991  0.5920779
##    1e-02   1e-03   50       0.7989002  0.5962895
##    1e-02   1e-03  100       0.7989002  0.5962534
##    1e-02   1e-03  150       0.7918505  0.5816562
##    1e-02   1e-03  200       0.7910752  0.5803013
##    1e-02   1e-03  250       0.7965441  0.5912807
##    1e-02   1e-02   50       0.7989493  0.5959013
##    1e-02   1e-02  100       0.8044427  0.6065880
##    1e-02   1e-02  150       0.7997671  0.5976010
##    1e-02   1e-02  200       0.8052175  0.6085573
##    1e-02   1e-02  250       0.8036305  0.6054588
##    1e-02   1e-01   50       0.7848859  0.5680917
##    1e-02   1e-01  100       0.7918806  0.5818803
##    1e-02   1e-01  150       0.7966049  0.5915145
##    1e-02   1e-01  200       0.7958299  0.5899191
```

```
##    1e-02   1e-01   250      0.7973924  0.5932490
##    1e-01   0e+00    50      0.7879562  0.5743817
##    1e-01   0e+00   100      0.7864119  0.5713114
##    1e-01   0e+00   150      0.7895309  0.5776237
##    1e-01   0e+00   200      0.7942368  0.5871749
##    1e-01   0e+00   250      0.7973619  0.5933139
##    1e-01   1e-04    50      0.7903427  0.5792903
##    1e-01   1e-04   100      0.7918564  0.5817421
##    1e-01   1e-04   150      0.7934494  0.5853833
##    1e-01   1e-04   200      0.8012867  0.6007985
##    1e-01   1e-04   250      0.8044178  0.6074000
##    1e-01   1e-03    50      0.7934620  0.5854748
##    1e-01   1e-03   100      0.7903123  0.5791110
##    1e-01   1e-03   150      0.7926501  0.5835578
##    1e-01   1e-03   200      0.7918871  0.5822555
##    1e-01   1e-03   250      0.7926868  0.5839328
##    1e-01   1e-02    50      0.7918993  0.5824580
##    1e-01   1e-02   100      0.7856307  0.5693689
##    1e-01   1e-02   150      0.7903428  0.5787425
##    1e-01   1e-02   200      0.7887621  0.5757647
##    1e-01   1e-02   250      0.7871933  0.5725978
##    1e-01   1e-01    50      0.7974049  0.5938090
##    1e-01   1e-01   100      0.7934435  0.5857668
##    1e-01   1e-01   150      0.7989614  0.5964540
##    1e-01   1e-01   200      0.7965930  0.5917967
##    1e-01   1e-01   250      0.7926683  0.5838032
##
## Tuning parameter 'eta' was held constant at a value of 0.3
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were nrounds = 250, lambda = 1e-04, alpha
##  = 0.1 and eta = 0.3.
```

```
ggplot(wine_xgbl)
```



```r
p_xgbl <- varImp(wine_xgbl,scale = F) %>%
  ggplot() + ggtitle("XGB L")
p_xgbl
```




```r
# Evaluate

confusionMatrix(predict(wine_xgbl, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 117  29
##          1  32 143
##
##                Accuracy : 0.81
##                  95% CI : (0.7627, 0.8514)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.6175
##
##  Mcnemar's Test P-Value : 0.7979
##
##             Sensitivity : 0.7852
##             Specificity : 0.8314
##          Pos Pred Value : 0.8014
##          Neg Pred Value : 0.8171
##              Prevalence : 0.4642
##          Detection Rate : 0.3645
##    Detection Prevalence : 0.4548
##       Balanced Accuracy : 0.8083
##
```

```
##        'Positive' Class : 0
##
```

```
xgbl_acc <- confusionMatrix(predict(wine_xgbl, test), test$quality)$overall["Accuracy"]
xgbl_acc
```

```
##  Accuracy
## 0.8099688
```

4.1.7 xgbDART

```
### XGBoost: xgbDART----

set.seed(1, sample.kind="Rounding")

# train the model

wine_xgbd <- train(
  quality ~ .,
  data = train,
  method = "xgbDART",
  trControl = trControl,
  tuneLength = 3
)
```

```
# Check the model

wine_xgbd
```

```
## eXtreme Gradient Boosting
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   max_depth  eta  rate_drop  skip_drop  subsample  colsample_bytree  nrounds
##   1          0.3  0.01       0.05       0.50       0.6                50
##   1          0.3  0.01       0.05       0.50       0.6               100
##   1          0.3  0.01       0.05       0.50       0.6               150
##   1          0.3  0.01       0.05       0.50       0.8                50
##   1          0.3  0.01       0.05       0.50       0.8               100
##   1          0.3  0.01       0.05       0.50       0.8               150
##   1          0.3  0.01       0.05       0.75       0.6                50
##   1          0.3  0.01       0.05       0.75       0.6               100
##   1          0.3  0.01       0.05       0.75       0.6               150
##   1          0.3  0.01       0.05       0.75       0.8                50
```

```
##   1           0.3  0.01        0.05        0.75        0.8                 100
##   1           0.3  0.01        0.05        0.75        0.8                 150
##   1           0.3  0.01        0.05        1.00        0.6                  50
##   1           0.3  0.01        0.05        1.00        0.6                 100
##   1           0.3  0.01        0.05        1.00        0.6                 150
##   1           0.3  0.01        0.05        1.00        0.8                  50
##   1           0.3  0.01        0.05        1.00        0.8                 100
##   1           0.3  0.01        0.05        1.00        0.8                 150
##   1           0.3  0.01        0.95        0.50        0.6                  50
##   1           0.3  0.01        0.95        0.50        0.6                 100
##   1           0.3  0.01        0.95        0.50        0.6                 150
##   1           0.3  0.01        0.95        0.50        0.8                  50
##   1           0.3  0.01        0.95        0.50        0.8                 100
##   1           0.3  0.01        0.95        0.50        0.8                 150
##   1           0.3  0.01        0.95        0.75        0.6                  50
##   1           0.3  0.01        0.95        0.75        0.6                 100
##   1           0.3  0.01        0.95        0.75        0.6                 150
##   1           0.3  0.01        0.95        0.75        0.8                  50
##   1           0.3  0.01        0.95        0.75        0.8                 100
##   1           0.3  0.01        0.95        0.75        0.8                 150
##   1           0.3  0.01        0.95        1.00        0.6                  50
##   1           0.3  0.01        0.95        1.00        0.6                 100
##   1           0.3  0.01        0.95        1.00        0.6                 150
##   1           0.3  0.01        0.95        1.00        0.8                  50
##   1           0.3  0.01        0.95        1.00        0.8                 100
##   1           0.3  0.01        0.95        1.00        0.8                 150
##   1           0.3  0.50        0.05        0.50        0.6                  50
##   1           0.3  0.50        0.05        0.50        0.6                 100
##   1           0.3  0.50        0.05        0.50        0.6                 150
##   1           0.3  0.50        0.05        0.50        0.8                  50
##   1           0.3  0.50        0.05        0.50        0.8                 100
##   1           0.3  0.50        0.05        0.50        0.8                 150
##   1           0.3  0.50        0.05        0.75        0.6                  50
##   1           0.3  0.50        0.05        0.75        0.6                 100
##   1           0.3  0.50        0.05        0.75        0.6                 150
##   1           0.3  0.50        0.05        0.75        0.8                  50
##   1           0.3  0.50        0.05        0.75        0.8                 100
##   1           0.3  0.50        0.05        0.75        0.8                 150
##   1           0.3  0.50        0.05        1.00        0.6                  50
##   1           0.3  0.50        0.05        1.00        0.6                 100
##   1           0.3  0.50        0.05        1.00        0.6                 150
##   1           0.3  0.50        0.05        1.00        0.8                  50
##   1           0.3  0.50        0.05        1.00        0.8                 100
##   1           0.3  0.50        0.05        1.00        0.8                 150
##   1           0.3  0.50        0.95        0.50        0.6                  50
##   1           0.3  0.50        0.95        0.50        0.6                 100
##   1           0.3  0.50        0.95        0.50        0.6                 150
##   1           0.3  0.50        0.95        0.50        0.8                  50
##   1           0.3  0.50        0.95        0.50        0.8                 100
##   1           0.3  0.50        0.95        0.50        0.8                 150
##   1           0.3  0.50        0.95        0.75        0.6                  50
##   1           0.3  0.50        0.95        0.75        0.6                 100
##   1           0.3  0.50        0.95        0.75        0.6                 150
##   1           0.3  0.50        0.95        0.75        0.8                  50
```

```
## 1 0.3 0.50 0.95 0.75 0.8 100
## 1 0.3 0.50 0.95 0.75 0.8 150
## 1 0.3 0.50 0.95 1.00 0.6  50
## 1 0.3 0.50 0.95 1.00 0.6 100
## 1 0.3 0.50 0.95 1.00 0.6 150
## 1 0.3 0.50 0.95 1.00 0.8  50
## 1 0.3 0.50 0.95 1.00 0.8 100
## 1 0.3 0.50 0.95 1.00 0.8 150
## 1 0.4 0.01 0.05 0.50 0.6  50
## 1 0.4 0.01 0.05 0.50 0.6 100
## 1 0.4 0.01 0.05 0.50 0.6 150
## 1 0.4 0.01 0.05 0.50 0.8  50
## 1 0.4 0.01 0.05 0.50 0.8 100
## 1 0.4 0.01 0.05 0.50 0.8 150
## 1 0.4 0.01 0.05 0.75 0.6  50
## 1 0.4 0.01 0.05 0.75 0.6 100
## 1 0.4 0.01 0.05 0.75 0.6 150
## 1 0.4 0.01 0.05 0.75 0.8  50
## 1 0.4 0.01 0.05 0.75 0.8 100
## 1 0.4 0.01 0.05 0.75 0.8 150
## 1 0.4 0.01 0.05 1.00 0.6  50
## 1 0.4 0.01 0.05 1.00 0.6 100
## 1 0.4 0.01 0.05 1.00 0.6 150
## 1 0.4 0.01 0.05 1.00 0.8  50
## 1 0.4 0.01 0.05 1.00 0.8 100
## 1 0.4 0.01 0.05 1.00 0.8 150
## 1 0.4 0.01 0.95 0.50 0.6  50
## 1 0.4 0.01 0.95 0.50 0.6 100
## 1 0.4 0.01 0.95 0.50 0.6 150
## 1 0.4 0.01 0.95 0.50 0.8  50
## 1 0.4 0.01 0.95 0.50 0.8 100
## 1 0.4 0.01 0.95 0.50 0.8 150
## 1 0.4 0.01 0.95 0.75 0.6  50
## 1 0.4 0.01 0.95 0.75 0.6 100
## 1 0.4 0.01 0.95 0.75 0.6 150
## 1 0.4 0.01 0.95 0.75 0.8  50
## 1 0.4 0.01 0.95 0.75 0.8 100
## 1 0.4 0.01 0.95 0.75 0.8 150
## 1 0.4 0.01 0.95 1.00 0.6  50
## 1 0.4 0.01 0.95 1.00 0.6 100
## 1 0.4 0.01 0.95 1.00 0.6 150
## 1 0.4 0.01 0.95 1.00 0.8  50
## 1 0.4 0.01 0.95 1.00 0.8 100
## 1 0.4 0.01 0.95 1.00 0.8 150
## 1 0.4 0.50 0.05 0.50 0.6  50
## 1 0.4 0.50 0.05 0.50 0.6 100
## 1 0.4 0.50 0.05 0.50 0.6 150
## 1 0.4 0.50 0.05 0.50 0.8  50
## 1 0.4 0.50 0.05 0.50 0.8 100
## 1 0.4 0.50 0.05 0.50 0.8 150
## 1 0.4 0.50 0.05 0.75 0.6  50
## 1 0.4 0.50 0.05 0.75 0.6 100
## 1 0.4 0.50 0.05 0.75 0.6 150
## 1 0.4 0.50 0.05 0.75 0.8  50
```

