Classification and Resampling of Wine Quality on Imbalanced Data Statistical Learning (STAT 983)

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April 18, 2021

Abstract

The ability to assess the quality of wine is essential in the wine industry in order to market and sell a wine. Currently quality assessment is done by the use of human experts, being costly and timely. In this paper, through the use of data mining techniques, wine quality is assessed through the use of easy available physiochemical properties of wine. Tree-based ensemble methods were tuned to classify the quality of future wines. We employed the use of eXtreme Gradiatent Boosting and Random Forest tree-based ensemble methods. Additionally, due to the imbalanced nature of the quality class, undersampling and oversampling resampling techniques were used on the data in order to evaluate the performance of our models. Utilizing cross-validation techniques, we saw immense benefits of oversampling the training data set reaching consistent performance of 100% classification rate of all quality classes with both classifiers. These results indicate that oversampling outperformed undersampling and that our two classifiers performed with similar accuracy with XGBoost having a slight advantage in classification of rare quality when no resampling or undersampling is performed.

1 Introduction

Successful marketing campaigns and productive selling strategies are directly linked to communication about key indicators of quality; hence, objective measurements of quality are essential. Within the wine industry, there are two types of quality assessment: physiochemical and sensory tests. Sensory tests require a human expert to assess the quality of wine based on visual, taste, and smell [Hu et al., 2016]. Hiring human experts to conduct sensory tests can take time and be expensive [Gupta, 2018]. In addition, taste is the least understood of all human senses, thus there is the potential for human bias to come into play with human testers [Cortez et al., 2009]. Unlike sensory tests, laboratory tests for measuring the physiochemical characteristics of wine such as acidity and alcohol content do not require a human expert. The relationship between physiochemcial and sensory analysis is not well understood. Recently, research in the food industry has utilized statistical learning techniques to evaluate widely available characteristics of wine. This type of evaluation allows the automation of quality assessment processes by minimizing the need of human experts [Gupta, 2018]. Additionally, if human experts are used, the classification model can be used to speed up and improve their quality assessment [Cortez et al., 2009].
These techniques also have the advantage of identifying the importantance of the phsiochemical characteristics that have an impact on the quality of wine as determined by a sensory test.

There have been a few previous papers that have looked into the classification of wine. Cortez et al. [2009] and Gupta [2018] examined the data using regression methods with their response being a quality rating from 0 to 10, with 0 being the worst quality and 10 being the highest quality. The methods that they employed were multiple regression, neural networks, and support vector machines, and they both found that support vector machines produced the lowest misclassification percentage. In Hu et al [2016], a different approach to this problem was employed where instead of using quality categories from 0-10, they grouped the qualities into three different categories: low, normal, and high. They looked at only data relating to white wine. The classification methods that they employed were Adaptive Boosting and Random Forest. Additionally, due to most of the qualities being classified as "normal", they employed an oversampling technique, SMOTE in order to develop better classification on the categories with not as much data, in this case "low" and "high". They found that Random Forest had the lowest misclassification rate of the two at 5.4% [Hu et al., 2016].

The goal of this paper, following Hu et al. [2016] is to train a model that would work well to classify wines into three categories, which are: low quality, normal quality and high quality. We evaluated two classification techniques, eXtreme Gradient Boosting (XGBoost) and Random Forest. Given prior investigation of the white wine data showed the Random Forests technique performed well; we would like to test this method using both white and red wine observations. Additionally, previous papers on the white wine data set have also applied different versions of gradient boosting such as adaptive boost; therefore we will apply XGBoost, an alternative gradient boosting technique. The quality categorization poses a challenge of working with imbalanced classes as there are many more normal quality wines than low or high quality wines [Figure 1]. To address this, we will evaluate different resampling techniques in order to determine if resampling improves performance and to identify which resampling method is best. Accuracy of each classification model applied in conjunction with each resampling method was compared. Initially, we first evaluated the classifier performance with no resampling. Since the quality class is highly imbalanced, we hypothesized no resampling to have low performance but provide a baseline. We will then apply a resampling method using SMOTE, which is an algorithm where the minority class (in this case low and high quality), will be oversampled, as this technique seemed to perform well in previous research [Hu et al., 2016]. The final resampling method we applied is a random undersampling method, where majority class data are randomly removed from the data set. We hypothesize random undersampling risks losing valuable information in our model. Accuracy of each classification method and resampling technique was evaluated by the overall correct classification rate and each individual group (low quality, normal quality, and high quality) correct classification rate.

2 Data Exploration

2.1 About the Data

In this paper, we applied classification and resampling techniques to the "Wine Quality Data Set" found on the UCI Data Repository [UCI]. The data consist of information from samples of Vinho Verde, which is a product from the northwest region of Portugal. The data was collected from May, 2004 to February, 2007, and is made up of 1599 red wines and 4898 white wines for a total of 6493 observations [Cortez et al., 2009]. For each of the wines in the dataset, 11 physiochemical variables were taken on it: fxed acidity, volatile acidity, citric acid, residual sugar, chlorides, free sulfur dioxide, total sulfur dioxide, density, pH, sulphates, and alcohol. Additionally, we classified the combined red and white wine data sets, and included an additional predictor variable categorizing the given observation as red or white wine. The response was measured as a quality rating based on a sensory test carried out by at least three sommeliers, where a 0 was considered very bad and a 10 was excellent Gupta [2018]. Following Hu et al. [2016], we separated the wine into three quality classes: Low Quality (≤ 4), Normal (5-7), and High quality (≥ 8). These response values are imbalanced as can be seen in Figure 1, with most of the wines having a response of "Normal".

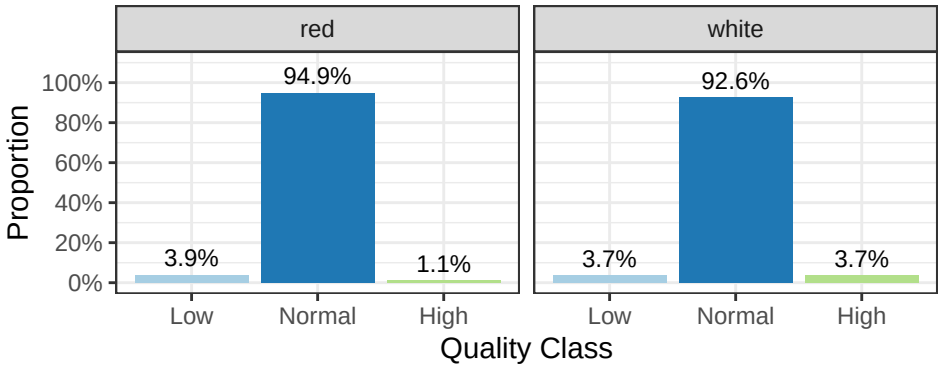

Figure 1: Wine quality class imbalance.

2.2 Exploring the Data

In Figure 2, boxplots of the 11 physiochemical variables are given. As can be see in this plot, for most of the predictor variables there are points that would be considered outliers, which are represented by black dots. We did not consider removing outliers, so no data points were removed for our final analysis. Looking at the boxplots, one can use these to give an idea of which of these predictor variables may be helpful in helping to determine the classification of the wines. For example, for alcohol, the interquartile range of the High category is above that of the Normal and Low class. Figure 3 gives the correlation plot for the 11 physiochemical variables, with also the 0-10 scale for the quality of the wines. Correlations that are not considered to be statistically significant are not shown. Most of the correlations seem to be on the lower end of the spectrum, so multicollinearity does not seem to be a huge issue that needs to be addressed among the predictor variables. It also shows that all of the predictor variables have a statistically significant correlation with the response of quality, so they should be helpful for classification.

