Random Forests tutorial

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Acknowledgments:

Awesome resources who inspired this tutorial, check them out!: - https://uc-r.github.io/random_forests - https://koalaverse.github.io/machine-learning-in-R/random-forest.html - https://www.blopig.com/blog/2017/04/a-very-basic-introduction-to-random-forests-using-r/ - https://towardsdatascience.com/understanding-auc-roc-curve-68b2303cc9c5

Data Preparation

```
## Preparation
# Load required packages
library(randomForest)
```

```
## randomForest 4.6-14
```

```
## Type rfNews() to see new features/changes/bug fixes.
```

```
library(caret)
```

```
## Loading required package: lattice
```

```
## Loading required package: ggplot2
```

```
##
## Attaching package: 'ggplot2'
```

```
## The following object is masked from 'package:randomForest':
##
##     margin
```

```
# Load datasets
red_dataset <- read.csv("http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequali
white_dataset <- read.csv("http://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequa

# Creating working dataframe
red_wine <- red_dataset
white_wine <- white_dataset

head(red_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.4             0.70        0.00            1.9     0.076
## 2           7.8             0.88        0.00            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             0.70        0.00            1.9     0.076
```

```
## 6           7.4             0.66        0.00            1.8     0.075
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  11                   34  0.9978 3.51      0.56     9.4
## 2                  25                   67  0.9968 3.20      0.68     9.8
## 3                  15                   54  0.9970 3.26      0.65     9.8
## 4                  17                   60  0.9980 3.16      0.58     9.8
## 5                  11                   34  0.9978 3.51      0.56     9.4
## 6                  13                   40  0.9978 3.51      0.56     9.4
##   quality
## 1       5
## 2       5
## 3       5
## 4       6
## 5       5
## 6       5
```

```
head(white_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.0             0.27        0.36           20.7     0.045
## 2           6.3             0.30        0.34            1.6     0.049
## 3           8.1             0.28        0.40            6.9     0.050
## 4           7.2             0.23        0.32            8.5     0.058
## 5           7.2             0.23        0.32            8.5     0.058
## 6           8.1             0.28        0.40            6.9     0.050
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  45                  170  1.0010 3.00      0.45     8.8
## 2                  14                  132  0.9940 3.30      0.49     9.5
## 3                  30                   97  0.9951 3.26      0.44    10.1
## 4                  47                  186  0.9956 3.19      0.40     9.9
## 5                  47                  186  0.9956 3.19      0.40     9.9
## 6                  30                   97  0.9951 3.26      0.44    10.1
##   quality
## 1       6
## 2       6
## 3       6
## 4       6
## 5       6
## 6       6
```

```
## Arrange dataset
# Add type
red_wine$type <- factor("red")
head(red_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.4             0.70        0.00            1.9     0.076
## 2           7.8             0.88        0.00            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             0.70        0.00            1.9     0.076
## 6           7.4             0.66        0.00            1.8     0.075
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  11                   34  0.9978 3.51      0.56     9.4
## 2                  25                   67  0.9968 3.20      0.68     9.8
## 3                  15                   54  0.9970 3.26      0.65     9.8
```

```
## 4                 17                  60  0.9980 3.16      0.58     9.8
## 5                 11                  34  0.9978 3.51      0.56     9.4
## 6                 13                  40  0.9978 3.51      0.56     9.4
##   quality type
## 1       5  red
## 2       5  red
## 3       5  red
## 4       6  red
## 5       5  red
## 6       5  red
```

```
white_wine$type <- factor("white")
head(white_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.0             0.27        0.36           20.7     0.045
## 2           6.3             0.30        0.34            1.6     0.049
## 3           8.1             0.28        0.40            6.9     0.050
## 4           7.2             0.23        0.32            8.5     0.058
## 5           7.2             0.23        0.32            8.5     0.058
## 6           8.1             0.28        0.40            6.9     0.050
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  45                  170  1.0010 3.00      0.45     8.8
## 2                  14                  132  0.9940 3.30      0.49     9.5
## 3                  30                   97  0.9951 3.26      0.44    10.1
## 4                  47                  186  0.9956 3.19      0.40     9.9
## 5                  47                  186  0.9956 3.19      0.40     9.9
## 6                  30                   97  0.9951 3.26      0.44    10.1
##   quality  type
## 1       6 white
## 2       6 white
## 3       6 white
## 4       6 white
## 5       6 white
## 6       6 white
```

```
# Join datasets
both_wine <- rbind(red_wine, white_wine)
head(both_wine)
```

```
##   fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1           7.4             0.70        0.00            1.9     0.076
## 2           7.8             0.88        0.00            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             0.70        0.00            1.9     0.076
## 6           7.4             0.66        0.00            1.8     0.075
##   free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates alcohol
## 1                  11                  34  0.9978 3.51      0.56     9.4
## 2                  25                  67  0.9968 3.20      0.68     9.8
## 3                  15                  54  0.9970 3.26      0.65     9.8
## 4                  17                  60  0.9980 3.16      0.58     9.8
## 5                  11                  34  0.9978 3.51      0.56     9.4
## 6                  13                  40  0.9978 3.51      0.56     9.4
##   quality type
## 1       5  red
```

```
## 2       5  red
## 3       5  red
## 4       6  red
## 5       5  red
## 6       5  red
```

```
tail(both_wine)
```

```
##      fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 6492           6.5             0.23        0.38            1.3     0.032
## 6493           6.2             0.21        0.29            1.6     0.039
## 6494           6.6             0.32        0.36            8.0     0.047
## 6495           6.5             0.24        0.19            1.2     0.041
## 6496           5.5             0.29        0.30            1.1     0.022
## 6497           6.0             0.21        0.38            0.8     0.020
##      free.sulfur.dioxide total.sulfur.dioxide density   pH sulphates
## 6492                  29                  112 0.99298 3.29      0.54
## 6493                  24                   92 0.99114 3.27      0.50
## 6494                  57                  168 0.99490 3.15      0.46
## 6495                  30                  111 0.99254 2.99      0.46
## 6496                  20                  110 0.98869 3.34      0.38
## 6497                  22                   98 0.98941 3.26      0.32
##      alcohol quality  type
## 6492     9.7       5 white
## 6493    11.2       6 white
## 6494     9.6       5 white
## 6495     9.4       6 white
## 6496    12.8       7 white
## 6497    11.8       6 white
```