```
##   1           0.4  0.50        0.05        0.75        0.8                 100
##   1           0.4  0.50        0.05        0.75        0.8                 150
##   1           0.4  0.50        0.05        1.00        0.6                  50
##   1           0.4  0.50        0.05        1.00        0.6                 100
##   1           0.4  0.50        0.05        1.00        0.6                 150
##   1           0.4  0.50        0.05        1.00        0.8                  50
##   1           0.4  0.50        0.05        1.00        0.8                 100
##   1           0.4  0.50        0.05        1.00        0.8                 150
##   1           0.4  0.50        0.95        0.50        0.6                  50
##   1           0.4  0.50        0.95        0.50        0.6                 100
##   1           0.4  0.50        0.95        0.50        0.6                 150
##   1           0.4  0.50        0.95        0.50        0.8                  50
##   1           0.4  0.50        0.95        0.50        0.8                 100
##   1           0.4  0.50        0.95        0.50        0.8                 150
##   1           0.4  0.50        0.95        0.75        0.6                  50
##   1           0.4  0.50        0.95        0.75        0.6                 100
##   1           0.4  0.50        0.95        0.75        0.6                 150
##   1           0.4  0.50        0.95        0.75        0.8                  50
##   1           0.4  0.50        0.95        0.75        0.8                 100
##   1           0.4  0.50        0.95        0.75        0.8                 150
##   1           0.4  0.50        0.95        1.00        0.6                  50
##   1           0.4  0.50        0.95        1.00        0.6                 100
##   1           0.4  0.50        0.95        1.00        0.6                 150
##   1           0.4  0.50        0.95        1.00        0.8                  50
##   1           0.4  0.50        0.95        1.00        0.8                 100
##   1           0.4  0.50        0.95        1.00        0.8                 150
##   2           0.3  0.01        0.05        0.50        0.6                  50
##   2           0.3  0.01        0.05        0.50        0.6                 100
##   2           0.3  0.01        0.05        0.50        0.6                 150
##   2           0.3  0.01        0.05        0.50        0.8                  50
##   2           0.3  0.01        0.05        0.50        0.8                 100
##   2           0.3  0.01        0.05        0.50        0.8                 150
##   2           0.3  0.01        0.05        0.75        0.6                  50
##   2           0.3  0.01        0.05        0.75        0.6                 100
##   2           0.3  0.01        0.05        0.75        0.6                 150
##   2           0.3  0.01        0.05        0.75        0.8                  50
##   2           0.3  0.01        0.05        0.75        0.8                 100
##   2           0.3  0.01        0.05        0.75        0.8                 150
##   2           0.3  0.01        0.05        1.00        0.6                  50
##   2           0.3  0.01        0.05        1.00        0.6                 100
##   2           0.3  0.01        0.05        1.00        0.6                 150
##   2           0.3  0.01        0.05        1.00        0.8                  50
##   2           0.3  0.01        0.05        1.00        0.8                 100
##   2           0.3  0.01        0.05        1.00        0.8                 150
##   2           0.3  0.01        0.95        0.50        0.6                  50
##   2           0.3  0.01        0.95        0.50        0.6                 100
##   2           0.3  0.01        0.95        0.50        0.6                 150
##   2           0.3  0.01        0.95        0.50        0.8                  50
##   2           0.3  0.01        0.95        0.50        0.8                 100
##   2           0.3  0.01        0.95        0.50        0.8                 150
##   2           0.3  0.01        0.95        0.75        0.6                  50
##   2           0.3  0.01        0.95        0.75        0.6                 100
##   2           0.3  0.01        0.95        0.75        0.6                 150
##   2           0.3  0.01        0.95        0.75        0.8                  50
```

```
##   2          0.3  0.01       0.95       0.75       0.8               100
##   2          0.3  0.01       0.95       0.75       0.8               150
##   2          0.3  0.01       0.95       1.00       0.6                50
##   2          0.3  0.01       0.95       1.00       0.6               100
##   2          0.3  0.01       0.95       1.00       0.6               150
##   2          0.3  0.01       0.95       1.00       0.8                50
##   2          0.3  0.01       0.95       1.00       0.8               100
##   2          0.3  0.01       0.95       1.00       0.8               150
##   2          0.3  0.50       0.05       0.50       0.6                50
##   2          0.3  0.50       0.05       0.50       0.6               100
##   2          0.3  0.50       0.05       0.50       0.6               150
##   2          0.3  0.50       0.05       0.50       0.8                50
##   2          0.3  0.50       0.05       0.50       0.8               100
##   2          0.3  0.50       0.05       0.50       0.8               150
##   2          0.3  0.50       0.05       0.75       0.6                50
##   2          0.3  0.50       0.05       0.75       0.6               100
##   2          0.3  0.50       0.05       0.75       0.6               150
##   2          0.3  0.50       0.05       0.75       0.8                50
##   2          0.3  0.50       0.05       0.75       0.8               100
##   2          0.3  0.50       0.05       0.75       0.8               150
##   2          0.3  0.50       0.05       1.00       0.6                50
##   2          0.3  0.50       0.05       1.00       0.6               100
##   2          0.3  0.50       0.05       1.00       0.6               150
##   2          0.3  0.50       0.05       1.00       0.8                50
##   2          0.3  0.50       0.05       1.00       0.8               100
##   2          0.3  0.50       0.05       1.00       0.8               150
##   2          0.3  0.50       0.95       0.50       0.6                50
##   2          0.3  0.50       0.95       0.50       0.6               100
##   2          0.3  0.50       0.95       0.50       0.6               150
##   2          0.3  0.50       0.95       0.50       0.8                50
##   2          0.3  0.50       0.95       0.50       0.8               100
##   2          0.3  0.50       0.95       0.50       0.8               150
##   2          0.3  0.50       0.95       0.75       0.6                50
##   2          0.3  0.50       0.95       0.75       0.6               100
##   2          0.3  0.50       0.95       0.75       0.6               150
##   2          0.3  0.50       0.95       0.75       0.8                50
##   2          0.3  0.50       0.95       0.75       0.8               100
##   2          0.3  0.50       0.95       0.75       0.8               150
##   2          0.3  0.50       0.95       1.00       0.6                50
##   2          0.3  0.50       0.95       1.00       0.6               100
##   2          0.3  0.50       0.95       1.00       0.6               150
##   2          0.3  0.50       0.95       1.00       0.8                50
##   2          0.3  0.50       0.95       1.00       0.8               100
##   2          0.3  0.50       0.95       1.00       0.8               150
##   2          0.4  0.01       0.05       0.50       0.6                50
##   2          0.4  0.01       0.05       0.50       0.6               100
##   2          0.4  0.01       0.05       0.50       0.6               150
##   2          0.4  0.01       0.05       0.50       0.8                50
##   2          0.4  0.01       0.05       0.50       0.8               100
##   2          0.4  0.01       0.05       0.50       0.8               150
##   2          0.4  0.01       0.05       0.75       0.6                50
##   2          0.4  0.01       0.05       0.75       0.6               100
##   2          0.4  0.01       0.05       0.75       0.6               150
##   2          0.4  0.01       0.05       0.75       0.8                50
```

```
##   2          0.4  0.01       0.05       0.75       0.8               100
##   2          0.4  0.01       0.05       0.75       0.8               150
##   2          0.4  0.01       0.05       1.00       0.6                50
##   2          0.4  0.01       0.05       1.00       0.6               100
##   2          0.4  0.01       0.05       1.00       0.6               150
##   2          0.4  0.01       0.05       1.00       0.8                50
##   2          0.4  0.01       0.05       1.00       0.8               100
##   2          0.4  0.01       0.05       1.00       0.8               150
##   2          0.4  0.01       0.95       0.50       0.6                50
##   2          0.4  0.01       0.95       0.50       0.6               100
##   2          0.4  0.01       0.95       0.50       0.6               150
##   2          0.4  0.01       0.95       0.50       0.8                50
##   2          0.4  0.01       0.95       0.50       0.8               100
##   2          0.4  0.01       0.95       0.50       0.8               150
##   2          0.4  0.01       0.95       0.75       0.6                50
##   2          0.4  0.01       0.95       0.75       0.6               100
##   2          0.4  0.01       0.95       0.75       0.6               150
##   2          0.4  0.01       0.95       0.75       0.8                50
##   2          0.4  0.01       0.95       0.75       0.8               100
##   2          0.4  0.01       0.95       0.75       0.8               150
##   2          0.4  0.01       0.95       1.00       0.6                50
##   2          0.4  0.01       0.95       1.00       0.6               100
##   2          0.4  0.01       0.95       1.00       0.6               150
##   2          0.4  0.01       0.95       1.00       0.8                50
##   2          0.4  0.01       0.95       1.00       0.8               100
##   2          0.4  0.01       0.95       1.00       0.8               150
##   2          0.4  0.50       0.05       0.50       0.6                50
##   2          0.4  0.50       0.05       0.50       0.6               100
##   2          0.4  0.50       0.05       0.50       0.6               150
##   2          0.4  0.50       0.05       0.50       0.8                50
##   2          0.4  0.50       0.05       0.50       0.8               100
##   2          0.4  0.50       0.05       0.50       0.8               150
##   2          0.4  0.50       0.05       0.75       0.6                50
##   2          0.4  0.50       0.05       0.75       0.6               100
##   2          0.4  0.50       0.05       0.75       0.6               150
##   2          0.4  0.50       0.05       0.75       0.8                50
##   2          0.4  0.50       0.05       0.75       0.8               100
##   2          0.4  0.50       0.05       0.75       0.8               150
##   2          0.4  0.50       0.05       1.00       0.6                50
##   2          0.4  0.50       0.05       1.00       0.6               100
##   2          0.4  0.50       0.05       1.00       0.6               150
##   2          0.4  0.50       0.05       1.00       0.8                50
##   2          0.4  0.50       0.05       1.00       0.8               100
##   2          0.4  0.50       0.05       1.00       0.8               150
##   2          0.4  0.50       0.95       0.50       0.6                50
##   2          0.4  0.50       0.95       0.50       0.6               100
##   2          0.4  0.50       0.95       0.50       0.6               150
##   2          0.4  0.50       0.95       0.50       0.8                50
##   2          0.4  0.50       0.95       0.50       0.8               100
##   2          0.4  0.50       0.95       0.50       0.8               150
##   2          0.4  0.50       0.95       0.75       0.6                50
##   2          0.4  0.50       0.95       0.75       0.6               100
##   2          0.4  0.50       0.95       0.75       0.6               150
##   2          0.4  0.50       0.95       0.75       0.8                50
```

```
##   2          0.4  0.50        0.95        0.75        0.8                100
##   2          0.4  0.50        0.95        0.75        0.8                150
##   2          0.4  0.50        0.95        1.00        0.6                 50
##   2          0.4  0.50        0.95        1.00        0.6                100
##   2          0.4  0.50        0.95        1.00        0.6                150
##   2          0.4  0.50        0.95        1.00        0.8                 50
##   2          0.4  0.50        0.95        1.00        0.8                100
##   2          0.4  0.50        0.95        1.00        0.8                150
##   3          0.3  0.01        0.05        0.50        0.6                 50
##   3          0.3  0.01        0.05        0.50        0.6                100
##   3          0.3  0.01        0.05        0.50        0.6                150
##   3          0.3  0.01        0.05        0.50        0.8                 50
##   3          0.3  0.01        0.05        0.50        0.8                100
##   3          0.3  0.01        0.05        0.50        0.8                150
##   3          0.3  0.01        0.05        0.75        0.6                 50
##   3          0.3  0.01        0.05        0.75        0.6                100
##   3          0.3  0.01        0.05        0.75        0.6                150
##   3          0.3  0.01        0.05        0.75        0.8                 50
##   3          0.3  0.01        0.05        0.75        0.8                100
##   3          0.3  0.01        0.05        0.75        0.8                150
##   3          0.3  0.01        0.05        1.00        0.6                 50
##   3          0.3  0.01        0.05        1.00        0.6                100
##   3          0.3  0.01        0.05        1.00        0.6                150
##   3          0.3  0.01        0.05        1.00        0.8                 50
##   3          0.3  0.01        0.05        1.00        0.8                100
##   3          0.3  0.01        0.05        1.00        0.8                150
##   3          0.3  0.01        0.95        0.50        0.6                 50
##   3          0.3  0.01        0.95        0.50        0.6                100
##   3          0.3  0.01        0.95        0.50        0.6                150
##   3          0.3  0.01        0.95        0.50        0.8                 50
##   3          0.3  0.01        0.95        0.50        0.8                100
##   3          0.3  0.01        0.95        0.50        0.8                150
##   3          0.3  0.01        0.95        0.75        0.6                 50
##   3          0.3  0.01        0.95        0.75        0.6                100
##   3          0.3  0.01        0.95        0.75        0.6                150
##   3          0.3  0.01        0.95        0.75        0.8                 50
##   3          0.3  0.01        0.95        0.75        0.8                100
##   3          0.3  0.01        0.95        0.75        0.8                150
##   3          0.3  0.01        0.95        1.00        0.6                 50
##   3          0.3  0.01        0.95        1.00        0.6                100
##   3          0.3  0.01        0.95        1.00        0.6                150
##   3          0.3  0.01        0.95        1.00        0.8                 50
##   3          0.3  0.01        0.95        1.00        0.8                100
##   3          0.3  0.01        0.95        1.00        0.8                150
##   3          0.3  0.50        0.05        0.50        0.6                 50
##   3          0.3  0.50        0.05        0.50        0.6                100
##   3          0.3  0.50        0.05        0.50        0.6                150
##   3          0.3  0.50        0.05        0.50        0.8                 50
##   3          0.3  0.50        0.05        0.50        0.8                100
##   3          0.3  0.50        0.05        0.50        0.8                150
##   3          0.3  0.50        0.05        0.75        0.6                 50
##   3          0.3  0.50        0.05        0.75        0.6                100
##   3          0.3  0.50        0.05        0.75        0.6                150
##   3          0.3  0.50        0.05        0.75        0.8                 50
```