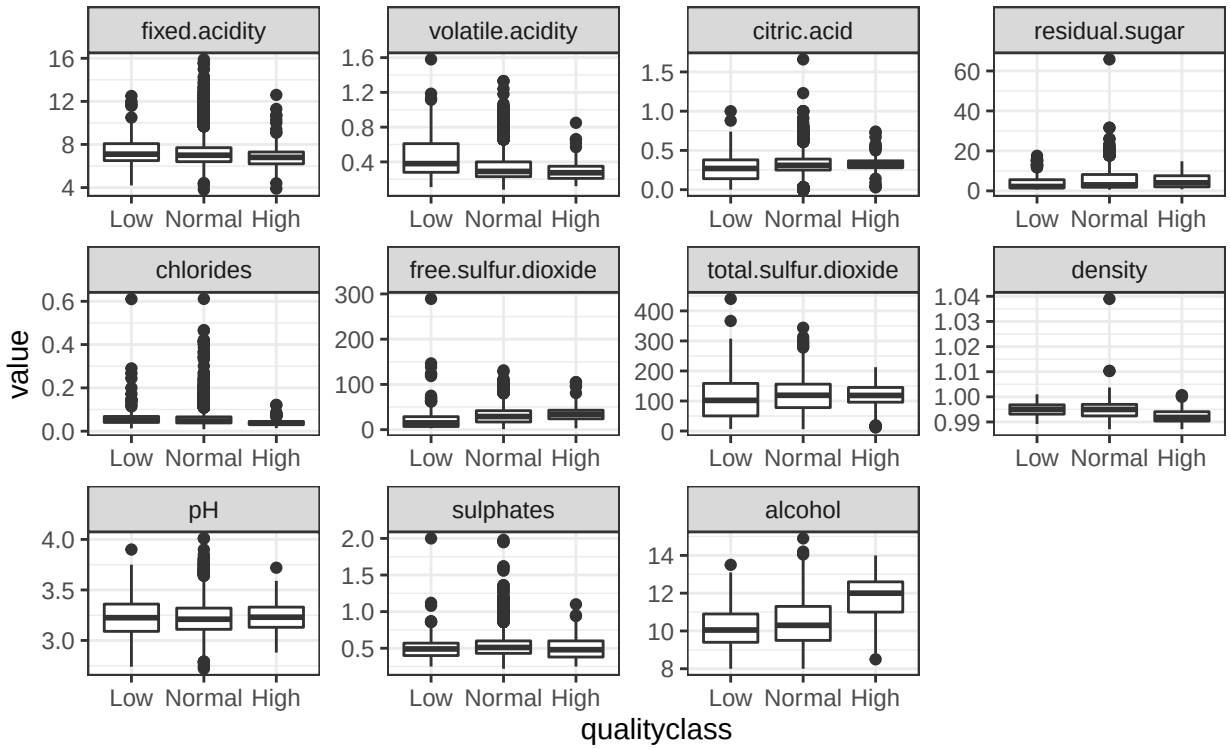

Figure 2: Distribution of the Predictor Variables

Table 1 provides physiochemical characteristics stratified by three quality classes. Continuous variables are presented as median and interquartile range (IQR) whereas discrete variables are presented as counts and proportions (%). Data were stratified by three classes of quality and comparisons were made with the Kruskal-Wallis and chi-square tests for continuous and discrete variables, respectively. We did not conduct post-hoc testing to further investigate pairwise differences. There was statistical evidence of a difference between the three classes of quality for all variables except for pH ($P < 0.001$, respectively) **I am not seeing any p-values in the table? Going back to the original table in the SJA file I am still not seeing them? -Emily**. The low designation of wine quality was associated with the highest amount of red wine, chlorides, density, fixed acidity, and volatile acidity, and the lowest amount of alcohol, citric acid, free sulfur dioxide, residual sugar, sulphates, and total sulfur dioxide **How was this determined? -Emily**. Again, we did not conduct post-hoc testing.

3 Statistical Methods

We applied two classification methods, Random Forest and eXtreme Gradient Boosting (XGBoost), on the original training set (no resampling), the undersampled training set, and the oversampled training set. Accuracy of each

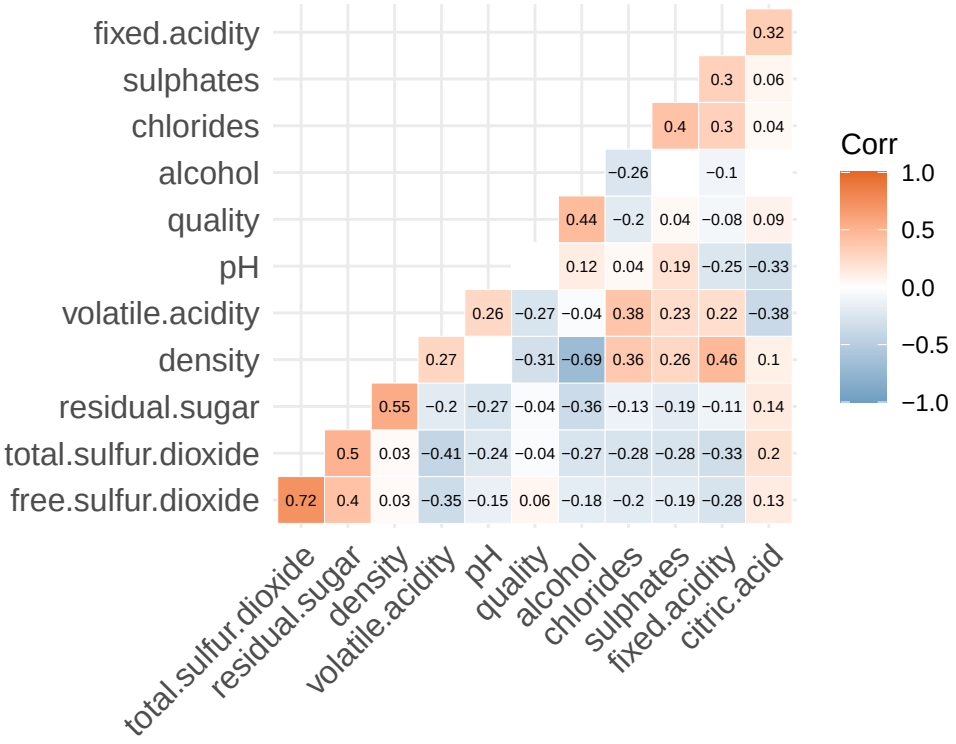

Figure 3: Correlation Plot

Table 1: Basic Descriptive Statistics from the Wine Quality Dataset.