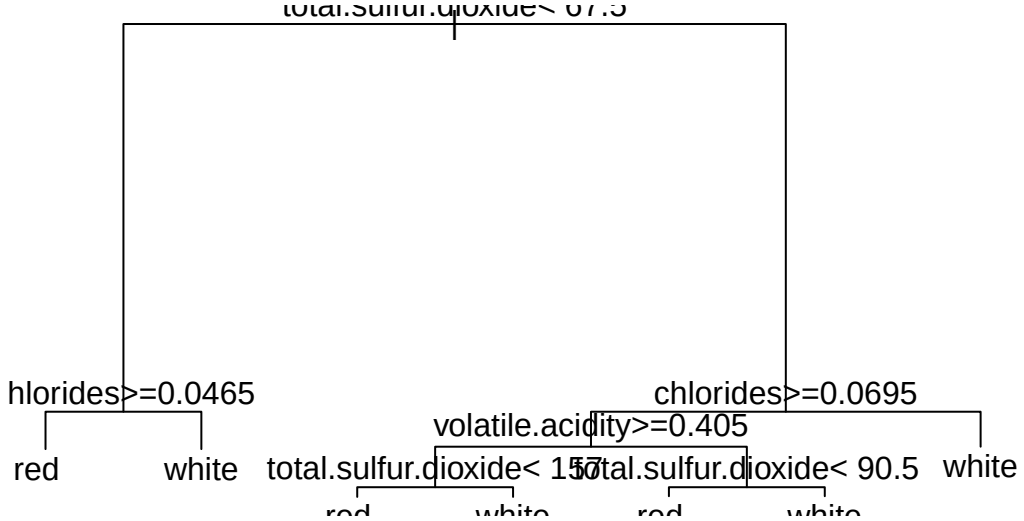
```
# Extract index of wine type
type_ind <- which(names(both_wine) == "type")
```

Decision Tree Example

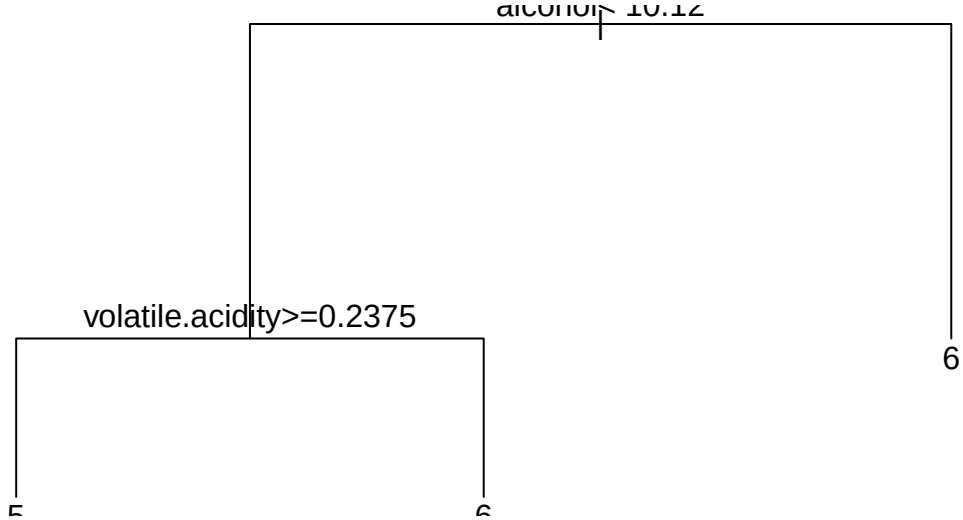
Decision Trees: - Predict a categorical/numeric response variable - Split points: nodes where decision is made - Terminal/leaf node: node without descendant - Pros: handling huge datasets, mixed predictors, ignore redundant variables - Cons: unstable trees, poor predictive accuracy & unstable predictions, high variance

Criterion & Best Split: - Gini Impurity: how often random element incorrectly labeled if labeled randomly, given label distribution - sum(fi * (1 - fi)) - Entropy: uncertainty in data set S, ~ data set (S), classes in S (X), ratio elem in x to elem in S p(x), 0 = perfect classification - Information gain: how much uncertainty reduced after splitting S on attribute A (diff in entropy) - Regression trees: minimize overall SSE (value vs constant for all trees) - Pruning, optimal subtree & cost complexity criterion: grow deep, prune back based on criterion (ex. number of terminal nodes)

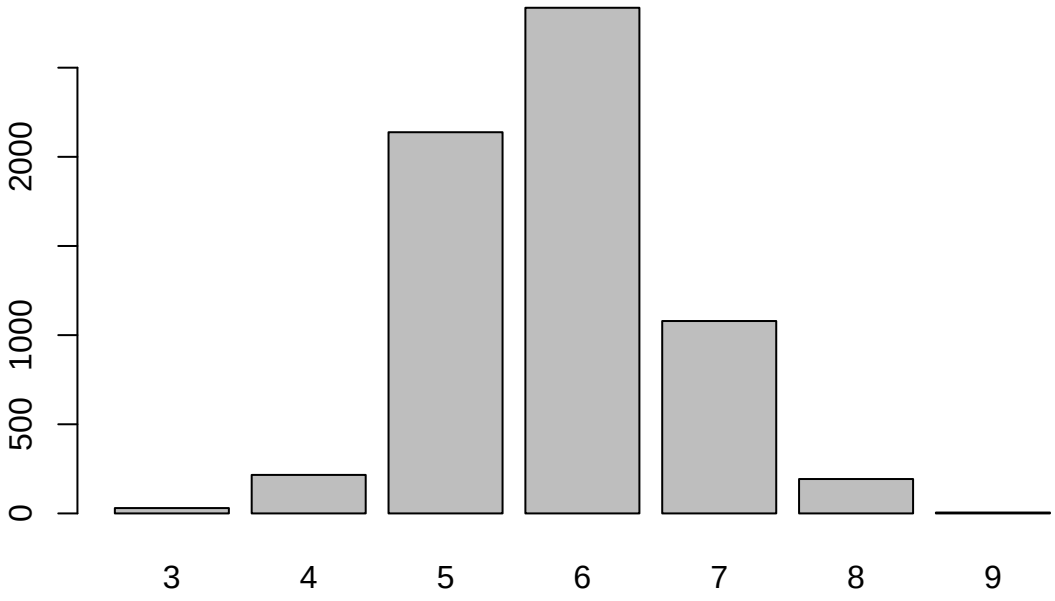
```
## Decision Tree Example
library(rpart)

set.seed(42)
decision_tree <- rpart(type ~ ., data = both_wine)
plot(decision_tree)
text(decision_tree)
```




```
set.seed(42)
decision_tree <- rpart(as.factor(quality) ~ ., data = both_wine)
plot(decision_tree)
text(decision_tree)
```




```
barplot(table(as.factor(both_wine$quality)))
```



Modelling wine type - Random Forest

Ensemble method: - Way to aggregate method from various models, should return better one

Random forests: - Bagging (boostrap aggregating): sampling with replacement, predict unseen samples by average/majority) - BUT still tree correlation, ~ same structure as all vars available at each split, doesn't optimally reduce variance of predictive values - Random Subspace/split-variable randomization: random subset of m features (variables) at each split (feature bagging) - Corrects overfitting, decorrelates trees, reduces variance - m: m = p/3 for regression trees, m = sqrt(p) for classification (?), m = p is bagging - OOB estimates: no need for cross-validation or separate test set for unbiased estimate of test set error, because estimated internally (tested in 1/3 of trees) - Efficient, no data sacrificed - BUT still differences between OOB error vs test error –> test set important if multiple models compared, complex loss functions –> cross-validation still possible - Variable importance: count correct OOB cases, permute var, recount correct –> big difference = important variable - Local importance score: ~ same as variable importance with percentage of votes instead of counts (?) - Overfitting: RF models more robust, possible with deep trees, but adding trees generally increases performance

```
### Prep the data

train_inds <- sample(1:nrow(both_wine), 0.7*nrow(both_wine))
train_wine <- both_wine[train_inds,]
table(train_wine$type, train_wine$quality)
```

```
##
##            3    4    5    6    7    8    9
##   red      9   35  468  450  138   12    0
##   white   15  107 1036 1517  635  122    3
```

```
valid_wine <- both_wine[-train_inds,]
table(train_wine$type, train_wine$quality)
```

```
##
##            3    4    5    6    7    8    9
##   red      9   35  468  450  138   12    0
##   white   15  107 1036 1517  635  122    3
```