```
##   3           0.3  0.50        0.05        0.75        0.8                 100
##   3           0.3  0.50        0.05        0.75        0.8                 150
##   3           0.3  0.50        0.05        1.00        0.6                  50
##   3           0.3  0.50        0.05        1.00        0.6                 100
##   3           0.3  0.50        0.05        1.00        0.6                 150
##   3           0.3  0.50        0.05        1.00        0.8                  50
##   3           0.3  0.50        0.05        1.00        0.8                 100
##   3           0.3  0.50        0.05        1.00        0.8                 150
##   3           0.3  0.50        0.95        0.50        0.6                  50
##   3           0.3  0.50        0.95        0.50        0.6                 100
##   3           0.3  0.50        0.95        0.50        0.6                 150
##   3           0.3  0.50        0.95        0.50        0.8                  50
##   3           0.3  0.50        0.95        0.50        0.8                 100
##   3           0.3  0.50        0.95        0.50        0.8                 150
##   3           0.3  0.50        0.95        0.75        0.6                  50
##   3           0.3  0.50        0.95        0.75        0.6                 100
##   3           0.3  0.50        0.95        0.75        0.6                 150
##   3           0.3  0.50        0.95        0.75        0.8                  50
##   3           0.3  0.50        0.95        0.75        0.8                 100
##   3           0.3  0.50        0.95        0.75        0.8                 150
##   3           0.3  0.50        0.95        1.00        0.6                  50
##   3           0.3  0.50        0.95        1.00        0.6                 100
##   3           0.3  0.50        0.95        1.00        0.6                 150
##   3           0.3  0.50        0.95        1.00        0.8                  50
##   3           0.3  0.50        0.95        1.00        0.8                 100
##   3           0.3  0.50        0.95        1.00        0.8                 150
##   3           0.4  0.01        0.05        0.50        0.6                  50
##   3           0.4  0.01        0.05        0.50        0.6                 100
##   3           0.4  0.01        0.05        0.50        0.6                 150
##   3           0.4  0.01        0.05        0.50        0.8                  50
##   3           0.4  0.01        0.05        0.50        0.8                 100
##   3           0.4  0.01        0.05        0.50        0.8                 150
##   3           0.4  0.01        0.05        0.75        0.6                  50
##   3           0.4  0.01        0.05        0.75        0.6                 100
##   3           0.4  0.01        0.05        0.75        0.6                 150
##   3           0.4  0.01        0.05        0.75        0.8                  50
##   3           0.4  0.01        0.05        0.75        0.8                 100
##   3           0.4  0.01        0.05        0.75        0.8                 150
##   3           0.4  0.01        0.05        1.00        0.6                  50
##   3           0.4  0.01        0.05        1.00        0.6                 100
##   3           0.4  0.01        0.05        1.00        0.6                 150
##   3           0.4  0.01        0.05        1.00        0.8                  50
##   3           0.4  0.01        0.05        1.00        0.8                 100
##   3           0.4  0.01        0.05        1.00        0.8                 150
##   3           0.4  0.01        0.95        0.50        0.6                  50
##   3           0.4  0.01        0.95        0.50        0.6                 100
##   3           0.4  0.01        0.95        0.50        0.6                 150
##   3           0.4  0.01        0.95        0.50        0.8                  50
##   3           0.4  0.01        0.95        0.50        0.8                 100
##   3           0.4  0.01        0.95        0.50        0.8                 150
##   3           0.4  0.01        0.95        0.75        0.6                  50
##   3           0.4  0.01        0.95        0.75        0.6                 100
##   3           0.4  0.01        0.95        0.75        0.6                 150
##   3           0.4  0.01        0.95        0.75        0.8                  50
```

```
##   3          0.4  0.01       0.95       0.75       0.8                 100
##   3          0.4  0.01       0.95       0.75       0.8                 150
##   3          0.4  0.01       0.95       1.00       0.6                  50
##   3          0.4  0.01       0.95       1.00       0.6                 100
##   3          0.4  0.01       0.95       1.00       0.6                 150
##   3          0.4  0.01       0.95       1.00       0.8                  50
##   3          0.4  0.01       0.95       1.00       0.8                 100
##   3          0.4  0.01       0.95       1.00       0.8                 150
##   3          0.4  0.50       0.05       0.50       0.6                  50
##   3          0.4  0.50       0.05       0.50       0.6                 100
##   3          0.4  0.50       0.05       0.50       0.6                 150
##   3          0.4  0.50       0.05       0.50       0.8                  50
##   3          0.4  0.50       0.05       0.50       0.8                 100
##   3          0.4  0.50       0.05       0.50       0.8                 150
##   3          0.4  0.50       0.05       0.75       0.6                  50
##   3          0.4  0.50       0.05       0.75       0.6                 100
##   3          0.4  0.50       0.05       0.75       0.6                 150
##   3          0.4  0.50       0.05       0.75       0.8                  50
##   3          0.4  0.50       0.05       0.75       0.8                 100
##   3          0.4  0.50       0.05       0.75       0.8                 150
##   3          0.4  0.50       0.05       1.00       0.6                  50
##   3          0.4  0.50       0.05       1.00       0.6                 100
##   3          0.4  0.50       0.05       1.00       0.6                 150
##   3          0.4  0.50       0.05       1.00       0.8                  50
##   3          0.4  0.50       0.05       1.00       0.8                 100
##   3          0.4  0.50       0.05       1.00       0.8                 150
##   3          0.4  0.50       0.95       0.50       0.6                  50
##   3          0.4  0.50       0.95       0.50       0.6                 100
##   3          0.4  0.50       0.95       0.50       0.6                 150
##   3          0.4  0.50       0.95       0.50       0.8                  50
##   3          0.4  0.50       0.95       0.50       0.8                 100
##   3          0.4  0.50       0.95       0.50       0.8                 150
##   3          0.4  0.50       0.95       0.75       0.6                  50
##   3          0.4  0.50       0.95       0.75       0.6                 100
##   3          0.4  0.50       0.95       0.75       0.6                 150
##   3          0.4  0.50       0.95       0.75       0.8                  50
##   3          0.4  0.50       0.95       0.75       0.8                 100
##   3          0.4  0.50       0.95       0.75       0.8                 150
##   3          0.4  0.50       0.95       1.00       0.6                  50
##   3          0.4  0.50       0.95       1.00       0.6                 100
##   3          0.4  0.50       0.95       1.00       0.6                 150
##   3          0.4  0.50       0.95       1.00       0.8                  50
##   3          0.4  0.50       0.95       1.00       0.8                 100
##   3          0.4  0.50       0.95       1.00       0.8                 150
##   Accuracy   Kappa
##   0.7497159  0.4983671
##   0.7442107  0.4873371
##   0.7575594  0.5135290
##   0.7473234  0.4918025
##   0.7426478  0.4828382
##   0.7403652  0.4784462
##   0.7528165  0.5045089
##   0.7520841  0.5027772
##   0.7614778  0.5217758
```

```
## 0.7457914 0.4898114
## 0.7551665 0.5086517
## 0.7481474 0.4939660
## 0.7442107 0.4869664
## 0.7442103 0.4862419
## 0.7450101 0.4883825
## 0.7458036 0.4898711
## 0.7465544 0.4915522
## 0.7442287 0.4867366
## 0.7614290 0.5205448
## 0.7599154 0.5179690
## 0.7544768 0.5078229
## 0.7536041 0.5056455
## 0.7481719 0.4946523
## 0.7598421 0.5177496
## 0.7465606 0.4918453
## 0.7583346 0.5151970
## 0.7504667 0.4984730
## 0.7411099 0.4806803
## 0.7370932 0.4722076
## 0.7449183 0.4868178
## 0.7520477 0.5026315
## 0.7450344 0.4881204
## 0.7450282 0.4879140
## 0.7520294 0.5026778
## 0.7504972 0.4992803
## 0.7465847 0.4913918
## 0.7340476 0.4661962
## 0.7340358 0.4662813
## 0.7363732 0.4705253
## 0.7184223 0.4356873
## 0.7277853 0.4536676
## 0.7316366 0.4616480
## 0.7340847 0.4667690
## 0.7332665 0.4651501
## 0.7340660 0.4665014
## 0.7184284 0.4370510
## 0.7278036 0.4549562
## 0.7261801 0.4515153
## 0.7230795 0.4447425
## 0.7301235 0.4587427
## 0.7269922 0.4531429
## 0.7129472 0.4256110
## 0.7145221 0.4283863
## 0.7207112 0.4402903
## 0.7465605 0.4922284
## 0.7473296 0.4925656
## 0.7559480 0.5101636
## 0.7504851 0.4998167
## 0.7512845 0.5008646
## 0.7481167 0.4939979
## 0.7418851 0.4821970
## 0.7450100 0.4881239
## 0.7512481 0.5001955
```

```
##   0.7426782  0.4835908
##   0.7465849  0.4908374
##   0.7481410  0.4942322
##   0.7496793  0.4982617
##   0.7527800  0.5040115
##   0.7457486  0.4898433
##   0.7489105  0.4960815
##   0.7489469  0.4963322
##   0.7418727  0.4817270
##   0.7465544  0.4913622
##   0.7402858  0.4790882
##   0.7527983  0.5036157
##   0.7505093  0.4986776
##   0.7488859  0.4957171
##   0.7481048  0.4946595
##   0.7528533  0.5042743
##   0.7575347  0.5135199
##   0.7575777  0.5141150
##   0.7473539  0.4928442
##   0.7418729  0.4817203
##   0.7434721  0.4858680
##   0.7457241  0.4891337
##   0.7465053  0.4910096
##   0.7473171  0.4930409
##   0.7395108  0.4774539
##   0.7348350  0.4683394
##   0.7371972  0.4730611
##   0.7575716  0.5137214
##   0.7558870  0.5103797
##   0.7488798  0.4956140
##   0.7512296  0.5002625
##   0.7528350  0.5034979
##   0.7396021  0.4784003
##   0.7528045  0.5037266
##   0.7496732  0.4978552
##   0.7551847  0.5091313
##   0.7434169  0.4847886
##   0.7458035  0.4897076
##   0.7591340  0.5170156
##   0.7418484  0.4823093
##   0.7387536  0.4757101
##   0.7442043  0.4867678
##   0.7528228  0.5043801
##   0.7434474  0.4855301
##   0.7403101  0.4788835
##   0.7372155  0.4722609
##   0.7426114  0.4831121
##   0.7418790  0.4815039
##   0.7254842  0.4511654
##   0.7379481  0.4745015
##   0.7465665  0.4919386
##   0.7293598  0.4582041
##   0.7347737  0.4683771
##   0.7379050  0.4749417
```

```
## 0.7333216 0.4658892
## 0.7285848 0.4557254
## 0.7324913 0.4647320
## 0.7301596 0.4590836
## 0.7309346 0.4606884
## 0.7324912 0.4630974
## 0.7199664 0.4393506
## 0.7176103 0.4340939
## 0.7301354 0.4583006
## 0.7481289 0.4940910
## 0.7544465 0.5069671
## 0.7489411 0.4959667
## 0.7441555 0.4858690
## 0.7464932 0.4911927
## 0.7481415 0.4943790
## 0.7481291 0.4948740
## 0.7449916 0.4869869
## 0.7543608 0.5063482
## 0.7559787 0.5106186
## 0.7536347 0.5057075
## 0.7442348 0.4861235
## 0.7457790 0.4906827
## 0.7434717 0.4854868
## 0.7465603 0.4914688
## 0.7457730 0.4906041
## 0.7450467 0.4886374
## 0.7411034 0.4804889
## 0.7552338 0.5082950
## 0.7685036 0.5357125
## 0.7606846 0.5204918
## 0.7434108 0.4857931
## 0.7685278 0.5354183
## 0.7646215 0.5278198
## 0.7520356 0.5019495
## 0.7559112 0.5096608
## 0.7622103 0.5232596
## 0.7575716 0.5141638
## 0.7512540 0.5017475
## 0.7645847 0.5282335
## 0.7512789 0.5008768
## 0.7544038 0.5075689
## 0.7567231 0.5120508
## 0.7536103 0.5051129
## 0.7535980 0.5049734
## 0.7590791 0.5163924
## 0.7598422 0.5182140
## 0.7677161 0.5341326
## 0.7629733 0.5242819
## 0.7504971 0.4988317
## 0.7567658 0.5113737
## 0.7614962 0.5215375
## 0.7598851 0.5186842
## 0.7606969 0.5196739
## 0.7739360 0.5463016
```