	Low No. 246	Normal No. 6,053	High No. 198
Fixed Acidity	7.10 (6.50 - 8.07)	7.00 (6.40 - 7.70)	6.80 (6.20 - 7.30)
Volatile Acidity	0.38 (0.28 - 0.61)	0.29 (0.23 - 0.40)	0.28 (0.21 - 0.35)
CitricAcidity	0.27 (0.14 - 0.38)	0.31 (0.25 - 0.39)	0.32 (0.28 - 0.37)
Residual Sugar	2.20 (1.50 - 5.60)	3.00 (1.80 - 8.20)	4.05 (2.00 - 7.57)
Chlorides	0.05 (0.04 - 0.07)	0.05 (0.04 - 0.07)	0.04 (0.03 - 0.04)
Free Sulfur Dioxide	15.00 (7.00 - 28.75)	29.00 (17.00 - 42.00)	34.00 (24.00 - 43.00)
Total Sulfur Dioxide	102.00 (50.25 - 158.50)	119.00 (78.00 - 156.00)	118.50 (96.00 - 145.00)
Density	1.00 (0.99 - 1.00)	0.99 (0.99 - 1.00)	0.99 (0.99 - 0.99)
pH	3.23 (3.09 - 3.36)	3.21 (3.11 - 3.32)	3.23 (3.13 - 3.33)
Sulphates	0.49 (0.40 - 0.57)	0.51 (0.43 - 0.60)	0.48 (0.38 - 0.60)
Alcohol	10.05 (9.40 - 10.90)	10.30 (9.50 - 11.30)	12.00 (11.00 - 12.60)

classification method and resampling technique was evaluated by the overall correct classification rate and each individual group (low quality, normal quality, and high quality) correct classification rate. Classification rate is calculated as:

$$\text{overall accuracy} = \frac{1}{n}\sum_{i=1}^{n} I_{[\widehat{class}_i = class_i]}$$

$$\text{accuracy for group k} = \frac{1}{n_k}\sum_{j=1}^{n_k} I_{[\widehat{class}_j = class_j]}.$$

Monte Carlo Cross-Validation (MCMC) was used to select tuning parameters and evaluate model performance. The MCMC algorithm repeatedly splits the data into training and testing sets (B = 50 for model tuning; B = 100 for final model comparison) by randomly selecting the designated proportions (70% training; 30% testing) of the overall data set to each. The undersampling and oversampling techniques as described below are then applied to the training set to obtain a final resampled training data set. For each split, the final resampled training data set is used to build the model; then accuracy is evaluated on the corresponding testing data set. The mean, 5th-quantile, and 95th-quantile of the correct classification rates are used to evaluate performance over the B splits. Both classification methods were tuned by conducting a hyperparameter grid search with MCMC (B = 50) to minimize the overall accuracy [Appendix A]; parallel computing with the `furrr` package in R was conducted to minimize computing time [Vaughan and Dancho, 2021].

3.1 Resampling Techniques

Before we are able to consider the different classification methods, the imbalanced issue in our data must be examined. This is because typical classifier algorithms assume a relatively balanced distribution, so with imbalanced data they tend to be biased towards the majority class [Sun et al., 2009]. Classification rules for the minority classes tend to be undiscovered or ignored, so the minority class is misclassified more often than the majority class. If we were to look at our data set from a binary standpoint where "Low Quality" and "High Quality" were classified as "rare", and "Normal Quality" was classified as "not rare", the majority (not rare) class has 6053 observations, and the minority (rare) class has 444 observations, which is a ratio of about 13:1. Due to this imbalanced nature in the data, classifying algorithms will be biased towards classifying wines as Normal Quality, causing poor predictions for the Low and High Quality classes. When creating the resampled data sets, the binary classification of "rare" and "not rare" is used due to the resampling algorithms relying on a binary class designation.

A method on how to deal with the imbalanced issue in the data is through resampling the original data set either by oversampling the majority class, or undersampling the minority class. The goal with these methods is to create a data set that has close to a balanced class distribution, so the classifying algorithms will have better predictions, so it will predict to the minority class more accurately [Hoens and Chawla, 2013]. The oversampling method involves replicating the minority class and creating synthetic data, or creating new instances using heuristics. This method tends to have an overfitting problem, where it will predict the minority class more than it should. The undersampling method removes instances from the majority class either randomly or using some heuristics. Since data is being removed, potentially valuable information is not considered [Hu et al., 2016]. To see how valuable resampling is in our data set, we ran the classifying algorithms with no resampling on the original imbalanced data set, randomly undersampling method, and SMOTE, which is an oversampling method.

The undersampling method that we considered is random undersampling. In this method, instances of the majority class are discarded at random until reaches balanced with the minority class [Hoens and Chawla, 2013]. For example, say there are 1000 observations in the majority class, and 100 in the minority class, observations in the majority class will be randomly discarded until this class is also 100. The benefit of this method is that since the data frame is being reduced, it is less costly. However, potentially useful information is discarded, which may make the decision boundary between the majority and minority class less clear, causing a decrease in overall prediction performance [Hoens and Chawla, 2013].

Synthetic Minority Over-Sampling Technique (SMOTE), is an oversampling technique which uses interpolation of the minority class to create synthetic data. The process begins by finding the k-nearest neighbors of each observation of the minority class based on some distance measure. Then a point between the minority class observation and one of its nearest neighbors is randomly picked by first finding the difference between the observation and its nearest neighbor. This difference is then multiplied by a random number between 0 and 1. This is then added to the observation, which becomes the new synthetic data point that is then added to the data set [Chawla et al., 2002]. In Hu et al. [2016], they used k = 5, so that is what we used to create our resampled

data set. **I did conduct a grid search over the k-value because I was curious and found that even k = 3 provides 100% classification! I have the output for k = 5 so we can certainly use that, let's just make sure we are consistent - Emily.** Oversampling tends to have an overfitting problem since now the minority class extends into the majority space, however this generally poses less of an issue with SMOTE [Luengo et al., 2011]. This was ran using the SMOTE function in the `smotefamily` package in R [Siriseriwan, 2019].

3.2 Classification Methods

We evaluated two classifiers, Random Forest and eXtreme Boosting (XGBoost), both tree based ensemble methods. First, we utilized the Random Forest algorithm and the associated selection of independent variables for the Random Forest with the `randomForest` and `tuneRF` functions [Liaw and Wiener, 2002]. In general, a Random Forest algorithm involves the generation of many classification trees, which are each grown through recursive partitioning of independent variable space. During the growth phase for each classification tree, split points of variable space are investigated to maximize the reduction of heterogeneity, which is measured with the Gini impurity index (a reflection of the probability of a variable being wrongly chosen through a stochastic process). Each tree is then grown to a phase where node(s) represent a delineation of data per split point of each variable, and leaves are the terminal points that represent the final classification of data. After the growth phase, a leaf is potentially pruned back to a node to maximize the trade-off between complexity and rate of misclassification. A Random Forest incorporates many trees and subsequently aggregates the predictions made by each tree. We initially selected 500 trees and four variables that could be randomly sampled from to generate a split point at each node. Finally, a stepwise function was created to iteratively conduct the Random Forest algorithm for the purposes of selection of the optimal number of variables to sample from. **Let's talk about tuning of our models, it seems we used different methods - which is fine! Let's just make sure our final results reflect our choice of tuning. -Emily**

We also applied eXtreme Gradient Boosting (XGBoost) using the `xgboost` function with the multiclass classification using the softmax objective function with three classes maximizing the multiclass misclassfication error evaluation metric in the xgboost library [Chen et al., 2021]. This method combines the tree-based model approach by implementing recursive partitioning and the boosting algorithm which repeatedly optimizes classification methods on the training set. In repeated optimization, a weak classifier is fit on the original data set with each observation having equal weight, the weight is then calculated for the current model based on the error rate and observations are assigned new weights used to fit the next weak classifier. This process is repeated for a final boosted classifier given by the weighted sum of our weak classifiers. XGBoost allows for a variety of evaluation metrics providing a benefit over other boosting methods. Tuning parameters for maximum tree depth, step size shrinkage to prevent overfitting (eta), maximum number of boosting iterations, and number of threads used for parallel computing were selected by conducting a hyperparameter grid search with MCMC [Appendix A.1].