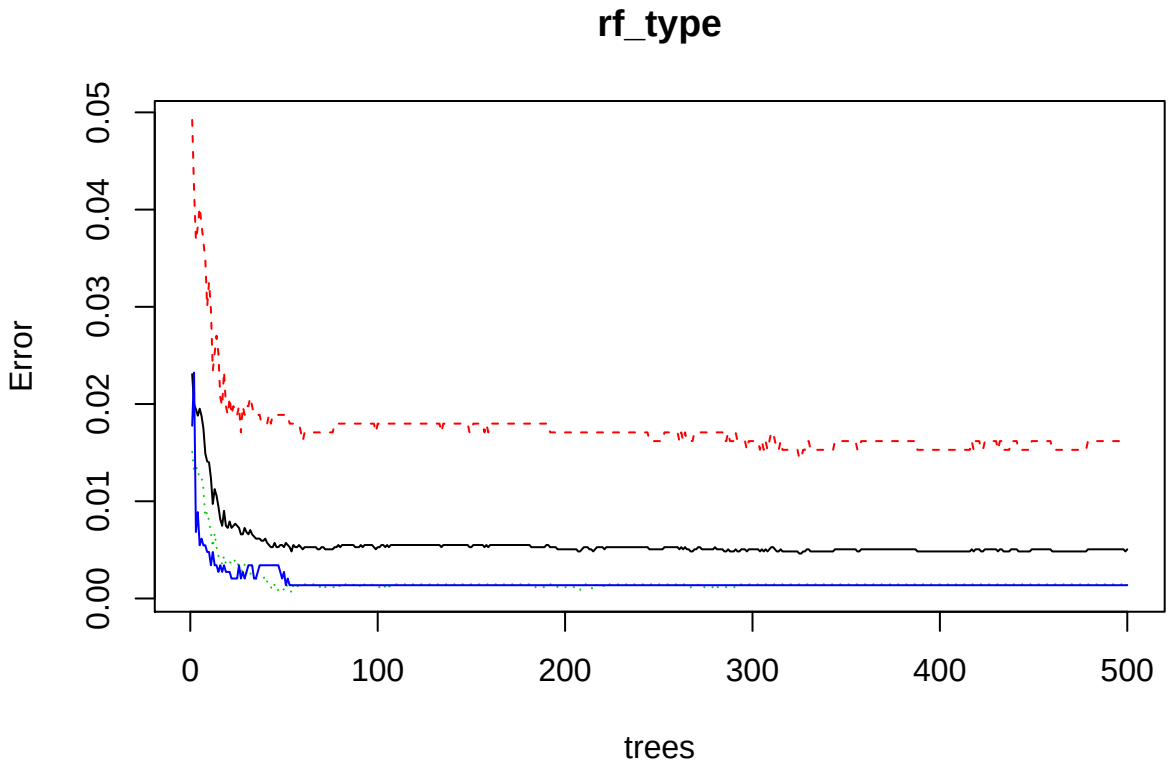
```
table(valid_wine$type, valid_wine$quality)
```

```
##
##            3   4   5   6   7   8   9
##   red      1  18 213 188  61   6   0
##   white    5  56 421 681 245  53   2
```

```
## Random Forest with default parameters
set.seed(42)
rf_type <- randomForest(type ~ ., data = train_wine, importance = TRUE)
rf_type
```

```
##
## Call:
##  randomForest(formula = type ~ ., data = train_wine, importance = TRUE)
##                Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 3
##
##         OOB estimate of  error rate: 0.51%
## Confusion matrix:
##        red white class.error
## red   1094    18 0.016187050
## white    5  3430 0.001455604
```

```
rf_type_test <- randomForest(type ~ ., data = train_wine, importance = TRUE,
                             xtest = valid_wine[,-type_ind], ytest = valid_wine$type)

plot(rf_type)
lines(1:500, rf_type_test$test$err.rate[,3], col="blue")
```



```r
pred_type <- predict(rf_type, valid_wine)
confusionMatrix(pred_type, valid_wine$type)
```

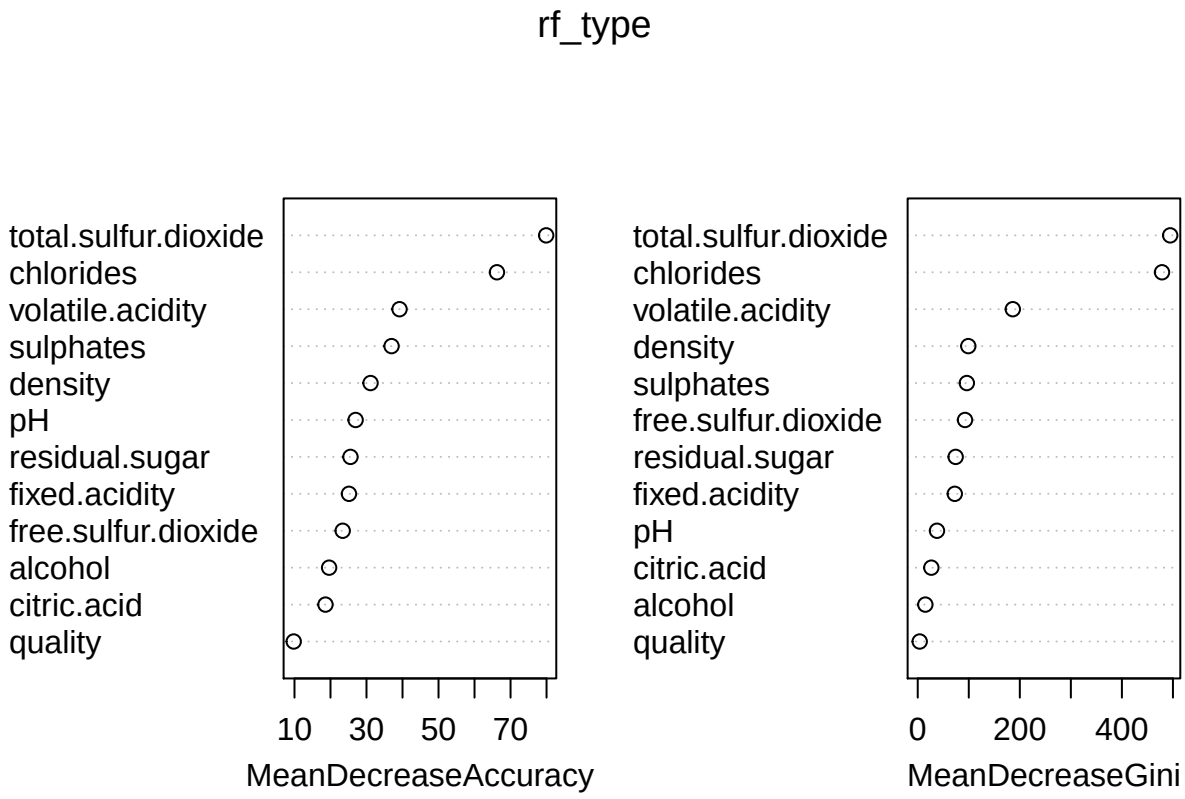
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  red white
##      red    477     2
##      white   10  1461
##
##                Accuracy : 0.9938
##                  95% CI : (0.9893, 0.9968)
##     No Information Rate : 0.7503
##     P-Value [Acc > NIR] : < 2e-16
##
##                   Kappa : 0.9835
##
##  Mcnemar's Test P-Value : 0.04331
##
##             Sensitivity : 0.9795
##             Specificity : 0.9986
##          Pos Pred Value : 0.9958
##          Neg Pred Value : 0.9932
##              Prevalence : 0.2497
##          Detection Rate : 0.2446
##    Detection Prevalence : 0.2456
##       Balanced Accuracy : 0.9890
##
##        'Positive' Class : red
##
```