```
##    0.7700844  0.5391434
##    0.7739539  0.5469298
##    0.7770667  0.5530386
##    0.7559172  0.5098241
##    0.7614535  0.5213812
##    0.7778664  0.5544467
##    0.7481781  0.4955339
##    0.7590423  0.5166632
##    0.7707740  0.5399312
##    0.7457912  0.4898446
##    0.7527801  0.5041687
##    0.7512173  0.5014254
##    0.7434539  0.4852334
##    0.7457914  0.4898988
##    0.7465786  0.4916078
##    0.7379236  0.4742573
##    0.7395107  0.4771375
##    0.7481599  0.4946190
##    0.7418971  0.4820953
##    0.7466215  0.4915612
##    0.7474274  0.4935907
##    0.7465911  0.4924985
##    0.7481535  0.4958670
##    0.7512542  0.5023151
##    0.7340480  0.4669078
##    0.7387357  0.4764342
##    0.7356043  0.4701281
##    0.7512545  0.5006750
##    0.7434357  0.4847269
##    0.7552032  0.5087446
##    0.7536716  0.5063743
##    0.7622288  0.5227966
##    0.7606603  0.5193616
##    0.7512481  0.5006576
##    0.7520659  0.5018525
##    0.7669164  0.5315431
##    0.7575411  0.5141819
##    0.7708349  0.5405970
##    0.7700657  0.5385503
##    0.7520600  0.5024529
##    0.7583103  0.5155132
##    0.7622104  0.5228007
##    0.7489349  0.4959772
##    0.7700966  0.5394220
##    0.7747843  0.5483670
##    0.7449857  0.4872838
##    0.7497591  0.4976229
##    0.7646153  0.5270106
##    0.7637912  0.5258442
##    0.7653967  0.5292132
##    0.7700599  0.5382093
##    0.7630218  0.5240992
##    0.7786785  0.5560278
##    0.7794227  0.5577162
```

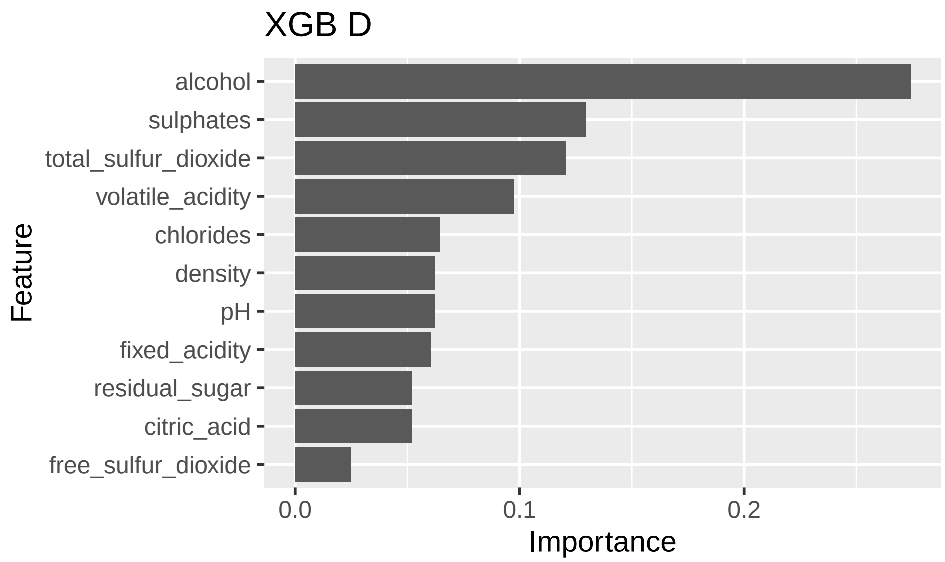
```
##   0.7536716  0.5056531
##   0.7559543  0.5097284
##   0.7661659  0.5303260
##   0.7450651  0.4885207
##   0.7513155  0.5013403
##   0.7661108  0.5308765
##   0.7489530  0.4959894
##   0.7535797  0.5055404
##   0.7567478  0.5118571
##   0.7536467  0.5060087
##   0.7637547  0.5267672
##   0.7629735  0.5240598
##   0.7333400  0.4653736
##   0.7590183  0.5160234
##   0.7551244  0.5079716
##   0.7513031  0.5019998
##   0.7661596  0.5309009
##   0.7622104  0.5227611
##   0.7543731  0.5070088
##   0.7684181  0.5356609
##   0.7731726  0.5448798
##   0.7551549  0.5082559
##   0.7669164  0.5319052
##   0.7739297  0.5456870
##   0.7567231  0.5120034
##   0.7716101  0.5415155
##   0.7739419  0.5459200
##   0.7512849  0.5012514
##   0.7488982  0.4960361
##   0.7504911  0.4996551
##   0.7457670  0.4899705
##   0.7481292  0.4943643
##   0.7434418  0.4844325
##   0.7356592  0.4698310
##   0.7411100  0.4814780
##   0.7488982  0.4963759
##   0.7434413  0.4852637
##   0.7442352  0.4870470
##   0.7348598  0.4682965
##   0.7418911  0.4814912
##   0.7410975  0.4804275
##   0.7457913  0.4905047
##   0.7356102  0.4702231
##   0.7364222  0.4720085
##   0.7426726  0.4840577
##   0.7551361  0.5090029
##   0.7606967  0.5199586
##   0.7661718  0.5312050
##   0.7504669  0.4988326
##   0.7496793  0.4977747
##   0.7637482  0.5248853
##   0.7497285  0.4980348
##   0.7528719  0.5051305
##   0.7630098  0.5245215
```

```
## 0.7505096 0.4993403
## 0.7599275 0.5184302
## 0.7606723 0.5196970
## 0.7512482 0.5003440
## 0.7661109 0.5305865
## 0.7629796 0.5247499
## 0.7590855 0.5163661
## 0.7707618 0.5399110
## 0.7778177 0.5542516
## 0.7582736 0.5143255
## 0.7661292 0.5301032
## 0.7739786 0.5458381
## 0.7661844 0.5314738
## 0.7662331 0.5304651
## 0.7708962 0.5403974
## 0.7763221 0.5508636
## 0.7817972 0.5626044
## 0.7848857 0.5686208
## 0.7770548 0.5529817
## 0.7802165 0.5587359
## 0.7911669 0.5807157
## 0.7708166 0.5404564
## 0.7801984 0.5589429
## 0.7856672 0.5693612
## 0.7677593 0.5344805
## 0.7755171 0.5494091
## 0.7746869 0.5477575
## 0.7653779 0.5291431
## 0.7755410 0.5488784
## 0.7849408 0.5677202
## 0.7685159 0.5365232
## 0.7802107 0.5591523
## 0.7848924 0.5686645
## 0.7669959 0.5331609
## 0.7723671 0.5431638
## 0.7731853 0.5443346
## 0.7684794 0.5354209
## 0.7731547 0.5437403
## 0.7872603 0.5723558
## 0.7692422 0.5374817
## 0.7832808 0.5645761
## 0.7966296 0.5913254
## 0.7693217 0.5378312
## 0.7865095 0.5719374
## 0.8013662 0.6013898
## 0.7441612 0.4871144
## 0.7536042 0.5057047
## 0.7622351 0.5233060
## 0.7535984 0.5062166
## 0.7598851 0.5189953
## 0.7543674 0.5073862
## 0.7552155 0.5093982
## 0.7567722 0.5126022
## 0.7528964 0.5044147
```

```
## 0.7450285 0.4888145
## 0.7528473 0.5041834
## 0.7544038 0.5072496
## 0.7489594 0.4966055
## 0.7528718 0.5050760
## 0.7489716 0.4969371
## 0.7465910 0.4922821
## 0.7489531 0.4971388
## 0.7473419 0.4937725
## 0.7654273 0.5289115
## 0.7896283 0.5777093
## 0.7801861 0.5579459
## 0.7559298 0.5094848
## 0.7629917 0.5237699
## 0.7700600 0.5374206
## 0.7708472 0.5407540
## 0.7716591 0.5423870
## 0.7841351 0.5664391
## 0.7544037 0.5078720
## 0.7802290 0.5593268
## 0.7895619 0.5767329
## 0.7637122 0.5257017
## 0.7793620 0.5573121
## 0.7848307 0.5679483
## 0.7739970 0.5474229
## 0.7935594 0.5862204
## 0.7934554 0.5854653
## 0.7606783 0.5203228
## 0.7567597 0.5125926
## 0.7708349 0.5401015
## 0.7685461 0.5356244
## 0.7692727 0.5370790
## 0.7777934 0.5540147
## 0.7676978 0.5339294
## 0.7872540 0.5731519
## 0.7770856 0.5522683
## 0.7614292 0.5216178
## 0.7802473 0.5590781
## 0.7935105 0.5855624
## 0.7769996 0.5527750
## 0.7840920 0.5668851
## 0.7918682 0.5819707
## 0.7653846 0.5291483
## 0.7849470 0.5688832
## 0.7856429 0.5699349
## 0.7700538 0.5380623
## 0.7693217 0.5366251
## 0.7779340 0.5546612
## 0.7645601 0.5278307
## 0.7825357 0.5640843
## 0.7887434 0.5756092
## 0.7748698 0.5480559
## 0.7888595 0.5754108
## 0.7880298 0.5732457
```

```
##   0.7801492  0.5590974
##   0.7950550  0.5878944
##   0.7871874  0.5720343
##   0.7786359  0.5556366
##   0.7919115  0.5822809
##   0.7918932  0.5823356
##   0.7661964  0.5322750
##   0.7825297  0.5640681
##   0.7778054  0.5541320
##   0.7520538  0.5022460
##   0.7583652  0.5154517
##   0.7598908  0.5186096
##   0.7512725  0.5018899
##   0.7504911  0.4986901
##   0.7528167  0.5029555
##   0.7426417  0.4838367
##   0.7551851  0.5091382
##   0.7575533  0.5141521
##   0.7465910  0.4915078
##   0.7481901  0.4951543
##   0.7481654  0.4944052
##   0.7340419  0.4666193
##   0.7473542  0.4939962
##   0.7528596  0.5046646
##   0.7489472  0.4966711
##   0.7520970  0.5034028
##   0.7544226  0.5082088
##   0.7558382  0.5097792
##   0.7613681  0.5207012
##   0.7731056  0.5443237
##   0.7512911  0.5009146
##   0.7739232  0.5464936
##   0.7856916  0.5699228
##   0.7754740  0.5494951
##   0.7872359  0.5722705
##   0.7840865  0.5662124
##   0.7661593  0.5314979
##   0.7809976  0.5604040
##   0.7833724  0.5650625
##   0.7770670  0.5533568
##   0.7864365  0.5718220
##   0.7817306  0.5619040
##   0.7802349  0.5591755
##   0.7841294  0.5665451
##   0.7856981  0.5697512
##
## Tuning parameter 'gamma' was held constant at a value of 0
## Tuning
##  parameter 'min_child_weight' was held constant at a value of 1
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were nrounds = 150, max_depth = 3, eta
##  = 0.3, gamma = 0, subsample = 1, colsample_bytree = 0.8, rate_drop =
##  0.01, skip_drop = 0.95 and min_child_weight = 1.
```

```r
p_xgbd <- varImp(wine_xgbd,scale = F) %>%
  ggplot() + ggtitle("XGB D")
p_xgbd
```




```r
# Evaluate

confusionMatrix(predict(wine_xgbd, test), test$quality)
```

```
## [23:49:02] WARNING: amalgamation/../src/c_api/c_api.cc:718: `ntree_limit` is deprecated, use `iterat

## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 118  27
##          1  31 145
##
##                Accuracy : 0.8193
##                  95% CI : (0.7728, 0.8598)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.6361
##
##  Mcnemar's Test P-Value : 0.6936
##
##             Sensitivity : 0.7919
##             Specificity : 0.8430
##          Pos Pred Value : 0.8138
##          Neg Pred Value : 0.8239
##              Prevalence : 0.4642
##          Detection Rate : 0.3676
##    Detection Prevalence : 0.4517
```

```
##       Balanced Accuracy : 0.8175
##
##        'Positive' Class : 0
##
```

```
xgbd_acc <- confusionMatrix(predict(wine_xgbd, test), test$quality)$overall["Accuracy"]
```

```
## [23:49:02] WARNING: amalgamation/../src/c_api/c_api.cc:718: `ntree_limit` is deprecated, use `iterat
```

```
xgbd_acc
```

```
##  Accuracy
## 0.8193146
```

4.1.8 xgbTree

```
### XGBoost: xgbTree----

set.seed(1, sample.kind="Rounding")

# train the model

wine_xgbt <- train(
  quality ~ .,
  data = train,
  method = "xgbTree",
  trControl = trControl,
  tuneLength = 5
)
```

```
# Check the model

wine_xgbt
```

```
## eXtreme Gradient Boosting
##
## 1278 samples
##   11 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1151, 1150, 1150, 1149, 1150, 1151, ...
## Resampling results across tuning parameters:
##
##   eta  max_depth  colsample_bytree  subsample  nrounds  Accuracy   Kappa
##   0.3  1          0.6               0.500       50      0.7496487  0.4979813
##   0.3  1          0.6               0.500      100      0.7449613  0.4873684
##   0.3  1          0.6               0.500      150      0.7465784  0.4910973
##   0.3  1          0.6               0.500      200      0.7434353  0.4853094
```