4 Results

A comparison of the best classifiers is shown in Figure 4. With no resampling, our overall baseline classification rate for Random Forest was between 93.7% and 94.9% while the rare classes had baseline classification rates of 9% and 30.9% for Low and High Quality respectively. The XGBoost had a similar overall baseline classification rate between 93.2% and 94.9% with a slight improvement in accuracy of Low and High Quality classes over Random Forest with 14.5% and 33% baseline classification rates. When undersampling on the training data set is conducted, Random Forest performs similar to the baseline in terms of overall accuracy with a classification rate between 93.4% to 94.9%, but performs better in terms of Low Quality and High Quality classification rates at 15% and 33% respectively. However, with undersampling, XGBoost results in a slight decrease from the baseline with an overall classification rate between 92.3% and 94%. We see this decrease occur from a sacrifice in classification of Normal Quality wines at 97.8%, but an increase in the Low Quality, 24.1%, and High Quality, 34.8% classification rates. We saw immense benefits of oversampling the training data set reaching consistent performance of 100% classification rate of all quality classes with both classifiers over all MCMC splits. These results indicate that oversampling outperformed undersampling and that accuracy is similar between classifiers with a slight advantage in the XGBoost classifier over Random Forest for the rare quality classification when no resampling or random undersampling is applied.

5 Discussion and Conclusion

Add discusssion about the project here. Beginning a bulletted list of possible discussion points.

- Random Forest rocks!

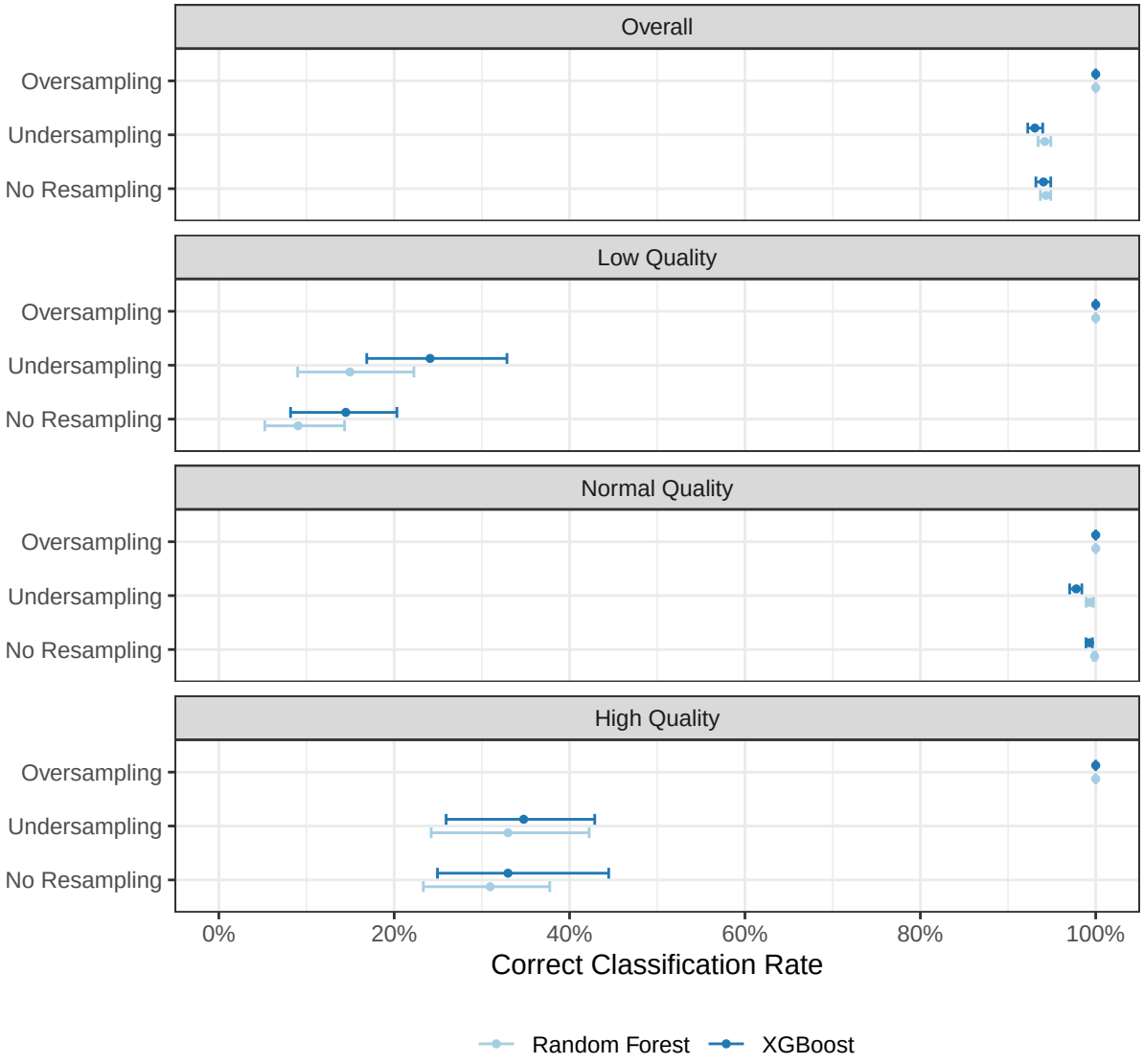

Figure 4: MCMC accuracy results for each classifier applied to each resampling technique.

- WOW, look at that oversampling method!
- Undersampling really helped increase the classification rate for rare classes.
- Tuning of XGBoost is not fun.
- As previously noted, the majority class had 6053 observations whereas the minority class had 444 observations, a ratio of about 13:1. Due to this imbalanced nature of these data, classifying algorithms were biased towards classifying wines as Normal quality, and causing poor predictions for the Low and High quality classes.

Supplementary Material

- **Data:** Data used was from the UCI Data Repository [UCI].
- **Code:** Access the final analysis code on GitHub.

Course Reflection

Discuss overall course lessons in this section. Beginning a bulleted list of possible discussion topics.

- Importance of cross validation.
- Interpretation and communication is key!
- Overall great job describing the methods in an understandable way, maybe a little more coding done in class? The homework was helpful for this!
- Instructor was well prepared for class and provided timely feedback.
- Overall really enjoyed the course!

References

Uci machine learning repository: Wine quality data set. URL https://archive.ics.uci.edu/ml/datasets/Wine+Quality.