```r
## Evaluate variable importance
# Show values
importance(rf_type)
```

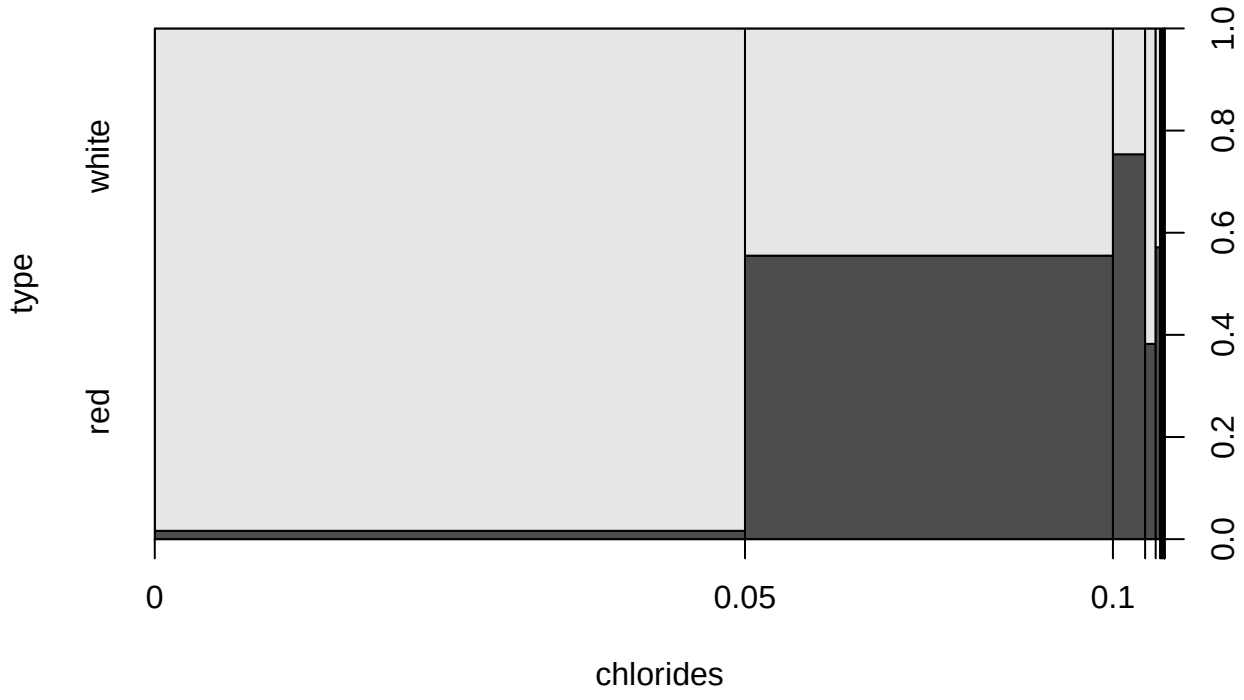
```
##                          red     white MeanDecreaseAccuracy
## fixed.acidity        18.344751 19.299763            25.129326
## volatile.acidity     31.524500 29.149741            39.172872
## citric.acid          14.744056 14.122003            18.604892
## residual.sugar       26.767727 13.388916            25.545957
## chlorides            55.999555 49.067543            66.229621
## free.sulfur.dioxide  14.766213 19.154661            23.390702
## total.sulfur.dioxide 63.538056 57.807278            79.899730
## density              32.650533 17.346005            31.123971
## pH                   21.834960 20.873625            26.977529
## sulphates            30.276471 32.566641            36.960562
## alcohol              17.350515 14.196691            19.621346
## quality               6.624782  7.133147             9.784119
##                      MeanDecreaseGini
## fixed.acidity               72.603109
## volatile.acidity           186.268988
## citric.acid                 26.645433
## residual.sugar              74.318811
## chlorides                  478.592287
```

```
## free.sulfur.dioxide          92.650773
## total.sulfur.dioxide        494.620358
## density                      99.098190
## pH                           37.736519
## sulphates                    96.195494
## alcohol                      14.930945
## quality                       3.876929
```

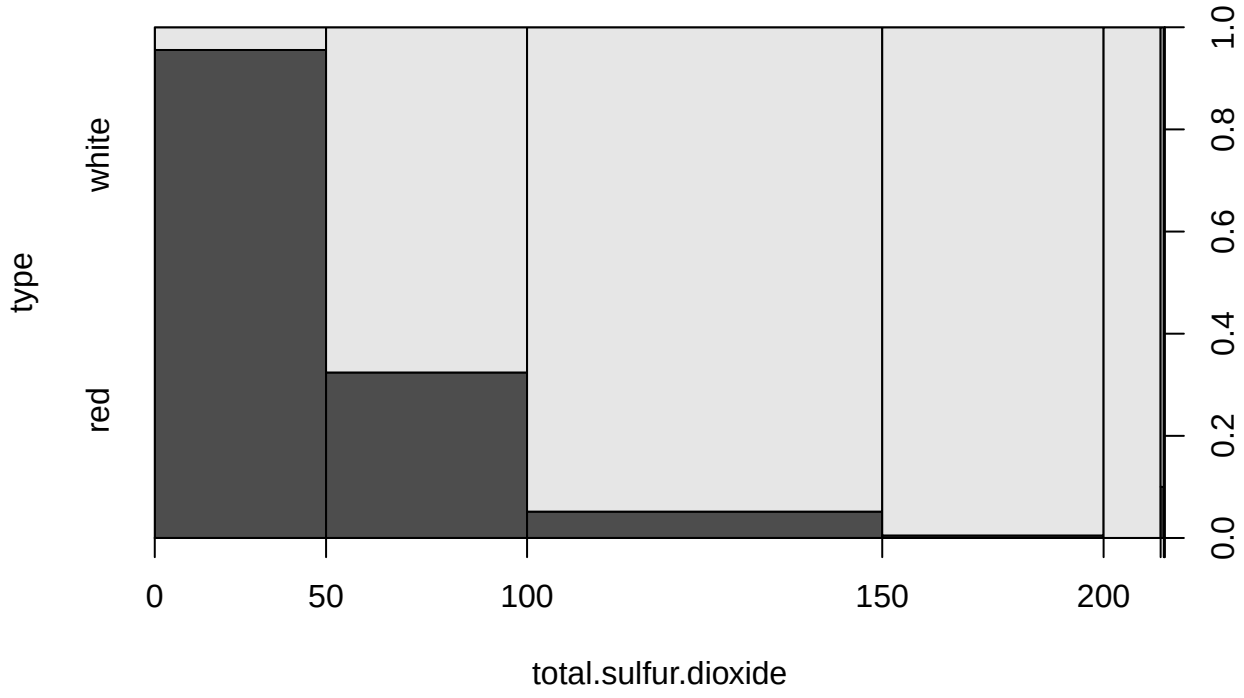
```r
# Plot importance values
varImpPlot(rf_type) # total.sulfur.dioxides & chlorides are clearly the best
```