```
##   0.3  1          0.6                0.500      250      0.7497222  0.4974293
##   0.3  1          0.6                0.625       50      0.7505154  0.4991680
##   0.3  1          0.6                0.625      100      0.7497162  0.4976127
##   0.3  1          0.6                0.625      150      0.7583225  0.5151200
##   0.3  1          0.6                0.625      200      0.7528229  0.5034805
##   0.3  1          0.6                0.625      250      0.7489410  0.4966740
##   0.3  1          0.6                0.750       50      0.7449430  0.4889398
##   0.3  1          0.6                0.750      100      0.7496672  0.4979979
##   0.3  1          0.6                0.750      150      0.7441860  0.4865818
##   0.3  1          0.6                0.750      200      0.7489043  0.4965776
##   0.3  1          0.6                0.750      250      0.7481413  0.4943523
##   0.3  1          0.6                0.875       50      0.7379540  0.4736665
##   0.3  1          0.6                0.875      100      0.7426722  0.4830625
##   0.3  1          0.6                0.875      150      0.7466215  0.4909662
##   0.3  1          0.6                0.875      200      0.7481595  0.4939573
##   0.3  1          0.6                0.875      250      0.7442349  0.4861466
##   0.3  1          0.6                1.000       50      0.7520355  0.5029666
##   0.3  1          0.6                1.000      100      0.7497281  0.4978286
##   0.3  1          0.6                1.000      150      0.7465848  0.4917048
##   0.3  1          0.6                1.000      200      0.7481351  0.4945275
##   0.3  1          0.6                1.000      250      0.7473417  0.4930898
##   0.3  1          0.8                0.500       50      0.7520966  0.5029548
##   0.3  1          0.8                0.500      100      0.7496979  0.4979277
##   0.3  1          0.8                0.500      150      0.7458158  0.4899657
##   0.3  1          0.8                0.500      200      0.7513032  0.5012891
##   0.3  1          0.8                0.500      250      0.7473725  0.4932435
##   0.3  1          0.8                0.625       50      0.7425990  0.4829670
##   0.3  1          0.8                0.625      100      0.7488492  0.4951492
##   0.3  1          0.8                0.625      150      0.7504604  0.4986381
##   0.3  1          0.8                0.625      200      0.7403529  0.4791129
##   0.3  1          0.8                0.625      250      0.7481901  0.4948563
##   0.3  1          0.8                0.750       50      0.7449856  0.4885751
##   0.3  1          0.8                0.750      100      0.7465605  0.4912466
##   0.3  1          0.8                0.750      150      0.7513091  0.5012014
##   0.3  1          0.8                0.750      200      0.7482025  0.4953127
##   0.3  1          0.8                0.750      250      0.7536409  0.5061851
##   0.3  1          0.8                0.875       50      0.7520477  0.5024606
##   0.3  1          0.8                0.875      100      0.7488919  0.4961297
##   0.3  1          0.8                0.875      150      0.7543486  0.5066420
##   0.3  1          0.8                0.875      200      0.7559296  0.5101490
##   0.3  1          0.8                0.875      250      0.7551726  0.5085133
##   0.3  1          0.8                1.000       50      0.7512664  0.5011293
##   0.3  1          0.8                1.000      100      0.7465724  0.4914618
##   0.3  1          0.8                1.000      150      0.7442408  0.4865798
##   0.3  1          0.8                1.000      200      0.7434473  0.4849342
##   0.3  1          0.8                1.000      250      0.7465726  0.4913530
##   0.3  2          0.6                0.500       50      0.7622592  0.5234359
##   0.3  2          0.6                0.500      100      0.7699925  0.5392508
##   0.3  2          0.6                0.500      150      0.7442104  0.4872543
##   0.3  2          0.6                0.500      200      0.7488980  0.4964396
##   0.3  2          0.6                0.500      250      0.7550994  0.5086932
##   0.3  2          0.6                0.625       50      0.7629729  0.5240823
##   0.3  2          0.6                0.625      100      0.7699984  0.5380904
##   0.3  2          0.6                0.625      150      0.7621798  0.5219712
```

```
##    0.3  2          0.6           0.625    200     0.7786599  0.5554678
##    0.3  2          0.6           0.625    250     0.7778603  0.5535694
##    0.3  2          0.6           0.750     50     0.7410791  0.4806174
##    0.3  2          0.6           0.750    100     0.7629854  0.5246135
##    0.3  2          0.6           0.750    150     0.7684727  0.5353029
##    0.3  2          0.6           0.750    200     0.7653720  0.5295794
##    0.3  2          0.6           0.750    250     0.7754860  0.5497023
##    0.3  2          0.6           0.875     50     0.7645847  0.5271147
##    0.3  2          0.6           0.875    100     0.7638098  0.5259728
##    0.3  2          0.6           0.875    150     0.7802410  0.5588354
##    0.3  2          0.6           0.875    200     0.7818585  0.5622250
##    0.3  2          0.6           0.875    250     0.7896165  0.5771385
##    0.3  2          0.6           1.000     50     0.7497223  0.4978322
##    0.3  2          0.6           1.000    100     0.7629916  0.5246452
##    0.3  2          0.6           1.000    150     0.7716040  0.5419000
##    0.3  2          0.6           1.000    200     0.7770610  0.5523641
##    0.3  2          0.6           1.000    250     0.7738871  0.5458254
##    0.3  2          0.8           0.500     50     0.7575290  0.5135304
##    0.3  2          0.8           0.500    100     0.7574617  0.5130588
##    0.3  2          0.8           0.500    150     0.7621982  0.5229346
##    0.3  2          0.8           0.500    200     0.7637605  0.5257170
##    0.3  2          0.8           0.500    250     0.7614355  0.5212132
##    0.3  2          0.8           0.625     50     0.7536407  0.5050883
##    0.3  2          0.8           0.625    100     0.7614105  0.5208827
##    0.3  2          0.8           0.625    150     0.7676244  0.5334112
##    0.3  2          0.8           0.625    200     0.7700845  0.5387586
##    0.3  2          0.8           0.625    250     0.7856856  0.5691240
##    0.3  2          0.8           0.750     50     0.7598358  0.5184010
##    0.3  2          0.8           0.750    100     0.7575288  0.5141114
##    0.3  2          0.8           0.750    150     0.7660557  0.5302995
##    0.3  2          0.8           0.750    200     0.7582738  0.5147619
##    0.3  2          0.8           0.750    250     0.7613988  0.5209545
##    0.3  2          0.8           0.875     50     0.7669104  0.5324161
##    0.3  2          0.8           0.875    100     0.7739174  0.5467007
##    0.3  2          0.8           0.875    150     0.7723363  0.5428081
##    0.3  2          0.8           0.875    200     0.7708042  0.5397119
##    0.3  2          0.8           0.875    250     0.7746924  0.5473674
##    0.3  2          0.8           1.000     50     0.7505098  0.4997416
##    0.3  2          0.8           1.000    100     0.7622166  0.5233791
##    0.3  2          0.8           1.000    150     0.7691993  0.5366535
##    0.3  2          0.8           1.000    200     0.7723060  0.5426161
##    0.3  2          0.8           1.000    250     0.7723122  0.5425294
##    0.3  3          0.6           0.500     50     0.7622348  0.5227416
##    0.3  3          0.6           0.500    100     0.7692298  0.5362816
##    0.3  3          0.6           0.500    150     0.7770304  0.5523454
##    0.3  3          0.6           0.500    200     0.7801680  0.5580750
##    0.3  3          0.6           0.500    250     0.7833053  0.5648145
##    0.3  3          0.6           0.625     50     0.7598790  0.5189398
##    0.3  3          0.6           0.625    100     0.7786173  0.5561995
##    0.3  3          0.6           0.625    150     0.7864731  0.5712056
##    0.3  3          0.6           0.625    200     0.7872788  0.5725230
##    0.3  3          0.6           0.625    250     0.7817974  0.5615035
##    0.3  3          0.6           0.750     50     0.7755534  0.5502194
##    0.3  3          0.6           0.750    100     0.7896348  0.5778411
```