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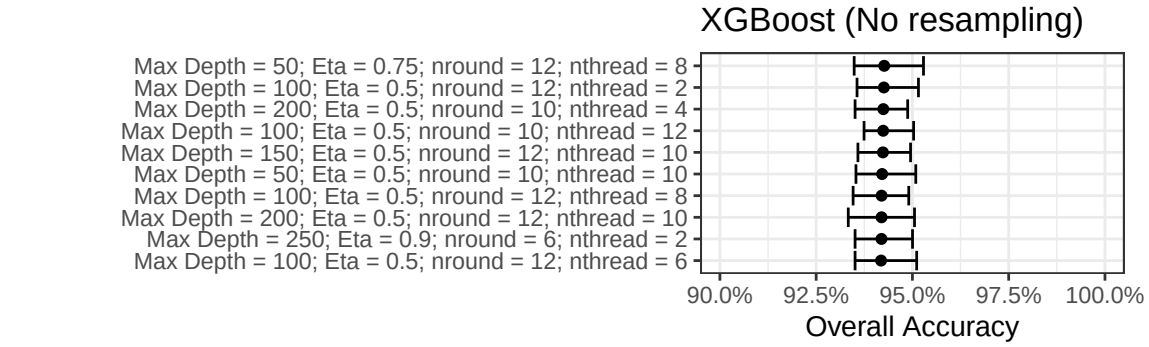
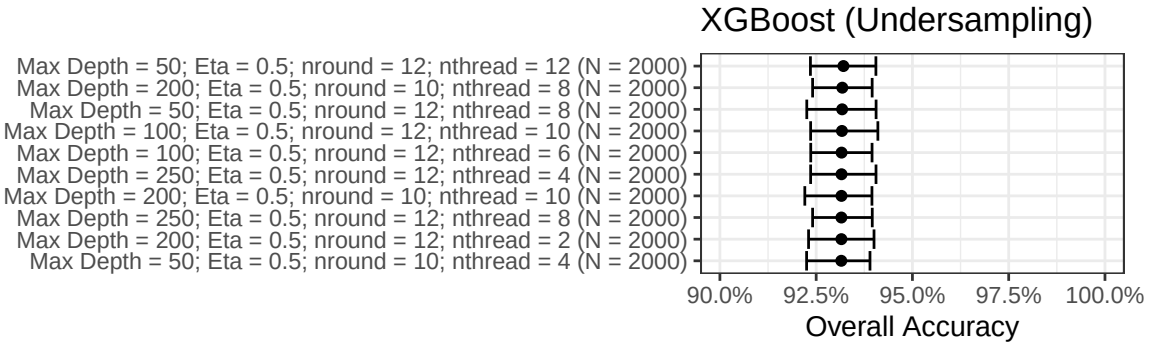
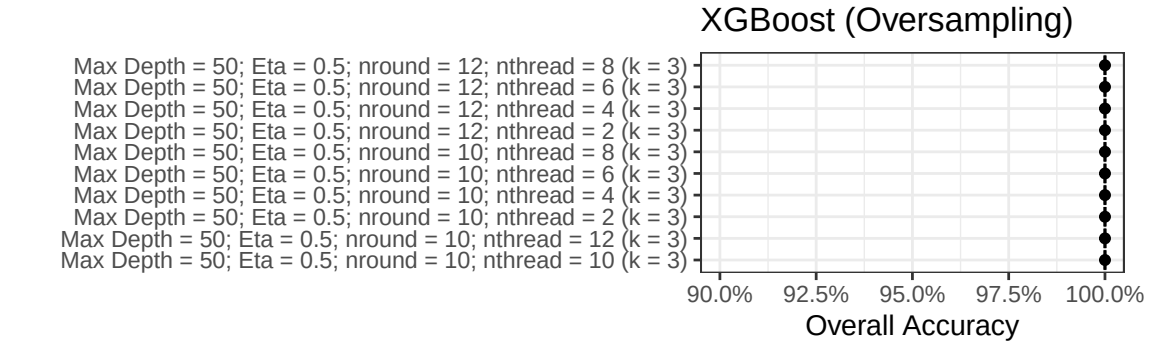
A Classification Tuning