```r
# Plot type as function of best parameters
plot(type ~ chlorides, data = both_wine)
```




```
plot(type ~ total.sulfur.dioxide, data = both_wine)
```



Modeling wine quality - Random Forest (classification analysis)

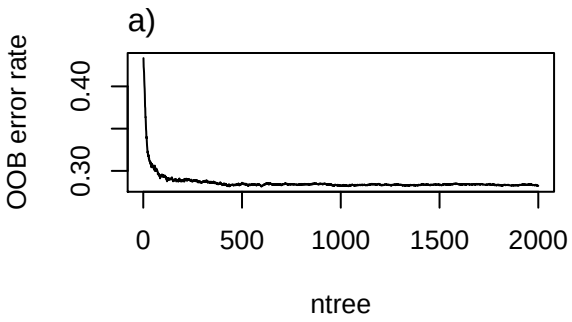
Tune model

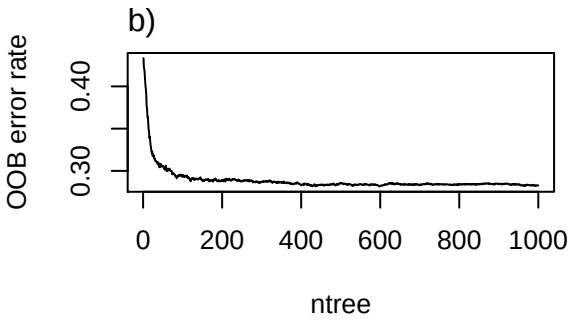
```
## 1. Model with default parameters
set.seed(42)
rf_qual <- randomForest(as.factor(quality) ~ ., data = both_wine)
```

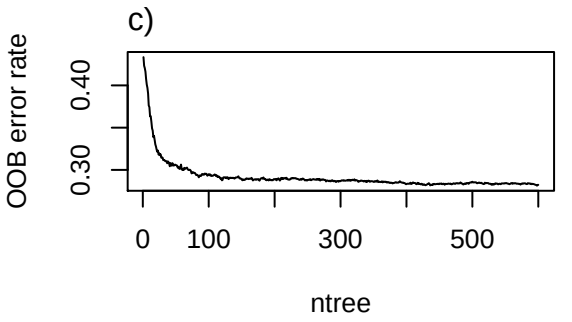
```
rf_qual
```

```
##
## Call:
##  randomForest(formula = as.factor(quality) ~ ., data = both_wine)
##                Type of random forest: classification
##                      Number of trees: 500
## No. of variables tried at each split: 3
##
##         OOB estimate of  error rate: 28.6%
## Confusion matrix:
##   3  4    5    6   7  8 9 class.error
## 3 0  1   17   12   0  0 0   1.0000000
## 4 1 32  111   68   4  0 0   0.8518519
## 5 0  9 1589  529  11  0 0   0.2567820
## 6 0  4  377 2305 148  2 0   0.1872355
## 7 0  0   21  419 631  8 0   0.4151993
## 8 0  0    1   66  44 82 0   0.5751295
## 9 0  0    0    3   2  0 0   1.0000000
```

```
# default ntree = 500
# default mtry = 3
# OOB error rate = 28.52%%

## 2. Choose ntree value (where OOB error rate stabilizes at minimum)

# Test model with ntree = 2000, 1000, and 600
set.seed(42)
rf_qual_2000 <- randomForest(as.factor(quality) ~ ., data = both_wine, ntree = 2000)
set.seed(42)
rf_qual_1000 <- randomForest(as.factor(quality) ~ ., data = both_wine, ntree = 1000)
set.seed(42)
rf_qual_600 <- randomForest(as.factor(quality) ~ ., data = both_wine, ntree = 600)

# Plot error rate ~ ntree

par(mfrow=c(2,2))
plot(rf_qual_2000$err.rate[,"OOB"], type = "l", xlab = "ntree",
     ylab = "OOB error rate")
mtext("a)", line = 0.5, adj = 0)
plot(rf_qual_1000$err.rate[,"OOB"], type = "l", xlab = "ntree",
     ylab = "OOB error rate")
mtext("b)", line = 0.5, adj = 0)
plot(rf_qual_600$err.rate[,"OOB"], type = "l", xlab = "ntree",
     ylab = "OOB error rate")
mtext("c)", line = 0.5, adj = 0)
par(mfrow=c(1,1))
```







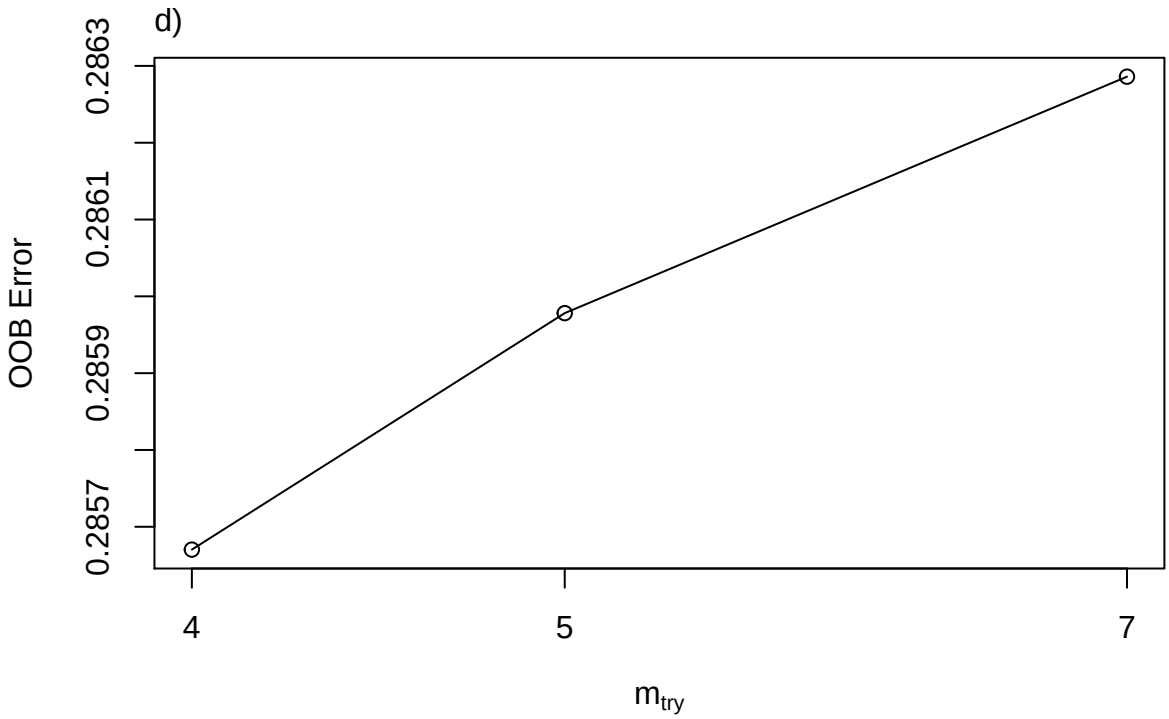