```
##   0.3  3          0.6             0.750      150      0.7934497  0.5851513
##   0.3  3          0.6             0.750      200      0.7919052  0.5818144
##   0.3  3          0.6             0.750      250      0.7911424  0.5804949
##   0.3  3          0.6             0.875       50      0.7739541  0.5472262
##   0.3  3          0.6             0.875      100      0.7879866  0.5743419
##   0.3  3          0.6             0.875      150      0.7895799  0.5775571
##   0.3  3          0.6             0.875      200      0.7809307  0.5599835
##   0.3  3          0.6             0.875      250      0.7785502  0.5549837
##   0.3  3          0.6             1.000       50      0.7707983  0.5398264
##   0.3  3          0.6             1.000      100      0.7763224  0.5512796
##   0.3  3          0.6             1.000      150      0.7887802  0.5759604
##   0.3  3          0.6             1.000      200      0.7935165  0.5856769
##   0.3  3          0.6             1.000      250      0.7888232  0.5760199
##   0.3  3          0.8             0.500       50      0.7622411  0.5227151
##   0.3  3          0.8             0.500      100      0.7731915  0.5442609
##   0.3  3          0.8             0.500      150      0.7786541  0.5551835
##   0.3  3          0.8             0.500      200      0.7880663  0.5743062
##   0.3  3          0.8             0.500      250      0.7755475  0.5491527
##   0.3  3          0.8             0.625       50      0.7567048  0.5114848
##   0.3  3          0.8             0.625      100      0.7645057  0.5272179
##   0.3  3          0.8             0.625      150      0.7832439  0.5639043
##   0.3  3          0.8             0.625      200      0.7848188  0.5671119
##   0.3  3          0.8             0.625      250      0.7800824  0.5579814
##   0.3  3          0.8             0.750       50      0.7614844  0.5224570
##   0.3  3          0.8             0.750      100      0.7888659  0.5771488
##   0.3  3          0.8             0.750      150      0.7872485  0.5729713
##   0.3  3          0.8             0.750      200      0.7841171  0.5661450
##   0.3  3          0.8             0.750      250      0.7872115  0.5725945
##   0.3  3          0.8             0.875       50      0.7732032  0.5451414
##   0.3  3          0.8             0.875      100      0.7880109  0.5746701
##   0.3  3          0.8             0.875      150      0.7872175  0.5723508
##   0.3  3          0.8             0.875      200      0.7919419  0.5820184
##   0.3  3          0.8             0.875      250      0.7911301  0.5804708
##   0.3  3          0.8             1.000       50      0.7615086  0.5214383
##   0.3  3          0.8             1.000      100      0.7715739  0.5407831
##   0.3  3          0.8             1.000      150      0.7887682  0.5754822
##   0.3  3          0.8             1.000      200      0.7840621  0.5658800
##   0.3  3          0.8             1.000      250      0.7840497  0.5660374
##   0.3  4          0.6             0.500       50      0.7700236  0.5385152
##   0.3  4          0.6             0.500      100      0.7902878  0.5784652
##   0.3  4          0.6             0.500      150      0.7957815  0.5893390
##   0.3  4          0.6             0.500      200      0.7879748  0.5732948
##   0.3  4          0.6             0.500      250      0.7879563  0.5735625
##   0.3  4          0.6             0.625       50      0.7802591  0.5587225
##   0.3  4          0.6             0.625      100      0.7857039  0.5697863
##   0.3  4          0.6             0.625      150      0.7817793  0.5618455
##   0.3  4          0.6             0.625      200      0.7918809  0.5820712
##   0.3  4          0.6             0.625      250      0.7848185  0.5682002
##   0.3  4          0.6             0.750       50      0.7856673  0.5694546
##   0.3  4          0.6             0.750      100      0.7927233  0.5833754
##   0.3  4          0.6             0.750      150      0.7888290  0.5760581
##   0.3  4          0.6             0.750      200      0.7919419  0.5822275
##   0.3  4          0.6             0.750      250      0.7919479  0.5822724
##   0.3  4          0.6             0.875       50      0.7833174  0.5651369
```

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##   0.3  4          0.6               0.875       100      0.7966236  0.5912135
##   0.3  4          0.6               0.875       150      0.7903734  0.5789977
##   0.3  4          0.6               0.875       200      0.7903977  0.5791135
##   0.3  4          0.6               0.875       250      0.7911971  0.5809806
##   0.3  4          0.6               1.000        50      0.7873399  0.5734610
##   0.3  4          0.6               1.000       100      0.7982229  0.5948509
##   0.3  4          0.6               1.000       150      0.7982351  0.5951877
##   0.3  4          0.6               1.000       200      0.8005421  0.5996593
##   0.3  4          0.6               1.000       250      0.7974476  0.5934838
##   0.3  4          0.8               0.500        50      0.7895979  0.5770846
##   0.3  4          0.8               0.500       100      0.7903793  0.5784700
##   0.3  4          0.8               0.500       150      0.7989489  0.5961828
##   0.3  4          0.8               0.500       200      0.7989735  0.5960480
##   0.3  4          0.8               0.500       250      0.7973862  0.5931361
##   0.3  4          0.8               0.625        50      0.7693028  0.5365449
##   0.3  4          0.8               0.625       100      0.7871750  0.5720375
##   0.3  4          0.8               0.625       150      0.7918931  0.5817755
##   0.3  4          0.8               0.625       200      0.7887434  0.5756207
##   0.3  4          0.8               0.625       250      0.7918747  0.5816409
##   0.3  4          0.8               0.750        50      0.7920027  0.5827138
##   0.3  4          0.8               0.750       100      0.7982959  0.5952875
##   0.3  4          0.8               0.750       150      0.7935534  0.5856912
##   0.3  4          0.8               0.750       200      0.7959156  0.5901755
##   0.3  4          0.8               0.750       250      0.7974293  0.5933849
##   0.3  4          0.8               0.875        50      0.7786357  0.5557589
##   0.3  4          0.8               0.875       100      0.7864058  0.5705646
##   0.3  4          0.8               0.875       150      0.7825175  0.5629837
##   0.3  4          0.8               0.875       200      0.7856733  0.5691224
##   0.3  4          0.8               0.875       250      0.7848981  0.5676694
##   0.3  4          0.8               1.000        50      0.7857040  0.5692326
##   0.3  4          0.8               1.000       100      0.7848799  0.5679847
##   0.3  4          0.8               1.000       150      0.7872234  0.5729158
##   0.3  4          0.8               1.000       200      0.7864119  0.5715685
##   0.3  4          0.8               1.000       250      0.7840680  0.5665247
##   0.3  5          0.6               0.500        50      0.7786298  0.5550211
##   0.3  5          0.6               0.500       100      0.7817488  0.5611171
##   0.3  5          0.6               0.500       150      0.7817490  0.5608772
##   0.3  5          0.6               0.500       200      0.7801679  0.5575508
##   0.3  5          0.6               0.500       250      0.7817978  0.5607806
##   0.3  5          0.6               0.625        50      0.7864364  0.5709254
##   0.3  5          0.6               0.625       100      0.8021110  0.6019869
##   0.3  5          0.6               0.625       150      0.8021046  0.6021478
##   0.3  5          0.6               0.625       200      0.7950793  0.5879980
##   0.3  5          0.6               0.625       250      0.7958482  0.5897298
##   0.3  5          0.6               0.750        50      0.7997670  0.5970532
##   0.3  5          0.6               0.750       100      0.8013175  0.6000909
##   0.3  5          0.6               0.750       150      0.7950613  0.5878309
##   0.3  5          0.6               0.750       200      0.7903737  0.5787964
##   0.3  5          0.6               0.750       250      0.7966362  0.5914354
##   0.3  5          0.6               0.875        50      0.7965930  0.5913410
##   0.3  5          0.6               0.875       100      0.7910933  0.5803737
##   0.3  5          0.6               0.875       150      0.7840008  0.5667238
##   0.3  5          0.6               0.875       200      0.7902878  0.5791474
##   0.3  5          0.6               0.875       250      0.7895185  0.5774600
```

```
##   0.3  5            0.6               1.000       50       0.7943777  0.5873877
##   0.3  5            0.6               1.000      100       0.7990223  0.5963210
##   0.3  5            0.6               1.000      150       0.7974355  0.5930620
##   0.3  5            0.6               1.000      200       0.7958363  0.5896841
##   0.3  5            0.6               1.000      250       0.7974110  0.5930618
##   0.3  5            0.8               0.500       50       0.7880783  0.5746859
##   0.3  5            0.8               0.500      100       0.7887988  0.5760596
##   0.3  5            0.8               0.500      150       0.7919178  0.5821667
##   0.3  5            0.8               0.500      200       0.7919362  0.5819467
##   0.3  5            0.8               0.500      250       0.7895495  0.5771379
##   0.3  5            0.8               0.625       50       0.7872114  0.5718813
##   0.3  5            0.8               0.625      100       0.7911118  0.5803600
##   0.3  5            0.8               0.625      150       0.7856487  0.5692072
##   0.3  5            0.8               0.625      200       0.7817180  0.5612785
##   0.3  5            0.8               0.625      250       0.7833112  0.5642046
##   0.3  5            0.8               0.750       50       0.7989124  0.5961500
##   0.3  5            0.8               0.750      100       0.7973744  0.5928058
##   0.3  5            0.8               0.750      150       0.7965871  0.5914180
##   0.3  5            0.8               0.750      200       0.7942676  0.5864553
##   0.3  5            0.8               0.750      250       0.7911487  0.5805282
##   0.3  5            0.8               0.875       50       0.7903121  0.5784018
##   0.3  5            0.8               0.875      100       0.8067679  0.6114529
##   0.3  5            0.8               0.875      150       0.8036062  0.6056872
##   0.3  5            0.8               0.875      200       0.8012684  0.6007662
##   0.3  5            0.8               0.875      250       0.8036245  0.6056663
##   0.3  5            0.8               1.000       50       0.8037041  0.6059577
##   0.3  5            0.8               1.000      100       0.8036489  0.6057016
##   0.3  5            0.8               1.000      150       0.8005115  0.5993210
##   0.3  5            0.8               1.000      200       0.8021108  0.6024151
##   0.3  5            0.8               1.000      250       0.8044364  0.6069584
##   0.4  1            0.6               0.500       50       0.7544035  0.5071352
##   0.4  1            0.6               0.500      100       0.7505402  0.4995513
##   0.4  1            0.6               0.500      150       0.7520113  0.5021209
##   0.4  1            0.6               0.500      200       0.7450039  0.4881901
##   0.4  1            0.6               0.500      250       0.7504545  0.4994772
##   0.4  1            0.6               0.625       50       0.7387353  0.4749176
##   0.4  1            0.6               0.625      100       0.7441798  0.4865656
##   0.4  1            0.6               0.625      150       0.7371971  0.4722709
##   0.4  1            0.6               0.625      200       0.7497465  0.4979282
##   0.4  1            0.6               0.625      250       0.7481599  0.4940845
##   0.4  1            0.6               0.750       50       0.7473235  0.4922806
##   0.4  1            0.6               0.750      100       0.7504607  0.4989944
##   0.4  1            0.6               0.750      150       0.7535982  0.5054597
##   0.4  1            0.6               0.750      200       0.7582860  0.5147886
##   0.4  1            0.6               0.750      250       0.7567662  0.5124845
##   0.4  1            0.6               0.875       50       0.7496794  0.4973059
##   0.4  1            0.6               0.875      100       0.7520477  0.5022188
##   0.4  1            0.6               0.875      150       0.7544220  0.5078791
##   0.4  1            0.6               0.875      200       0.7552031  0.5089141
##   0.4  1            0.6               0.875      250       0.7543912  0.5073940
##   0.4  1            0.6               1.000       50       0.7497037  0.4982648
##   0.4  1            0.6               1.000      100       0.7489652  0.4969808
##   0.4  1            0.6               1.000      150       0.7473904  0.4931745
##   0.4  1            0.6               1.000      200       0.7489225  0.4962205
```

```
##   0.4  1          0.6           1.000     250      0.7450037  0.4886313
##   0.4  1          0.8           0.500      50      0.7434779  0.4848276
##   0.4  1          0.8           0.500     100      0.7481961  0.4945737
##   0.4  1          0.8           0.500     150      0.7606296  0.5192571
##   0.4  1          0.8           0.500     200      0.7606786  0.5199217
##   0.4  1          0.8           0.500     250      0.7528111  0.5033873
##   0.4  1          0.8           0.625      50      0.7481780  0.4956870
##   0.4  1          0.8           0.625     100      0.7473843  0.4932674
##   0.4  1          0.8           0.625     150      0.7419339  0.4823654
##   0.4  1          0.8           0.625     200      0.7395841  0.4779688
##   0.4  1          0.8           0.625     250      0.7372524  0.4741210
##   0.4  1          0.8           0.750      50      0.7536102  0.5058429
##   0.4  1          0.8           0.750     100      0.7520479  0.5022340
##   0.4  1          0.8           0.750     150      0.7536286  0.5061993
##   0.4  1          0.8           0.750     200      0.7496978  0.4977901
##   0.4  1          0.8           0.750     250      0.7497526  0.4981361
##   0.4  1          0.8           0.875      50      0.7457486  0.4901998
##   0.4  1          0.8           0.875     100      0.7426724  0.4836051
##   0.4  1          0.8           0.875     150      0.7442351  0.4864002
##   0.4  1          0.8           0.875     200      0.7387660  0.4759706
##   0.4  1          0.8           0.875     250      0.7521028  0.5029076
##   0.4  1          0.8           1.000      50      0.7457791  0.4905375
##   0.4  1          0.8           1.000     100      0.7442408  0.4873412
##   0.4  1          0.8           1.000     150      0.7442530  0.4872146
##   0.4  1          0.8           1.000     200      0.7395165  0.4773847
##   0.4  1          0.8           1.000     250      0.7426724  0.4840272
##   0.4  2          0.6           0.500      50      0.7465725  0.4912467
##   0.4  2          0.6           0.500     100      0.7551666  0.5073021
##   0.4  2          0.6           0.500     150      0.7676369  0.5334014
##   0.4  2          0.6           0.500     200      0.7770733  0.5519552
##   0.4  2          0.6           0.500     250      0.7708595  0.5399003
##   0.4  2          0.6           0.625      50      0.7700111  0.5378942
##   0.4  2          0.6           0.625     100      0.7622475  0.5221865
##   0.4  2          0.6           0.625     150      0.7699930  0.5376726
##   0.4  2          0.6           0.625     200      0.7583105  0.5145056
##   0.4  2          0.6           0.625     250      0.7574803  0.5119854
##   0.4  2          0.6           0.750      50      0.7621554  0.5228829
##   0.4  2          0.6           0.750     100      0.7614475  0.5210616
##   0.4  2          0.6           0.750     150      0.7716103  0.5415674
##   0.4  2          0.6           0.750     200      0.7739357  0.5464037
##   0.4  2          0.6           0.750     250      0.7770854  0.5524646
##   0.4  2          0.6           0.875      50      0.7465665  0.4917192
##   0.4  2          0.6           0.875     100      0.7731910  0.5450811
##   0.4  2          0.6           0.875     150      0.7692845  0.5366366
##   0.4  2          0.6           0.875     200      0.7747352  0.5478288
##   0.4  2          0.6           0.875     250      0.7708288  0.5395609
##   0.4  2          0.6           1.000      50      0.7544219  0.5073866
##   0.4  2          0.6           1.000     100      0.7739173  0.5461292
##   0.4  2          0.6           1.000     150      0.7700294  0.5383173
##   0.4  2          0.6           1.000     200      0.7652745  0.5286024
##   0.4  2          0.6           1.000     250      0.7621553  0.5218868
##   0.4  2          0.8           0.500      50      0.7582488  0.5152597
##   0.4  2          0.8           0.500     100      0.7536161  0.5058953
##   0.4  2          0.8           0.500     150      0.7630590  0.5241268
```