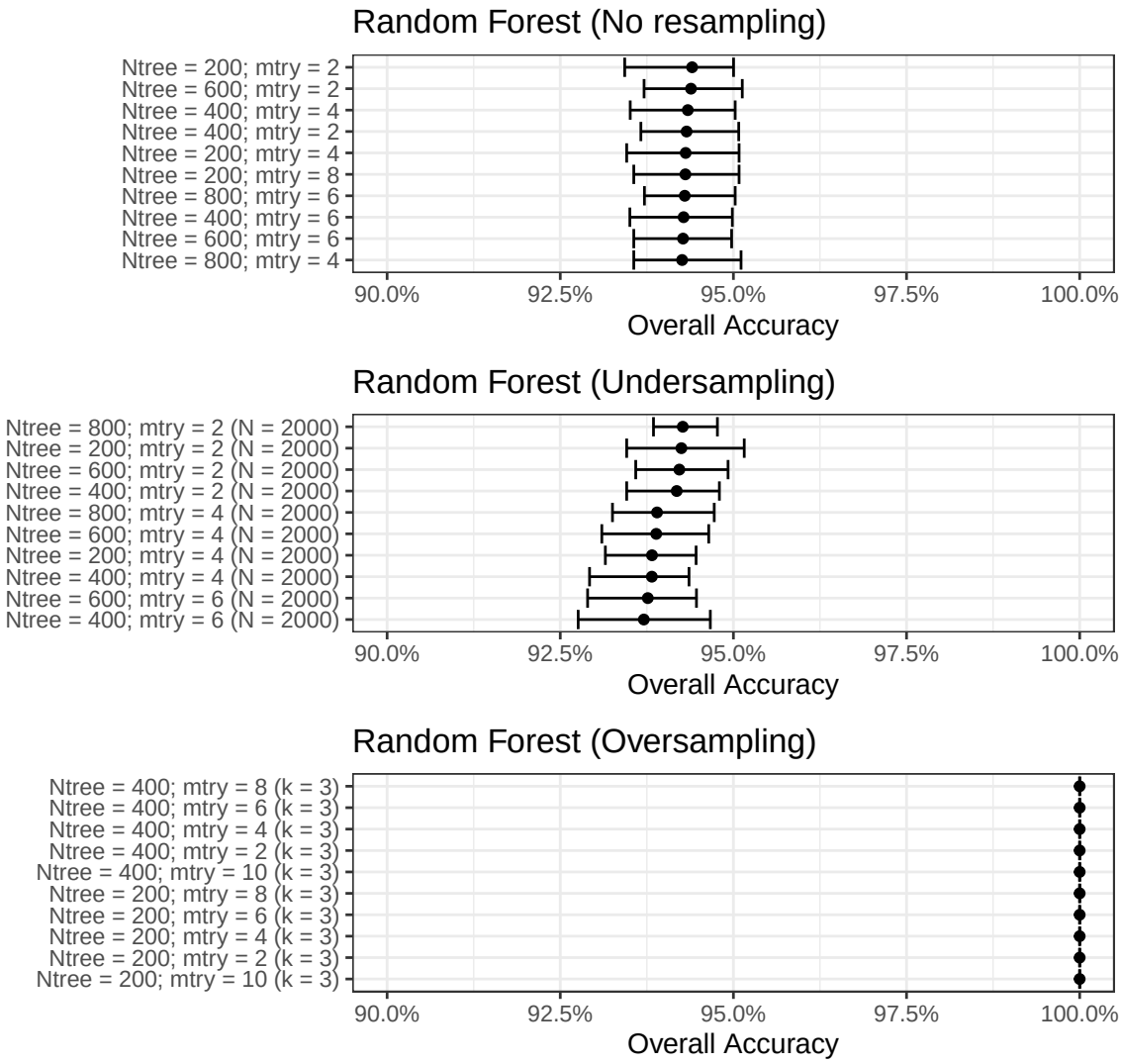
A.1 XGBoost







A.2 Random Forest



B Code

```
# LOAD LIBRARIES -------------------------------------------------------------
library(tidyverse)
library(readr)
library(xgboost)
library(Matrix)
library(tictoc)
library(furrr)
library(smotefamily)
# IMPORT DATA, RELEVEL FACTOR COLUMNS ----------------------------------------
winequality <- read_csv("data/winequality-all.csv") %>%
  mutate(type = factor(type, levels = c("red", "white")),
         type01 = as.numeric(ifelse(type == "white", 0, 1)),
         qualityclass = factor(qualityclass, levels = c("Low", "Normal", "High")),
         under_class = ifelse(qualityclass == "Normal", 0, 1),
```

```
        over_class = ifelse(qualityclass == "Low", 0,
                            ifelse(qualityclass == "Normal", 1, 2)))
colnames(winequality) <- make.names(names(winequality), unique=TRUE)
summary(winequality)
# RESAMPLING FUNCTIONS ------------------------------------------------
# FUNCTION FOR UNDERSAMPLING
undersample <- function(train_df, nsample){
  df_wine_0_ind <- which(train_df$under_class == 0)
  df_wine_1_ind <- which(train_df$under_class == 1)
  pick_0 <- sample(df_wine_0_ind, nsample)
  undersample_wine <- train_df[c(df_wine_1_ind,pick_0),] #Final Data frame
  undersample_wine <- undersample_wine %>%
    dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                  residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                  density, pH, sulphates, alcohol)
  # table(undersample_wine$under_class) # have just to make sure it's all balancing out how I think
  return(undersample_wine)
}
# FUNCTION FOR OVERSAMPLING
oversample <- function(train_df, k){

  winequality_low <- filter(winequality, qualityclass %in% c('Low'))
  winequality_normal <- filter(winequality, qualityclass %in% c('Normal'))
  winequality_high <- filter(winequality, qualityclass %in% c('High'))

  wine <- sort(sample(nrow(winequality_normal), nrow(winequality_normal)*0.5))
  winequality_norm1 <- winequality_normal[wine,]
  winequality_norm2 <- winequality_normal[-wine,]

  wine_LN <- rbind(winequality_low,winequality_norm1)
  wine_HN <- rbind(winequality_high,winequality_norm2)
  SMOTEData1 <- SMOTE(wine_LN[,c("fixed.acidity", "volatile.acidity", "citric.acid",
                                 "residual.sugar", "chlorides", "free.sulfur.dioxide",
                                 "total.sulfur.dioxide", "density", "pH", "sulphates", "alcohol",
                                 "type01")], wine_LN[,"over_class"], K = k, dup_size = 0)
  SMOTEData2 <- SMOTE(wine_HN[,c("fixed.acidity", "volatile.acidity", "citric.acid",
                                 "residual.sugar", "chlorides", "free.sulfur.dioxide",
                                 "total.sulfur.dioxide", "density", "pH", "sulphates", "alcohol",
                                 "type01")], wine_HN[,"over_class"], K = k, dup_size = 0)
  oversample_df1 <- SMOTEData1$data #Final data frame
  oversample_df2 <- SMOTEData2$data #Final data frame
  oversample_df <- rbind(oversample_df1,oversample_df2) %>%
    mutate(type01 = round(type01)) %>%
    mutate(type = as.factor(ifelse(type01 == 0, "white","red")),
           qualityclass = ifelse(class == 0, "Low",
                                 ifelse(class == "1", "Normal","High"))) %>%
    mutate(qualityclass = factor(qualityclass, levels = c("Low", "Normal", "High"))) %>%
    dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                  residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                  density, pH, sulphates, alcohol)
  #table(oversample_df$class) have just to make sure it's all balancing out how I think
  return(oversample_df)
}
# XGBOOST FUNCTIONS ---------------------------------------------------------
# SET UP FUNCTION TO EVALUATE XGBOOST
xgbFunc <-
  function(df = winequality, samplingMethod = "none", nUndersample = 2000, kOversample = 5,
           trainPct = 0.7, max.depth, eta, nround = 2, nthread = 2, show.table = F){
```

```r
require(Matrix)
require(xgboost)

# set up training/testing sets
n <- nrow(df)
train.index <- sample(seq(1,n), floor(n*trainPct), replace = F)

# create dgCMatrix for modeling

# training
train.data <-  df[train.index,] # Normal

if(samplingMethod == "undersample"){
  train.data <- undersample(train.data, nUndersample) # Undersample
}

if(samplingMethod == "oversample"){
  train.data <- oversample(train.data, kOversample) # Oversample
}

train.data <- train.data %>%
  dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                density, pH, sulphates, alcohol)

train.datamatrix   <- sparse.model.matrix(qualityclass ~ ., data = train.data)[,-1]
train.qualityclass <- train.data$qualityclass
train.label        <- as.integer(train.data$qualityclass)-1 # label conversion
xgb.train          <- list(data = train.datamatrix, label = train.label)

# testing
test.data         <- df[-train.index,] %>%
  dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                density, pH, sulphates, alcohol)
test.datamatrix   <- sparse.model.matrix(qualityclass ~ ., data = test.data)[,-1]
test.qualityclass <- test.data$qualityclass
test.label        <- as.integer(test.data$qualityclass)-1 # label conversion
xgb.test          <- list(data = test.datamatrix, label = test.label)


# fit xgboost model
xgb.fit <- xgboost(data  = xgb.train$data,
                   label = xgb.train$label,
                   booster ="gbtree",
                   max.depth = max.depth,
                   eta = eta,
                   nround = nround,
                   nthread = nthread,
                   objective = "multi:softprob",
                   eval_metric = "merror",
                   num_class = length(levels(train.qualityclass)),
                   verbose = 0
)

# predict
xgb.pred = predict(xgb.fit, xgb.test$data, reshape = T) %>% as.data.frame()
colnames(xgb.pred) = levels(train.qualityclass)
```

```
    xgb.pred$prediction = apply(xgb.pred, 1, function(x) colnames(xgb.pred)[which.max(x)])
    xgb.pred$label = levels(train.qualityclass)[test.label + 1]
    xgb.pred <- xgb.pred %>%
      mutate(prediction = factor(prediction, levels = c("Low", "Normal", "High")),
             label = factor(label, levels = c("Low", "Normal", "High")))
    # evaluated prediction
    accuracy.all  <- mean(xgb.pred$prediction==xgb.pred$label)
    table    <- with(xgb.pred, table(label, prediction))
    prop.table <- table/rowSums(table)
    accuracy.low    <- prop.table[1,1]
    accuracy.normal <- prop.table[2,2]
    accuracy.high   <- prop.table[3,3]
    accuracy <- cbind(accuracy.all, accuracy.low, accuracy.normal, accuracy.high)

    if(show.table){
      return(list(accuracy = accuracy, table = table, prop.table = prop.table))
    } else{
      return(accuracy)
    }

  }
# XGBOOST MCMC FUNCTION WITH PARALLEL COMPUTING
xgbMCMC <-
  function(samplingMethod = "none", nUndersample = 2000, kOversample = 5,
           B = 5, trainPct = 0.7, max.depth, eta, nround = 2, nthread = 2){
    require(furrr)

    # Create Parameter Grid
    mcmc.grid <- expand_grid(B = seq(1,B),
                             samplingMethod = samplingMethod,
                             nUndersample = nUndersample,
                             kOversample = kOversample,
                             trainPct = trainPct,
                             max.depth = max.depth,
                             eta = eta,
                             nround = nround,
                             nthread = nthread)

    # Obtain Accuracy
    accuracyList <- furrr::future_pmap(mcmc.grid[,-1], xgbFunc)
    xgbAccuracy <- matrix(unlist(accuracyList, use.names = TRUE), ncol = 4, nrow = nrow(mcmc.grid), byrow = T)