```
# stabilizes around n=500, same as default value. Let's select it

## 3. Find optimal mtry value
set.seed(42)
mtry <- tuneRF(x = both_wine[-which(names(both_wine)=="quality")], y = as.factor(both_wine$quality),
               ntreeTry=500, mtryStart = 5,stepFactor=1.5,improve=0.01, trace=TRUE, plot=TRUE)
```

```
## mtry = 5  OOB error = 28.6%
## Searching left ...
## mtry = 4     OOB error = 28.57%
## 0.001076426 0.01
## Searching right ...
## mtry = 7     OOB error = 28.63%
## -0.001076426 0.01
```

```
# Plot mtry values
mtry
```

```
##       mtry  OOBError
## 4.OOB    4 0.2856703
## 5.OOB    5 0.2859781
## 7.OOB    7 0.2862860
```

```
mtext("d)", line = 0.5, adj = 0)
```




```
# Best mtry = 3, same as default
```

Modeling wine quality - Random Forest (regression analysis)

```
## Modeling wine quality - Random Forest (regression analysis)

## Random forest with default parameters
set.seed(42)
rf_qual_reg <- randomForest(quality ~ ., data = both_wine, importance=TRUE)
rf_qual_reg
```

```
##
## Call:
##  randomForest(formula = quality ~ ., data = both_wine, importance = TRUE)
##                Type of random forest: regression
##                      Number of trees: 500
## No. of variables tried at each split: 4
##
##           Mean of squared residuals: 0.3388956
##                     % Var explained: 55.55
```

```
# default ntree = 500
# default mtry = 4
# Mean of squared residuals = 0.339
# % Var explained = 55.55

## Verify model accuracy with predicted values as integers
# Extract OOB testing and predicted values from model
testing_qual_reg <- rf_qual_reg$y
predicted_qual_reg <- rf_qual_reg$predicted
```

```r
## Function to rearrange numeric predictions to integers as in
## Cortez et al. 2009
# Tolerance range is used to determine if predicted value is correct
rf_reg_accuracy <- function(tolerance){ # Wrapped in a function

  # Loop for all predicted values
  for(j in 1:length(predicted_qual_reg)){

    # Conditional operators to determine if predicted value is within tolerance
    # range of real value
    if(abs(predicted_qual_reg[j]-testing_qual_reg[j]) < tolerance) {
      # if TRUE, predicted value is within tolerance range and considered
      # correct; # hence, real value is selected
      predicted_qual_reg[j] <- testing_qual_reg[j]
    } else {
      # if FALSE, predicted value is incorrect; hence, predicted value is simply
      # rounded to closest integer
      predicted_qual_reg[j] <- round(predicted_qual_reg[j], digits = 0)
    }

  }
  # Define datasets as factors with same levels (warnings if not)
  testing_qual_reg <- as.factor(testing_qual_reg)
  predicted_qual_reg <- factor(predicted_qual_reg,
                               levels = levels(testing_qual_reg))
  # Check confusion matrix of predicted values
  print(confusionMatrix(predicted_qual_reg, testing_qual_reg))
}

# Verify model accuracy
library(caret)
rf_reg_accuracy(tolerance = 0.5) # accuracy = 0.700, similar to classification
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    3    4    5    6    7    8    9
##          3    0    0    0    0    0    0    0
##          4    1    6    2    0    0    0    0
##          5   19  160 1574  358   12    3    0
##          6   10   48  551 2324  465   50    1
##          7    0    2   11  154  602  107    4
##          8    0    0    0    0    0   33    0
##          9    0    0    0    0    0    0    0
##
## Overall Statistics
##
##                Accuracy : 0.6986
##                  95% CI : (0.6873, 0.7098)
##     No Information Rate : 0.4365
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.5276
##
```

```
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 3  Class: 4 Class: 5 Class: 6 Class: 7
## Sensitivity          0.000000 0.0277778   0.7362   0.8195  0.55792
## Specificity          1.000000 0.9995224   0.8734   0.6927  0.94869
## Pos Pred Value            NaN 0.6666667   0.7404   0.6738  0.68409
## Neg Pred Value       0.995382 0.9676326   0.8710   0.8320  0.91508
## Prevalence           0.004618 0.0332461   0.3291   0.4365  0.16608
## Detection Rate       0.000000 0.0009235   0.2423   0.3577  0.09266
## Detection Prevalence 0.000000 0.0013853   0.3272   0.5309  0.13545
## Balanced Accuracy    0.500000 0.5136501   0.8048   0.7561  0.75331
##                      Class: 8  Class: 9
## Sensitivity          0.170984 0.0000000
## Specificity          1.000000 1.0000000
## Pos Pred Value       1.000000       NaN
## Neg Pred Value       0.975248 0.9992304
## Prevalence           0.029706 0.0007696
## Detection Rate       0.005079 0.0000000
## Detection Prevalence 0.005079 0.0000000
## Balanced Accuracy    0.585492 0.5000000
```