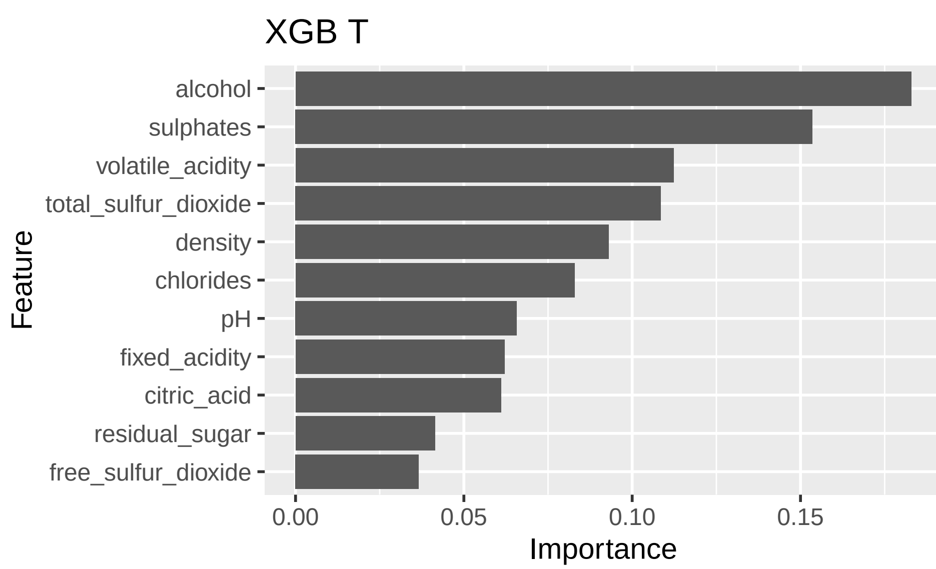
```
##   0.4  2          0.8              0.500     200        0.7591159  0.5163147
##   0.4  2          0.8              0.500     250        0.7622720  0.5225858
##   0.4  2          0.8              0.625      50        0.7497098  0.4978863
##   0.4  2          0.8              0.625     100        0.7676914  0.5340577
##   0.4  2          0.8              0.625     150        0.7630406  0.5246388
##   0.4  2          0.8              0.625     200        0.7684667  0.5355369
##   0.4  2          0.8              0.625     250        0.7692784  0.5370459
##   0.4  2          0.8              0.750      50        0.7567477  0.5110766
##   0.4  2          0.8              0.750     100        0.7692299  0.5368833
##   0.4  2          0.8              0.750     150        0.7684670  0.5347091
##   0.4  2          0.8              0.750     200        0.7692359  0.5354977
##   0.4  2          0.8              0.750     250        0.7692116  0.5357602
##   0.4  2          0.8              0.875      50        0.7473480  0.4926257
##   0.4  2          0.8              0.875     100        0.7637667  0.5265237
##   0.4  2          0.8              0.875     150        0.7762308  0.5505359
##   0.4  2          0.8              0.875     200        0.7785930  0.5554309
##   0.4  2          0.8              0.875     250        0.7864243  0.5710801
##   0.4  2          0.8              1.000      50        0.7410914  0.4800247
##   0.4  2          0.8              1.000     100        0.7653297  0.5293098
##   0.4  2          0.8              1.000     150        0.7754985  0.5497422
##   0.4  2          0.8              1.000     200        0.7707986  0.5401593
##   0.4  2          0.8              1.000     250        0.7684362  0.5352763
##   0.4  3          0.6              0.500      50        0.7591218  0.5161441
##   0.4  3          0.6              0.500     100        0.7597811  0.5183969
##   0.4  3          0.6              0.500     150        0.7637184  0.5254795
##   0.4  3          0.6              0.500     200        0.7792953  0.5563617
##   0.4  3          0.6              0.500     250        0.7770002  0.5518933
##   0.4  3          0.6              0.625      50        0.7653725  0.5293958
##   0.4  3          0.6              0.625     100        0.7801803  0.5583352
##   0.4  3          0.6              0.625     150        0.7825671  0.5630908
##   0.4  3          0.6              0.625     200        0.7887990  0.5759191
##   0.4  3          0.6              0.625     250        0.7856616  0.5691764
##   0.4  3          0.6              0.750      50        0.7716467  0.5415899
##   0.4  3          0.6              0.750     100        0.7887678  0.5752194
##   0.4  3          0.6              0.750     150        0.7919602  0.5817174
##   0.4  3          0.6              0.750     200        0.7888108  0.5755013
##   0.4  3          0.6              0.750     250        0.7848677  0.5679389
##   0.4  3          0.6              0.875      50        0.7880597  0.5754887
##   0.4  3          0.6              0.875     100        0.7981737  0.5944221
##   0.4  3          0.6              0.875     150        0.7973437  0.5926874
##   0.4  3          0.6              0.875     200        0.8091423  0.6161452
##   0.4  3          0.6              0.875     250        0.8091300  0.6163746
##   0.4  3          0.6              1.000      50        0.7731604  0.5453262
##   0.4  3          0.6              1.000     100        0.7793865  0.5573107
##   0.4  3          0.6              1.000     150        0.7848555  0.5677303
##   0.4  3          0.6              1.000     200        0.7871931  0.5729692
##   0.4  3          0.6              1.000     250        0.7864302  0.5715116
##   0.4  3          0.8              0.500      50        0.7598483  0.5177128
##   0.4  3          0.8              0.500     100        0.7802101  0.5595100
##   0.4  3          0.8              0.500     150        0.7856976  0.5698723
##   0.4  3          0.8              0.500     200        0.7903548  0.5794422
##   0.4  3          0.8              0.500     250        0.7833111  0.5648440
##   0.4  3          0.8              0.625      50        0.7770611  0.5523875
##   0.4  3          0.8              0.625     100        0.7801374  0.5585931
```

```
##   0.4  3          0.8             0.625      150      0.7808882  0.5603335
##   0.4  3          0.8             0.625      200      0.7824507  0.5631224
##   0.4  3          0.8             0.625      250      0.7934253  0.5852960
##   0.4  3          0.8             0.750       50      0.7614598  0.5214419
##   0.4  3          0.8             0.750      100      0.7715739  0.5405223
##   0.4  3          0.8             0.750      150      0.7793501  0.5561831
##   0.4  3          0.8             0.750      200      0.7824935  0.5626371
##   0.4  3          0.8             0.750      250      0.7817245  0.5613200
##   0.4  3          0.8             0.875       50      0.7638340  0.5262589
##   0.4  3          0.8             0.875      100      0.7786355  0.5555425
##   0.4  3          0.8             0.875      150      0.7817241  0.5620034
##   0.4  3          0.8             0.875      200      0.7746866  0.5477905
##   0.4  3          0.8             0.875      250      0.7770243  0.5526511
##   0.4  3          0.8             1.000       50      0.7699989  0.5388049
##   0.4  3          0.8             1.000      100      0.7817427  0.5614696
##   0.4  3          0.8             1.000      150      0.7793927  0.5566184
##   0.4  3          0.8             1.000      200      0.7770428  0.5517042
##   0.4  3          0.8             1.000      250      0.7832928  0.5645620
##   0.4  4          0.6             0.500       50      0.7724219  0.5436088
##   0.4  4          0.6             0.500      100      0.7755411  0.5499737
##   0.4  4          0.6             0.500      150      0.7833294  0.5659513
##   0.4  4          0.6             0.500      200      0.7849105  0.5687607
##   0.4  4          0.6             0.500      250      0.7919725  0.5830506
##   0.4  4          0.6             0.625       50      0.7888168  0.5762247
##   0.4  4          0.6             0.625      100      0.7895614  0.5774059
##   0.4  4          0.6             0.625      150      0.7770365  0.5527530
##   0.4  4          0.6             0.625      200      0.7707557  0.5403766
##   0.4  4          0.6             0.625      250      0.7770060  0.5522986
##   0.4  4          0.6             0.750       50      0.7958543  0.5899334
##   0.4  4          0.6             0.750      100      0.7934677  0.5848521
##   0.4  4          0.6             0.750      150      0.7903425  0.5782535
##   0.4  4          0.6             0.750      200      0.7958053  0.5894562
##   0.4  4          0.6             0.750      250      0.7973496  0.5923393
##   0.4  4          0.6             0.875       50      0.7863632  0.5710464
##   0.4  4          0.6             0.875      100      0.7949511  0.5880819
##   0.4  4          0.6             0.875      150      0.7934373  0.5851609
##   0.4  4          0.6             0.875      200      0.7911057  0.5807260
##   0.4  4          0.6             0.875      250      0.7871870  0.5726445
##   0.4  4          0.6             1.000       50      0.7911913  0.5803608
##   0.4  4          0.6             1.000      100      0.7864364  0.5705533
##   0.4  4          0.6             1.000      150      0.7864606  0.5706509
##   0.4  4          0.6             1.000      200      0.7895920  0.5776188
##   0.4  4          0.6             1.000      250      0.7927171  0.5838385
##   0.4  4          0.8             0.500       50      0.7935777  0.5859454
##   0.4  4          0.8             0.500      100      0.7966905  0.5915286
##   0.4  4          0.8             0.500      150      0.7958604  0.5897004
##   0.4  4          0.8             0.500      200      0.7973619  0.5930356
##   0.4  4          0.8             0.500      250      0.7895614  0.5775327
##   0.4  4          0.8             0.625       50      0.7865400  0.5711051
##   0.4  4          0.8             0.625      100      0.7801614  0.5577822
##   0.4  4          0.8             0.625      150      0.7817790  0.5618127
##   0.4  4          0.8             0.625      200      0.7786540  0.5554546
##   0.4  4          0.8             0.625      250      0.7771037  0.5526345
##   0.4  4          0.8             0.750       50      0.7824933  0.5628723
```

```
##   0.4  4          0.8              0.750      100      0.7762800  0.5505003
##   0.4  4          0.8              0.750      150      0.7848984  0.5677250
##   0.4  4          0.8              0.750      200      0.7895860  0.5772952
##   0.4  4          0.8              0.750      250      0.7840988  0.5663714
##   0.4  4          0.8              0.875       50      0.7887497  0.5759867
##   0.4  4          0.8              0.875      100      0.7856550  0.5694797
##   0.4  4          0.8              0.875      150      0.7848555  0.5679448
##   0.4  4          0.8              0.875      200      0.7926867  0.5840442
##   0.4  4          0.8              0.875      250      0.7934680  0.5856940
##   0.4  4          0.8              1.000       50      0.7801618  0.5585827
##   0.4  4          0.8              1.000      100      0.7918749  0.5816219
##   0.4  4          0.8              1.000      150      0.7895494  0.5770301
##   0.4  4          0.8              1.000      200      0.7895309  0.5770918
##   0.4  4          0.8              1.000      250      0.7934923  0.5849133
##   0.4  5          0.6              0.500       50      0.7723858  0.5432220
##   0.4  5          0.6              0.500      100      0.7856673  0.5684486
##   0.4  5          0.6              0.500      150      0.7739543  0.5451944
##   0.4  5          0.6              0.500      200      0.7755048  0.5478901
##   0.4  5          0.6              0.500      250      0.7786666  0.5548965
##   0.4  5          0.6              0.625       50      0.7982106  0.5940758
##   0.4  5          0.6              0.625      100      0.7974479  0.5925025
##   0.4  5          0.6              0.625      150      0.7903856  0.5785752
##   0.4  5          0.6              0.625      200      0.7911670  0.5802035
##   0.4  5          0.6              0.625      250      0.7864916  0.5712987
##   0.4  5          0.6              0.750       50      0.7880478  0.5741964
##   0.4  5          0.6              0.750      100      0.7942616  0.5870650
##   0.4  5          0.6              0.750      150      0.7864363  0.5716711
##   0.4  5          0.6              0.750      200      0.7926989  0.5841424
##   0.4  5          0.6              0.750      250      0.7903428  0.5792474
##   0.4  5          0.6              0.875       50      0.7888472  0.5754737
##   0.4  5          0.6              0.875      100      0.7865220  0.5710718
##   0.4  5          0.6              0.875      150      0.7919911  0.5821772
##   0.4  5          0.6              0.875      200      0.7911793  0.5805115
##   0.4  5          0.6              0.875      250      0.7896228  0.5774629
##   0.4  5          0.6              1.000       50      0.8044487  0.6069289
##   0.4  5          0.6              1.000      100      0.7966174  0.5910181
##   0.4  5          0.6              1.000      150      0.8013051  0.6006953
##   0.4  5          0.6              1.000      200      0.7989430  0.5953441
##   0.4  5          0.6              1.000      250      0.7981740  0.5941187
##   0.4  5          0.8              0.500       50      0.7856732  0.5696933
##   0.4  5          0.8              0.500      100      0.7895738  0.5772457
##   0.4  5          0.8              0.500      150      0.7864181  0.5706418
##   0.4  5          0.8              0.500      200      0.7887987  0.5754746
##   0.4  5          0.8              0.500      250      0.7958362  0.5896496
##   0.4  5          0.8              0.625       50      0.7949328  0.5874869
##   0.4  5          0.8              0.625      100      0.7941945  0.5860809
##   0.4  5          0.8              0.625      150      0.7887193  0.5752835
##   0.4  5          0.8              0.625      200      0.7926685  0.5830595
##   0.4  5          0.8              0.625      250      0.7903124  0.5784105
##   0.4  5          0.8              0.750       50      0.7934558  0.5846526
##   0.4  5          0.8              0.750      100      0.7997119  0.5973215
##   0.4  5          0.8              0.750      150      0.8075431  0.6134020
##   0.4  5          0.8              0.750      200      0.8044300  0.6071978
##   0.4  5          0.8              0.750      250      0.8028674  0.6041606
```

```
##   0.4  5          0.8                0.875       50      0.7919233  0.5816062
##   0.4  5          0.8                0.875      100      0.7919540  0.5814025
##   0.4  5          0.8                0.875      150      0.7903671  0.5785885
##   0.4  5          0.8                0.875      200      0.7919541  0.5823326
##   0.4  5          0.8                0.875      250      0.7943103  0.5869851
##   0.4  5          0.8                1.000       50      0.7981737  0.5945265
##   0.4  5          0.8                1.000      100      0.7958300  0.5894348
##   0.4  5          0.8                1.000      150      0.7958179  0.5896373
##   0.4  5          0.8                1.000      200      0.7942920  0.5864927
##   0.4  5          0.8                1.000      250      0.7927172  0.5834134
##
## Tuning parameter 'gamma' was held constant at a value of 0
## Tuning
##  parameter 'min_child_weight' was held constant at a value of 1
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were nrounds = 200, max_depth = 3, eta
##  = 0.4, gamma = 0, colsample_bytree = 0.6, min_child_weight = 1 and subsample
##  = 0.875.
```

```r
p_xgbt <- varImp(wine_xgbt,scale = F) %>%
  ggplot() + ggtitle("XGB T")
p_xgbt
```




```r
# Evaluate

confusionMatrix(predict(wine_xgbt, test), test$quality)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 115  25
##          1  34 147
##
```

```
##                Accuracy : 0.8162
##                  95% CI : (0.7694, 0.857)
##     No Information Rate : 0.5358
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.629
##
##  Mcnemar's Test P-Value : 0.2976
##
##             Sensitivity : 0.7718
##             Specificity : 0.8547
##          Pos Pred Value : 0.8214
##          Neg Pred Value : 0.8122
##              Prevalence : 0.4642
##          Detection Rate : 0.3583
##    Detection Prevalence : 0.4361
##       Balanced Accuracy : 0.8132
##
##        'Positive' Class : 0
##
```

```r
xgbt_acc <- confusionMatrix(predict(wine_xgbt, test), test$quality)$overall["Accuracy"]
xgbt_acc
```

```
##  Accuracy
## 0.8161994
```

4.1.9 torch

```r
### Torch / Deep Learning -----

# Change the type from factor to numeric for DNN
train_torch <-
  train %>% mutate(
    quality = as.numeric(quality) - 1
    )

test_torch <-
  test %>% mutate(
    quality = as.numeric(quality) - 1
  )

# check the quality

table(train$quality,train_torch$quality) %>% kable()
```