    colnames(xgbAccuracy) <- colnames(accuracyList[[1]])

    # Summarize Accuracy
    results <- cbind(mcmc.grid, xgbAccuracy) %>%
      pivot_longer(cols = c("accuracy.all", "accuracy.low", "accuracy.normal", "accuracy.high"),
                   names_to = "accuracyGroup",
                   values_to = "accuracy") %>%
      mutate(Method = "XGBoost") %>%
      dplyr::group_by(Method, accuracyGroup, samplingMethod, nUndersample, kOversample, max.depth, eta, nround, n
      summarise(B = n(),
                mean  = mean(accuracy),
                lower = quantile(accuracy, probs = c(0.05)),
                upper = quantile(accuracy, probs = c(0.95))) %>%
      ungroup()

    return(results)
```

```
  }
# RANDOM FOREST FUNCTIONS ----------------------------------------
# SET UP FUNCTION TO EVALUATE RANDOM FOREST
rfFunc <-
  function(df = winequality, samplingMethod = "none", nUndersample = 2000, kOversample = 5,
           trainPct = 0.7, importance = F, mtry = 4, ntree = 500, show.table = F){

    require(randomForest)

    # set up training/testing sets
    n <- nrow(df)
    train.index <- sample(seq(1,n), floor(n*trainPct), replace = F)

    # training
    train.data <-  df[train.index,] # Normal

    if(samplingMethod == "undersample"){
      train.data <- undersample(train.data, nUndersample)
    }

    if(samplingMethod == "oversample"){
      train.data <- oversample(train.data, kOversample)
    }

    train.data <- train.data %>%
      dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                    residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                    density, pH, sulphates, alcohol)

    # testing
    test.data  <- df[-train.index,] %>%
      dplyr::select(qualityclass, type, fixed.acidity, volatile.acidity, citric.acid,
                    residual.sugar, chlorides, free.sulfur.dioxide, total.sulfur.dioxide,
                    density, pH, sulphates, alcohol)

    # Fit that Random Forest!
    rf.fit <- randomForest(qualityclass ~ .,
                           data=train.data,
                           method="class",
                           ntree=ntree,
                           mtry = mtry,
                           importance=importance
    )

    # Get that Prediction!
    rf.pred = predict(rf.fit, newdata = test.data)

    # Evaluate Prediction
    accuracy.all  <- mean(rf.pred==test.data$qualityclass) #this is not working SJA
    table    <- table(test.data$qualityclass, rf.pred)
    prop.table <- table/rowSums(table)
    accuracy.low    <- prop.table[1,1]
    accuracy.normal <- prop.table[2,2]
    accuracy.high   <- prop.table[3,3]
    accuracy <- cbind(accuracy.all, accuracy.low, accuracy.normal, accuracy.high)

    if(show.table){
      return(list(accuracy = accuracy, table = table, prop.table = prop.table))
```

```
    } else{
      return(accuracy)
    }

  }
# RANDOM FOREST MCMC FUNCTION WITH PARALLEL COMPUTING
rfMCMC <-
  function(B = 5, samplingMethod = "none", nUndersample = 2000, kOversample = 5, trainPct = 0.7, ntree = 500, mtry
    require(furrr)

    # Create Parameter Grid
    mcmc.grid <- expand_grid(B = seq(1,B),
                             samplingMethod = samplingMethod,
                             nUndersample = nUndersample,
                             kOversample = kOversample,
                             trainPct = trainPct,
                             ntree = ntree,
                             mtry = mtry)

    # Obtain Accuracy
    accuracyList <- furrr::future_pmap(mcmc.grid[,-1], rfFunc)
    rfAccuracy <- matrix(unlist(accuracyList, use.names = TRUE), ncol = 4, nrow = nrow(mcmc.grid), byrow = T)
    colnames(rfAccuracy) <- colnames(accuracyList[[1]])

    # Summarize Accuracy
    results <- cbind(mcmc.grid, rfAccuracy) %>%
      pivot_longer(cols = c("accuracy.all", "accuracy.low", "accuracy.normal", "accuracy.high"),
                   names_to = "accuracyGroup",
                   values_to = "accuracy") %>%
      mutate(Method = "Random Forest") %>%
      dplyr::group_by(Method, accuracyGroup, samplingMethod, nUndersample, kOversample, ntree, mtry) %>%
      summarise(B = n(),
                mean  = mean(accuracy),
                lower = quantile(accuracy, probs = c(0.05)),
                upper = quantile(accuracy, probs = c(0.95))) %>%
      ungroup()

    return(results)

  }
# HYPERPARAMETER GRID SEARCH ---------------------------------------
setB = 50
# XGBOOST
tic()
xgbMCMC.none.gridsearch <- xgbMCMC(samplingMethod = "none",
                                   nUndersample = NA,
                                   kOversample = NA,
                                   trainPct = 0.7,
                                   B = setB,
                                   max.depth = seq(50, 250, 50),
                                   eta = c(0.05, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95),
                                   nround = seq(2,12,2),
                                   nthread = seq(2,12,2)
                                   )
toc()
xgbMCMC.none.gridsearch <- xgbMCMC.none.gridsearch %>%
  filter(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
```

```
xgbMCMC.none.gridsearch
# write.csv(xgbMCMC.none.gridsearch, file = "reports/xgbMCMC.none.gridsearch.csv", row.names = F, na = "")
xgbMCMC.none.gridsearch.plot <- xgbMCMC.none.gridsearch[c(0:10),] %>%
  mutate(label = paste("Max Depth = ", max.depth, "; Eta = ", eta, "; nround = ", nround, "; nthread = ", nthread
ggplot(aes(x = mean, y = reorder(label, mean))) +
  geom_point() +
  geom_errorbar(aes(xmin = lower, xmax = upper)) +
  theme_bw() +
  scale_y_discrete("") +
  scale_x_continuous("Overall Accuracy", labels = scales::percent) +
  ggtitle("XGBoost (No resampling)")
xgbMCMC.none.gridsearch.plot
tic()
xgbMCMC.undersample.gridsearch <- xgbMCMC(samplingMethod = "undersample",
                                          nUndersample = seq(1000, 2000, 500),
                                          kOversample = NA,
                                          trainPct = 0.7,
                                          B = setB,
                                          max.depth = seq(50, 250, 50),
                                          eta = c(0.5, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95),
                                          nround = seq(2,12,2),
                                          nthread = seq(2,12,2)
                                          )
toc()
xgbMCMC.undersample.gridsearch <- xgbMCMC.undersample.gridsearch %>%
  select(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
xgbMCMC.undersample.gridsearch
# write.csv(xgbMCMC.undersample.gridsearch, file = "reports/xgbMCMC.undersample.gridsearch.csv", row.names = F, n
xgbMCMC.undersample.gridsearch.plot <- xgbMCMC.undersample.gridsearch[c(0:10),] %>%
  mutate(label = paste("Max Depth = ", max.depth, "; Eta = ", eta, "; nround = ", nround, "; nthread = ", nthread
ggplot(aes(x = mean, y = reorder(label, mean))) +
  geom_point() +
  geom_errorbar(aes(xmin = lower, xmax = upper)) +
  theme_bw() +
  scale_y_discrete("") +
  scale_x_continuous("Overall Accuracy", labels = scales::percent) +
  ggtitle("XGBoost (Undersampling)")
xgbMCMC.undersample.gridsearch.plot
tic()
xgbMCMC.oversample.gridsearch <- xgbMCMC(samplingMethod = "oversample",
                                         nUndersample = NA,
                                         kOversample = seq(3,7,2),
                                         trainPct = 0.7,
                                         B = setB,
                                         max.depth = seq(50, 250, 50),
                                         eta = c(0.5, 0.1, 0.25, 0.5, 0.75, 0.9, 0.95),
                                         nround = seq(2,12,2),