```
rf_reg_accuracy(tolerance = 1.0) # accuracy = 0.913
```

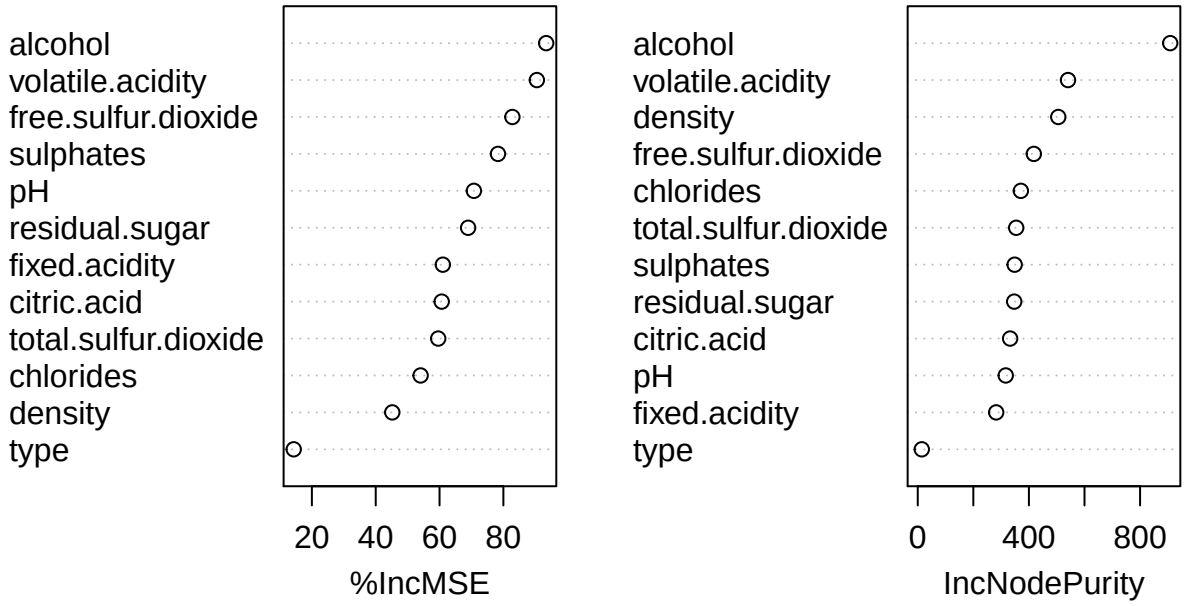
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    3    4    5    6    7    8    9
##          3    0    0    0    0    0    0    0
##          4    1   69    0    0    0    0    0
##          5   19   97 2019   15   12    3    0
##          6   10   48  108 2814  119   50    1
##          7    0    2   11    7  948   51    4
##          8    0    0    0    0    0   89    0
##          9    0    0    0    0    0    0    0
##
## Overall Statistics
##
##                Accuracy : 0.9141
##                  95% CI : (0.907, 0.9208)
##     No Information Rate : 0.4365
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.8682
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 3 Class: 4 Class: 5 Class: 6 Class: 7 Class: 8
## Sensitivity          0.000000  0.31944   0.9443   0.9922   0.8786  0.46114
## Specificity          1.000000  0.99984   0.9665   0.9082   0.9862  1.00000
## Pos Pred Value            NaN  0.98571   0.9326   0.8933   0.9267  1.00000
## Neg Pred Value       0.995382  0.97713   0.9725   0.9934   0.9761  0.98377
```

```
## Prevalence           0.004618  0.03325   0.3291   0.4365   0.1661  0.02971
## Detection Rate       0.000000  0.01062   0.3108   0.4331   0.1459  0.01370
## Detection Prevalence 0.000000  0.01077   0.3332   0.4848   0.1575  0.01370
## Balanced Accuracy    0.500000  0.65964   0.9554   0.9502   0.9324  0.73057
##                       Class: 9
## Sensitivity          0.0000000
## Specificity          1.0000000
## Pos Pred Value             NaN
## Neg Pred Value       0.9992304
## Prevalence           0.0007696
## Detection Rate       0.0000000
## Detection Prevalence 0.0000000
## Balanced Accuracy    0.5000000
```

```r
## Evaluate variable importance
# Show values
importance(rf_qual_reg)
```

```
##                       %IncMSE IncNodePurity
## fixed.acidity        61.02999     282.24308
## volatile.acidity     90.48706     540.75877
## citric.acid          60.66902     332.37285
## residual.sugar       68.95193     347.08741
## chlorides            54.06412     371.02795
## free.sulfur.dioxide  82.81470     417.69809
## total.sulfur.dioxide 59.57786     354.29125
## density              45.18951     505.73845
## pH                   70.75994     316.61830
## sulphates            78.29823     348.70583
## alcohol              93.41057     908.41400
## type                 14.30684      14.49352
```

```r
# Plot importance values
varImpPlot(rf_qual_reg, main = NULL) # alcohol is the best predictor
```



Party

```
# library(party)
# rf <- cforest(as.factor(quality) ~ .,
#               data = train_wine,
#               control = cforest_unbiased(mtry = 2, ntree = 500))
#
# (vars_imp <- varimp(rf, conditional = T))
# (vars_imp <- varimp(rf))
#
# pred_wine <- predict(rf, valid_wine, OOB=TRUE)
#
# confusionMatrix(pred_wine, as.factor(train_wine$quality))
```

```
library(ranger)
```