	0	1
0	595	0
1	0	683

```r
# Create {torch} dataset

df_dataset <- dataset(

  "wine",

  initialize = function(df, response_variable) {
    self$df <- df[,-which(names(df) == response_variable)]
    self$response_variable <- df[[response_variable]]
  },

  .getitem = function(index) {
    response <- torch_tensor(self$response_variable[index])
    x <- torch_tensor(as.numeric(self$df[index,]))

    list(x = x, y = response)
  },

  .length = function() {
    length(self$response_variable)
  }

)

# Create the data set train and test

train_torch_ds <- df_dataset(train_torch, "quality")
test_torch_ds <- df_dataset(test_torch, "quality")

# Create the data loader train and test

train_torch_dl <- dataloader(train_torch_ds, batch_size = 32, shuffle = T)
test_torch_dl <- dataloader(test_torch_ds, batch_size = 1, shuffle = F)

# Define a network / fc1 - 3 and dropout

net <- nn_module(

  "wine_DNN",

  initialize = function() {
    self$fc1 <- nn_linear(11, 66)
    self$fc2 <- nn_linear(66, 44)
    self$fc3 <- nn_linear(44, 1)
    self$dropout <- nn_dropout(0.5)
  },

  forward = function(x) {
    x %>%
      self$fc1() %>%
      nnf_relu() %>%
      self$fc2() %>%
      nnf_relu() %>%
```

```r
      self$dropout() %>%
      self$fc3() %>%
      nnf_sigmoid()
  }
)

# Use CPU version

model <- net()
model$to(device = "cpu")

# Set the optimizer condition

optimizer <- optim_adam(model$parameters,lr = 0.01)
```

```r
# Run a learning iteration

coro::loop(for (epoch in 1:20) {

  l <- c()

  coro::loop(for (b in enumerate(train_torch_dl)) {
    optimizer$zero_grad()
    output <- model(b[[1]]$to(device = "cpu"))
    loss <- nnf_binary_cross_entropy_with_logits(output, b[[2]]$to(device = "cpu"))
    loss$backward()
    optimizer$step()
    l <- c(l, loss$item())
  })

  cat(sprintf("Loss at epoch %d: %3f\n", epoch, mean(l)))
})

# Model prediction

model$eval()

i <- 1
pred_labels <- rep(0, nrow(test_torch))

coro::loop(for (b in enumerate(test_torch_dl)) {
  output <- model(b[[1]]$to(device = "cpu"))
  pred_labels[i] <- round(output$item(), 0)
  i <- i + 1
})
```

```r
# Evaluate

table(test=test_torch$quality, pred_labels)
```

```
##     pred_labels
## test   0   1
##    0 125  24
```

```
##    1  74  98
```

```
torch_acc <- sum(diag(table(test_torch$quality, pred_labels))) / nrow(test_torch)
torch_acc
```

```
## [1] 0.694704
```

4.1.10 Tabnet

```
### Tabnet -----

# splits the data (set vfold to 4 because it takes time)

splits <-
  vfold_cv(train, v = 4, strata = "quality") %>%
  with_seed(1, .)

# Create rule "classification"

rule <- tabnet(
  epochs = tune(),
  penalty = tune(),
  batch_size = tune(),
  decision_width = tune(),
  attention_width =tune(),
  num_steps = tune(),
  learn_rate = 0.08,
  momentum = 0.6) %>%
  set_engine("torch", verbose = TRUE) %>%
  set_mode("classification")

# making a recipe

rec <- recipe(quality ~ ., data = train) %>%
  step_nzv(all_predictors())

# making a work flow

wf <- workflow() %>%
  add_model(rule) %>%
  add_recipe(rec)

# range of hyper parameter

range_hypara <-
  wf %>%
  parameters() %>%
  update(
    epochs = epochs(c(50, 70)),
    decision_width = decision_width(range = c(20, 40)),
    attention_width = attention_width(range = c(20, 40)),
    num_steps = num_steps(range = c(4, 8))
```

```
  ) %>%
  finalize(train)

# making a grid

grid <- range_hypara %>%
  grid_latin_hypercube(size = 1) %>%
  with_seed(1, .)
```

```
# tuning of hyper parameters (long time)

tune <-
  wf %>%
  tune_grid(
    resamples = splits,
    grid = grid,
    control = control_grid(save_pred = TRUE),
    metrics = metric_set(accuracy)
  )

# select the best hyper parameters

good_hypara <-
  tune %>%
  show_best() %>%
  dplyr::slice(1)

# update the rule with best parameters

upd_rule <-
  tabnet(
    epochs = good_hypara %>% pull(epochs),
    penalty = good_hypara %>% pull(penalty),
    batch_size = good_hypara %>% pull(batch_size),
    decision_width = good_hypara %>% pull(decision_width),
    attention_width = good_hypara %>% pull(attention_width),
    num_steps = good_hypara %>% pull(num_steps),
    learn_rate = 0.08,
    momentum = 0.6) %>%
  set_engine("torch", verbose = TRUE) %>%
  set_mode("classification")


# update the work flow with updated rule

upd_wf <-
  workflow() %>%
  add_model(upd_rule) %>%
  add_recipe(rec)

# build the model

model_tn <-
```

```
  upd_wf %>%
  fit(train) %>%
  with_seed(1,.)


# Predict

pred_tabnet <-
  predict(model_tn,new_data = test, type = "class")
```

```
# Evaluate

table(test=test$quality, pred= pred_tabnet$.pred_class)
```

```
##      pred
## test   0   1
##    0 111  38
##    1  49 123
```

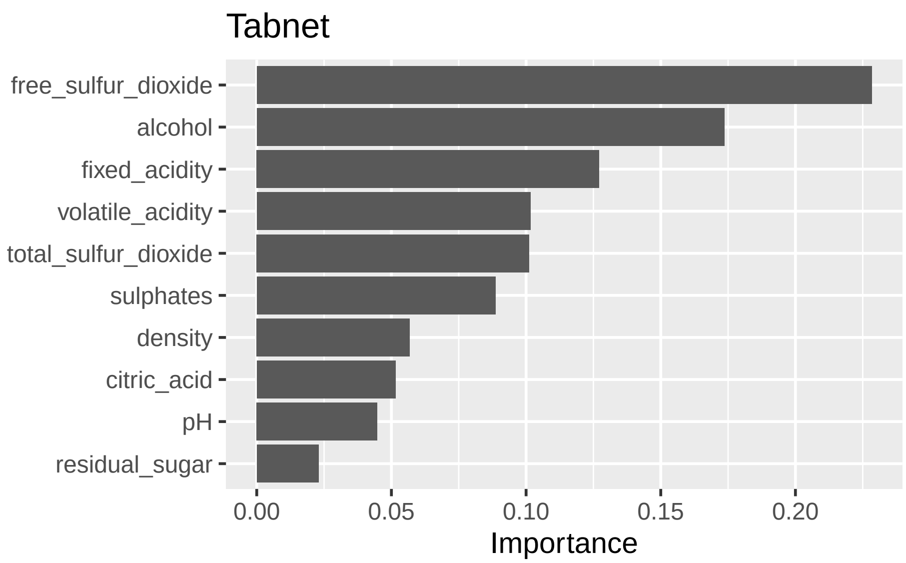
```
tabnet_acc <- sum(diag(table(test$quality, pred_tabnet$.pred_class))) /
    nrow(test)

tabnet_acc
```

```
## [1] 0.728972
```

```
# Check the importance

fit <- extract_fit_parsnip(model_tn)
p_tabnet <- vip(fit) + ggtitle("Tabnet")
p_tabnet
```



4.2 Compare the models

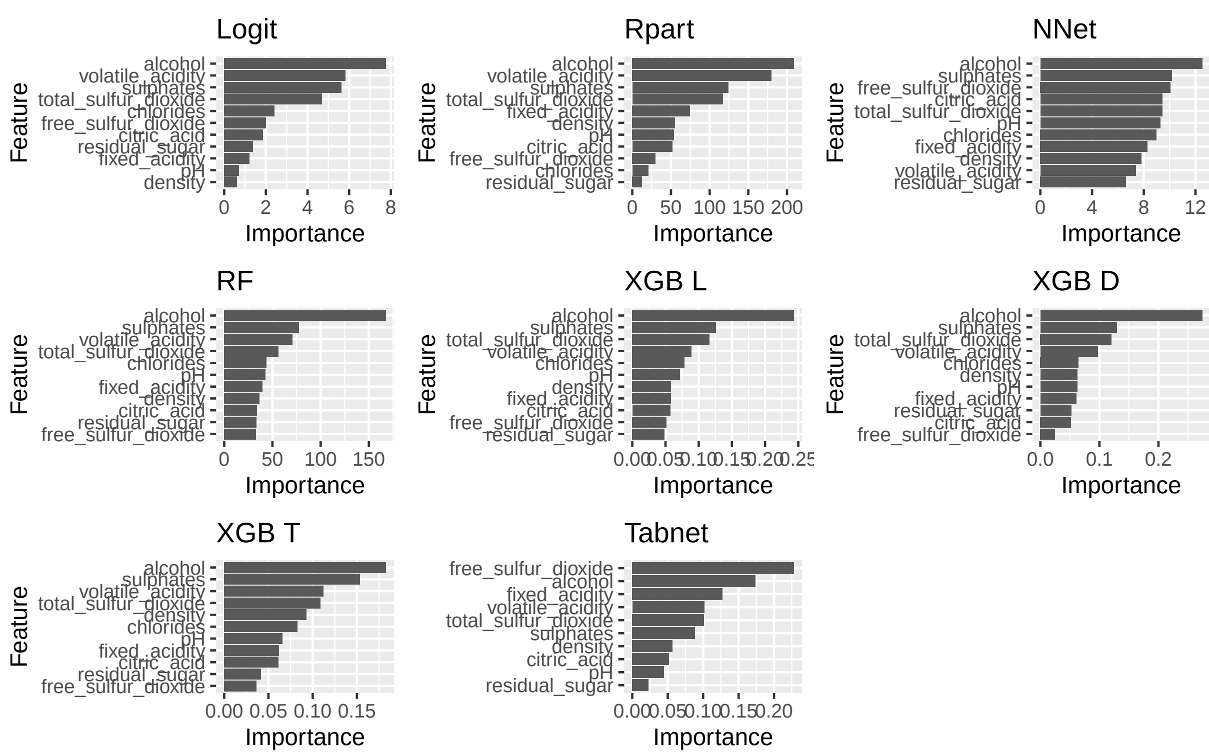
As a result of comparing each model using Accuracy, the DART model of XGBoost showed the highest score. Since we have not yet reached the optimal tuning for each model, we cannot judge which model is the best, but XGBoost was able to calculate a high score with a short code for all of them. In the Importance comparison, all models except Tabnet showed the highest score for Alchol, while Tabnet showed the highest score for free sulfur dioxide. The ability to obtain multiple features in real work is attractive, and in competitions such as Kaggle, we believe it can be used to build ensembles.

```r
### Compare the models -----

rbind(logit_acc, rpart_acc, rf_acc, svm_acc, nnet_acc,
      xgbl_acc, xgbd_acc, xgbt_acc, torch_acc, tabnet_acc) %>% kable()
```

	Accuracy
logit_acc	0.7258567
rpart_acc	0.7476636
rf_acc	0.7912773
svm_acc	0.7476636
nnet_acc	0.7819315
xgbl_acc	0.8099688
xgbd_acc	0.8193146
xgbt_acc	0.8161994
torch_acc	0.6947040
tabnet_acc	0.7289720

```r
wrap_plots(p_logit, p_rpart, p_nnet, p_rf, p_xgbl, p_xgbd, p_xgbt, p_tabnet)
```



4.3 Additional: Google Colaboratory

In order to perform deep learning using GPU, we tried to calculate with R/torch using Google Colaboratory, where we can build a GPU environment for free. Link of the code and calculation results: **Google Colab: CYO_colab**

> Note: The library will automatically determine whether the environment is CPU or GPU and install the library, so you need to set the runtime to GPU first and then run the installation.

The number of epochs was set to 20 in this report, but 2000 in the Google Colaboratory calculation. 53 minutes was required in the CPU environment, but 35 minutes in the GPU environment, which reduced the calculation time.

5 conclusion

Following the previous MovieLens project, we worked on machine learning about classification using a small data table: Wine Quality dataset, assuming a BtoB business.

We were able to build models not only using the methods from the edx course and the widely used gradient boosting, but also using a library newly incorporated into R in 2020. In search of a better computing environment, we took advantage of the external environment and actually reduced the computation time.

Through this series of initiatives, we were able to learn how to work with data science, which will continue to grow in the future. By creating many models for the same data set, we were able to learn about the characteristics of each model. On the other hand, we have not yet calculated the optimal values of hyper-parameters for each model, so we think this is a future work to be done with better resources such as GPU environment.

Reference

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- UCI: Machine Learning Repository https://archive.ics.uci.edu/ml/index.php
- Pandoc https://pandoc.org/index.html
- The caret Package https://topepo.github.io/caret/index.html
- Tidymodels https://www.tidymodels.org/
- XGBoost.ai https://xgboost.ai/
- DART: Dropouts meet Multiple Additive Regression Trees (2015) https://arxiv.org/pdf/1505.01866.pdf
- torch for R https://torch.mlverse.org/
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- GitHub: mlverse/tabnet https://github.com/mlverse/tabnet
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- kaggle: Simple R - xgboost - caret kernel https://www.kaggle.com/nagsdata/simple-r-xgboost-caret-kernel
- towards data science: How to use R in Google Colab https://towardsdatascience.com/how-to-use-r-in-google-colab-b6e02d736497
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