                                         nthread = seq(2,12,2)
                                         )
toc()
xgbMCMC.oversample.gridsearch <- xgbMCMC.oversample.gridsearch %>%
  select(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
xgbMCMC.oversample.gridsearch
# write.csv(xgbMCMC.oversample.gridsearch, file = "reports/xgbMCMC.oversample.gridsearch.csv", row.names = F, na
xgbMCMC.oversample.gridsearch.plot <- xgbMCMC.oversample.gridsearch[c(0:10),] %>%
  mutate(label = paste("Max Depth = ", max.depth, "; Eta = ", eta, "; nround = ", nround, "; nthread = ", nthread
```

```
  ggplot(aes(x = mean, y = reorder(label, mean))) +
    geom_point() +
    geom_errorbar(aes(xmin = lower, xmax = upper)) +
    theme_bw() +
    scale_y_discrete("") +
    scale_x_continuous("Overall Accuracy", labels = scales::percent) +
    ggtitle("XGBoost (Oversampling)")
xgbMCMC.oversample.gridsearch.plot
# RANDOM FOREST
# No resampling
tic()
rfMCMC.none.gridsearch <- rfMCMC(samplingMethod = "none",
                                 nUndersample = NA,
                                 kOversample = NA,
                                 trainPct = 0.7,
                                 B = setB,
                                 ntree = seq(200, 800, 200),
                                 mtry = seq(2,10,2) # Default should be 4
                                )
toc()
rfMCMC.none.gridsearch <- rfMCMC.none.gridsearch %>%
  filter(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
rfMCMC.none.gridsearch
# write.csv(rfMCMC.none.gridsearch, file = "reports/rfMCMC.none.gridsearch.csv", row.names = F, na = "")
rfMCMC.none.gridsearch.plot <- rfMCMC.none.gridsearch[c(0:10),] %>%
  mutate(label = paste("Ntree = ", ntree, "; mtry = ", mtry, sep = "")) %>%
  ggplot(aes(x = mean, y = reorder(label, mean))) +
  geom_point() +
  geom_errorbar(aes(xmin = lower, xmax = upper)) +
  theme_bw() +
  scale_y_discrete("") +
  scale_x_continuous("Overall Accuracy", labels = scales::percent) +
  ggtitle("Random Forest (No resampling)")
rfMCMC.none.gridsearch.plot
# Undersample
tic()
rfMCMC.undersample.gridsearch <- rfMCMC(samplingMethod = "undersample",
                                 nUndersample = seq(1000, 2000, 500),
                                 kOversample = NA,
                                 trainPct = 0.7,
                                 B = setB,
                                 ntree = seq(200, 800, 200),
                                 mtry = seq(2,10,2) # Default should be 4
)
toc()
rfMCMC.undersample.gridsearch <- rfMCMC.undersample.gridsearch %>%
  filter(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
rfMCMC.undersample.gridsearch
# write.csv(rfMCMC.undersample.gridsearch, file = "reports/rfMCMC.undersample.gridsearch.csv", row.names = F, na
rfMCMC.undersample.gridsearch.plot <- rfMCMC.undersample.gridsearch[c(0:10),] %>%
  mutate(label = paste("Ntree = ", ntree, "; mtry = ", mtry, " (N = ", nUndersample, ")", sep = "")) %>%
  ggplot(aes(x = mean, y = reorder(label, mean))) +
  geom_point() +
  geom_errorbar(aes(xmin = lower, xmax = upper)) +
  theme_bw() +
  scale_y_discrete("") +
```

```
  scale_x_continuous("Overall Accuracy", labels = scales::percent) +
  ggtitle("Random Forest (Undersampling)")
rfMCMC.undersample.gridsearch.plot
# Oversample
tic()
rfMCMC.oversample.gridsearch <- rfMCMC(samplingMethod = "oversample",
                                       nUndersample = NA,
                                       kOversample = seq(3,7,2),
                                       trainPct = 0.7,
                                       B = setB,
                                       ntree = seq(200, 800, 200),
                                       mtry = seq(2,10,2) # Default should be 4
)
toc()
rfMCMC.oversample.gridsearch <- rfMCMC.oversample.gridsearch %>%
  filter(accuracyGroup == "accuracy.all") %>%
  arrange(-mean)
rfMCMC.oversample.gridsearch
# write.csv(rfMCMC.oversample.gridsearch, file = "reports/rfMCMC.oversample.gridsearch.csv", row.names = F, na =
rfMCMC.oversample.gridsearch.plot <- rfMCMC.oversample.gridsearch[c(0:10),] %>%
  mutate(label = paste("Ntree = ", ntree, "; mtry = ", mtry, " (k = ", kOversample, ")", sep = "")) %>%
  ggplot(aes(x = mean, y = reorder(label, mean))) +
  geom_point() +
  geom_errorbar(aes(xmin = lower, xmax = upper)) +
  theme_bw() +
  scale_y_discrete("") +
  scale_x_continuous("Overall Accuracy", labels = scales::percent) +
  ggtitle("Random Forest (Oversampling)")
rfMCMC.oversample.gridsearch.plot

# FINAL RESULTS ----------------------------------------------
# XGBOOST MCMC RESULTS
setB = 100
tic()
xgbMCMC.none.results <- xgbMCMC(samplingMethod = "none", nUndersample = NA, kOversample = NA,
                                trainPct = 0.7, B = setB, max.depth = 50, eta = 0.75, nround = 12, nthread = 8)
toc()
tic()
xgbMCMC.undersample.results <- xgbMCMC(samplingMethod = "undersample", nUndersample = 1000, kOversample = NA,
                                       trainPct = 0.7, B = setB, max.depth = 50, eta = 0.10, nround = 2, nthread =
toc()
tic()
xgbMCMC.oversample.results <- xgbMCMC(samplingMethod = "oversample", nUndersample = NA, kOversample = 3,
                                      trainPct = 0.7, B = setB, max.depth = 50, eta = 0.10, nround = 2, nthread =
toc()
xgbMCMC.results <- rbind(xgbMCMC.none.results,
                         xgbMCMC.undersample.results,
                         xgbMCMC.oversample.results) %>%
  mutate(label = paste("Max Depth = ", max.depth, "; Eta = ", eta, sep = "")) %>%
  select(-max.depth, -eta, -nround, - nthread)
# RANDOM FORST MCMC RESULTS
tic()
rfMCMC.none.results <- rfMCMC(B = setB, samplingMethod = "none", nUndersample = NA, kOversample = NA,
                              trainPct = 0.7, ntree = 200, mtry = 2)
toc()
tic()
rfMCMC.undersample.results <- rfMCMC(B = setB, samplingMethod = "undersample", nUndersample = 2000, kOversample =
                                     trainPct = 0.7, ntree = 800, mtry = 2)
```

```r
toc()
tic()
rfMCMC.oversample.results <- rfMCMC(B = setB, samplingMethod = "oversample", nUndersample = NA, kOversample = 3,
                                    trainPct = 0.7, ntree = 200, mtry = 3)
toc()
rfMCMC.results <- rbind(rfMCMC.none.results,
                        rfMCMC.undersample.results,
                        rfMCMC.oversample.results) %>%
  mutate(label = paste("N Trees = ", ntree, "; Mtry = ", mtry, sep = "")) %>%
  select(-ntree, -mtry)
# COMBINE XGBOOST AND RANDOM FOREST RESULTS & PLOT
MCMC.results <- rbind(xgbMCMC.results, rfMCMC.results)
write.csv(MCMC.results, "reports/MCMC.results.csv", row.names = F, na = "")
MCMC.results <- read_csv("reports/MCMC.results.csv")
# new facet labels
accuracyGroup.labs <- c("Overall", "Low Quality", "Normal Quality", "High Quality")
names(accuracyGroup.labs) <- c("accuracy.all", "accuracy.low", "accuracy.normal", "accuracy.high")
# plot accuracy
MCMC.results %>%
  mutate(samplingMethod = factor(samplingMethod, levels = c("none", "undersample", "oversample")),
         accuracyGroup = factor(accuracyGroup, levels = c("accuracy.all", "accuracy.low", "accuracy.normal", "accu
  ggplot(aes(x = mean, y = samplingMethod, group = Method, color = Method)) +
  geom_point(size = 1, position = position_dodge(width = 0.5)) +
  geom_errorbar(aes(xmin = lower, xmax = upper), position = position_dodge(width = 0.5), width = 0.4) +
  facet_wrap(~accuracyGroup, ncol = 1, labeller = labeller(accuracyGroup = accuracyGroup.labs)) +
  theme_bw() +
  theme(aspect.ratio = 0.2) +
  scale_y_discrete("Resampling Method") +
  scale_x_continuous("Accuracy", limits = c(0,1), breaks = seq(0,1,0.2), labels = scales::percent) +
  scale_color_brewer("", palette = "Paired")
```