Ranger

```
##
## Attaching package: 'ranger'
```

```
## The following object is masked from 'package:randomForest':
##
##     importance
```

```
# time models
system.time(rf_qual <- randomForest(as.factor(quality) ~ ., data = train_wine))
```

```
##    user  system elapsed
##   3.697   0.064   3.761
```

```
system.time(ranger_qual <- ranger(as.factor(quality) ~ ., data = train_wine, importance = "impurity"))
```

```
##    user  system elapsed
##   6.394   0.044   0.663
```

```
## Fine tuning
# hyperparameter grid search
hyper_grid <- expand.grid(
  mtry       = seq(2, 6, by = 1),
  node_size  = seq(1, 5, by = 1),
  sampe_size = c(.55, .632, .70),
  OOB   = 0
)

# total number of combinations
nrow(hyper_grid)
```

```
## [1] 75
```

```
## [1] 160

system.time(
  for(i in 1:nrow(hyper_grid)) {

    # train model
    model <- ranger(formula = as.factor(quality) ~ .,
```

```
                    data = train_wine,
                    num.trees = 500,
                    mtry = hyper_grid$mtry[i],
                    min.node.size = hyper_grid$node_size[i],
                    sample.fraction = hyper_grid$sampe_size[i],
                    importance = "impurity",
                    seed = 42
                    )

    # add OOB error to grid
    hyper_grid$OOB[i] <- model$prediction.error
  }
)
```

```
##    user  system elapsed
## 390.882   1.460  40.075
```

```
hyper_grid
```

```
##    mtry node_size sampe_size       OOB
## 1     2         1      0.550 0.3217506
## 2     3         1      0.550 0.3206510
## 3     4         1      0.550 0.3243897
## 4     5         1      0.550 0.3268089
## 5     6         1      0.550 0.3254893
## 6     2         2      0.550 0.3272487
## 7     3         2      0.550 0.3276886
## 8     4         2      0.550 0.3305476
## 9     5         2      0.550 0.3301078
## 10    6         2      0.550 0.3325269
## 11    2         3      0.550 0.3301078
## 12    3         3      0.550 0.3287882
## 13    4         3      0.550 0.3316472
## 14    5         3      0.550 0.3316472
## 15    6         3      0.550 0.3367055
## 16    2         4      0.550 0.3296679
## 17    3         4      0.550 0.3422037
## 18    4         4      0.550 0.3384649
## 19    5         4      0.550 0.3415439
## 20    6         4      0.550 0.3384649
## 21    2         5      0.550 0.3422037
## 22    3         5      0.550 0.3408841
## 23    4         5      0.550 0.3408841
## 24    5         5      0.550 0.3466022
## 25    6         5      0.550 0.3424236
## 26    2         1      0.632 0.3206510
## 27    3         1      0.632 0.3235100
## 28    4         1      0.632 0.3239499
## 29    5         1      0.632 0.3237299
## 30    6         1      0.632 0.3215307
## 31    2         2      0.632 0.3208709
## 32    3         2      0.632 0.3241698
## 33    4         2      0.632 0.3230702
## 34    5         2      0.632 0.3268089
## 35    6         2      0.632 0.3268089
```

```
## 36    2         3      0.632 0.3285683
## 37    3         3      0.632 0.3290081
## 38    4         3      0.632 0.3235100
## 39    5         3      0.632 0.3285683
## 40    6         3      0.632 0.3259292
## 41    2         4      0.632 0.3263690
## 42    3         4      0.632 0.3347262
## 43    4         4      0.632 0.3272487
## 44    5         4      0.632 0.3358258
## 45    6         4      0.632 0.3303277
## 46    2         5      0.632 0.3349461
## 47    3         5      0.632 0.3362657
## 48    4         5      0.632 0.3345063
## 49    5         5      0.632 0.3369254
## 50    6         5      0.632 0.3345063
## 51    2         1      0.700 0.3202111
## 52    3         1      0.700 0.3237299
## 53    4         1      0.700 0.3221905
## 54    5         1      0.700 0.3210908
## 55    6         1      0.700 0.3309875
## 56    2         2      0.700 0.3208709
## 57    3         2      0.700 0.3257093
## 58    4         2      0.700 0.3221905
## 59    5         2      0.700 0.3237299
## 60    6         2      0.700 0.3305476
## 61    2         3      0.700 0.3217506
## 62    3         3      0.700 0.3246096
## 63    4         3      0.700 0.3254893
## 64    5         3      0.700 0.3259292
## 65    6         3      0.700 0.3301078
## 66    2         4      0.700 0.3259292
## 67    3         4      0.700 0.3246096
## 68    4         4      0.700 0.3303277
## 69    5         4      0.700 0.3285683
## 70    6         4      0.700 0.3303277
## 71    2         5      0.700 0.3316472
## 72    3         5      0.700 0.3331867
## 73    4         5      0.700 0.3294480
## 74    5         5      0.700 0.3360457
## 75    6         5      0.700 0.3371454
```

AUC

```
# Validation set assessment #2: ROC curves and AUC
# Needs to import ROCR package for ROC curve plotting:
library(ROCR)
```

```
## Loading required package: gplots
```

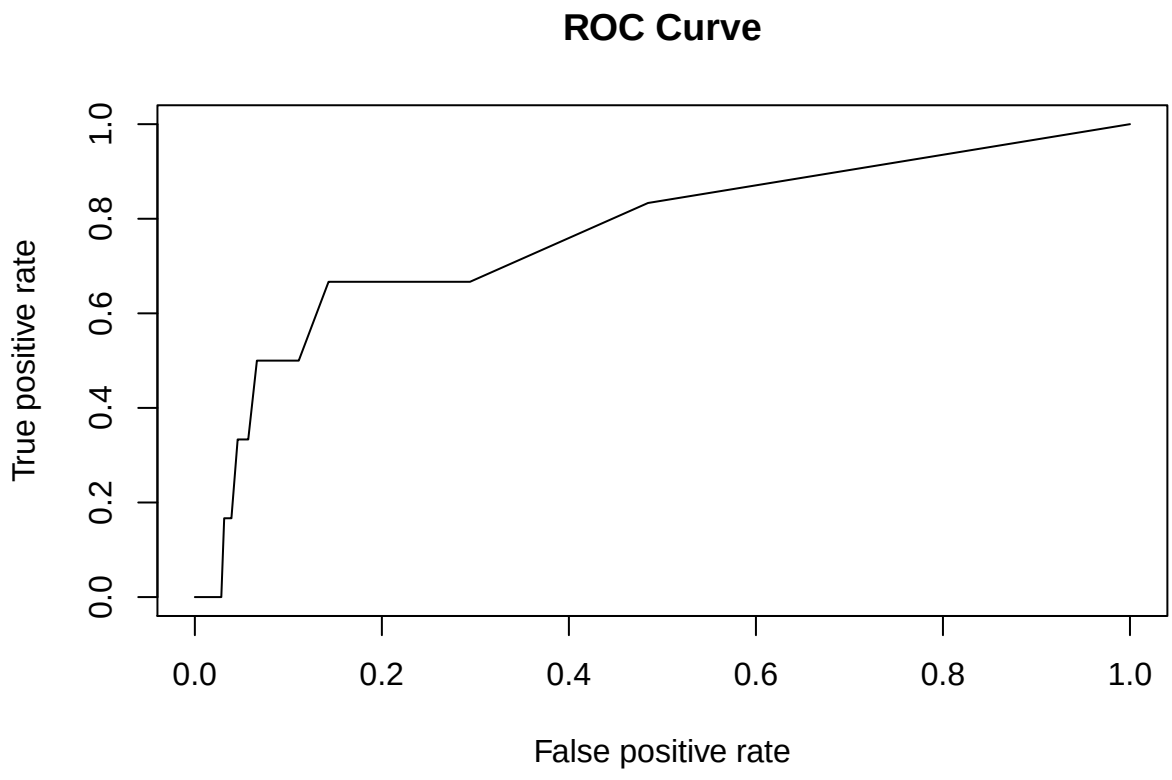
```
##
## Attaching package: 'gplots'
```

```
## The following object is masked from 'package:stats':
##
##     lowess
```

```r
# Calculate the probability of new observations belonging to each class
# prediction_for_roc_curve will be a matrix with dimensions data_set_size x number_of_classes
valid_wine$quality <- as.factor(valid_wine$quality)
prediction_for_roc_curve <- predict(rf_qual, valid_wine, type="prob")
# Use pretty colours:
# pretty_colours <- c("#F8766D","#00BA38","#619CFF")
# Specify the different classes
(classes <- levels(as.factor(valid_wine$quality)))
```

```
## [1] "3" "4" "5" "6" "7" "8" "9"
```

```r
# For each class
for (i in 1:length(class)){
 # Define which observations belong to class[i]
 true_values <- ifelse(as.factor(valid_wine$quality) == classes[i], 1, 0)
 # Assess the performance of classifier for class[i]
 pred <- prediction(prediction_for_roc_curve[,i], true_values)
 perf <- performance(pred, "tpr", "fpr")
 if (i == 1)
 {
     plot(perf, main="ROC Curve")
 }
 else
 {
     plot(perf, main="ROC Curve",add=TRUE)
 }
 # Calculate the AUC and print it to screen
 auc.perf <- performance(pred, measure = "auc")
 print(auc.perf@y.values)
}
```



```
## [[1]]
## [1] 0.7678755
```