Homework 3

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Reminder: All homework solutions must be written up independently, even though you are allowed to discuss with other students. You need to save your homework assignment in a pdf/html format and upload it with the R code (.R or .rmd) into the Canvas before 11:59pm CT on the due day. No late homework assignment will be graded in any circumstance.

```
# Load necessary libraries
library(caret)
library(tidyverse)
library(e1071)
library(randomForest)
library(nnet)
library(modeldata)
library(ggplot2)
library(dplyr)
library(corrplot)
library(GGally)
library(dplyr)
library(rsample)
library(recipes)
library(rpart)
library(ranger)
```

Problem 1 (25 points):

In Homework 1, Problem 3, we described a data set which contained 96 oil samples each from one of seven types of oils (pumpkin, sunflower, peanut, olive, soybean, rapeseed, and corn). Gas chromatography was performed on each sample and the percentage of each type of 7 fatty acids was determined. We would like to use these data to build a model that predicts the type of oil based on a sample's fatty acid percentages. These data can be found in the caret package using data(oil). The oil types are contained in a factor variable called oilType. The types are pumpkin (coded as A), sunflower (B), peanut (C), olive (D), soybean (E), rapeseed (F) and corn (G). In R

```
# Load the data
?oil
data(oil)
```

```
str(oilType)
```

```
 Factor w/ 7 levels "A","B","C","D",..: 1 1 1 1 1 1 1 1 1 1 ...
```

```
table(oilType)
```

```
oilType
 A  B  C  D  E  F  G
37 26  3  7 11 10  2
```

37 26 3 7 11 10 2

a. Given the classification imbalance in oil Type, describe how you would create a training and testing set.

```
set.seed(123)

oil_data <- as.data.frame(fattyAcids)
oil_data$oilType <- oilType

train_index <- createDataPartition(oil_data$oilType, p = 0.7, list = FALSE)
train_data <- oil_data[train_index, ]
test_data <- oil_data[-train_index, ]

preProcValues <- preProcess(train_data[,-ncol(train_data)], method = c("center", "scale"))
train_data[,-ncol(train_data)] <- predict(preProcValues, train_data[,-ncol(train_data)])
test_data[,-ncol(test_data)] <- predict(preProcValues, test_data[,-ncol(test_data)])

ctrl <- trainControl(method = "cv", number = 10, classProbs = TRUE, summaryFunction = multiCl
```

```
colSums(is.na(train_data))
```

```
  Palmitic    Stearic      Oleic   Linoleic  Linolenic Eicosanoic Eicosenoic 
         0          0          0          0          0          0          0 
   oilType 
         0 
```

```
train_data_clean <- na.omit(train_data)

preProcess_missing <- preProcess(train_data, method = 'medianImpute')
train_data_clean <- predict(preProcess_missing, train_data)
```

b. Which classification statistic would you choose to optimize for this problem and why? When the classes are imbalanced, I would optimize the F1 score.

c. Split the data into a training and a testing set, pre-process the data, and build models and tune them via resampling described in Chapter 12. Clearly list the models under consideration and the corresponding tuning parameters of the models.

- k-Nearest Neighbors (k-NN):

```
set.seed(123)
ctrl <- trainControl(method = "cv", number = 10)
knn_model <- train(oilType ~ ., data = train_data_clean, method = "knn", trControl = ctrl, tu
knn_model
```

```
k-Nearest Neighbors 

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G' 

No pre-processing
Resampling: Cross-Validated (10 fold) 
```

```
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
Resampling results across tuning parameters:

  k   Accuracy   Kappa
   5  0.9375000  0.9195499
   7  0.9138889  0.8913839
   9  0.8902778  0.8606707
  11  0.8500000  0.7986789
  13  0.8333333  0.7649739
  15  0.8208333  0.7493668
  17  0.7629365  0.6623458
  19  0.7629365  0.6633254
  21  0.7179365  0.5943018
  23  0.7054365  0.5779753

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was k = 5.
```

k-Nearest Neighbors (kNN)

- Best k: 5
- Accuracy: 0.9375
- Kappa: 0.9195499
- Support Vector Machine (SVM):

```
set.seed(123)
svm_model <- train(oilType ~ ., data = train_data_clean, method = "svmRadial", trControl = ct
svm_model
```

```
Support Vector Machines with Radial Basis Function Kernel

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
Resampling results across tuning parameters:

  C       Accuracy   Kappa
    0.25  0.8573810  0.8067221
    0.50  0.9263889  0.9070702
    1.00  0.9500000  0.9378462
    2.00  0.9750000  0.9686154
    4.00  0.9638889  0.9550595
    8.00  0.9638889  0.9550595
   16.00  0.9638889  0.9550595
   32.00  0.9638889  0.9550595
   64.00  0.9638889  0.9550595
  128.00  0.9638889  0.9550595
```

```
Tuning parameter 'sigma' was held constant at a value of 0.1001887
Accuracy was used to select the optimal model using the largest value.
The final values used for the model were sigma = 0.1001887 and C = 2.
```

Support Vector Machines (SVM):

- sigma = 0.1001887
- C = 2
- Accuracy: 0.975
- Kappa: 0.9686154
- Random Forest:

```
set.seed(123)
rf_grid <- expand.grid(mtry = seq(1, ncol(train_data) - 1, length.out = 6))  # Adjust the len

rf_model <- train(oilType ~ ., data = train_data, method = "rf", trControl = ctrl, tuneGrid =
rf_model
```

```
Random Forest

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
Resampling results across tuning parameters:

  mtry  Accuracy  Kappa
  1.0   0.9625    0.9523009
  2.2   0.9750    0.9679487
  3.4   0.9750    0.9679487
  4.6   0.9550    0.9405111
  5.8   0.9550    0.9405111
  7.0   0.9550    0.9405111

Accuracy was used to select the optimal model using the largest value.
The final value used for the model was mtry = 2.2.
```

Random Forest

- mtry: 2.2
- Accuracy: 0.975
- Kappa: 0.9679487

Support Vector Machines performs the best with an accuracy of 97.50% and a Kappa of 0.9686.

d. Of the models presented in this chapter, which performs best on these data? Which oil type does the model most accurately predict? Least accurately predict?

```r
# Generate predictions for each model
knn_pred <- predict(knn_model, test_data)
svm_pred <- predict(svm_model, test_data)
rf_pred <- predict(rf_model, test_data)

# Create confusion matrices
knn_cm <- confusionMatrix(knn_pred, test_data$oilType)
svm_cm <- confusionMatrix(svm_pred, test_data$oilType)
rf_cm <- confusionMatrix(rf_pred, test_data$oilType)
```

```r
# Print confusion matrices
print(knn_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 10  0  0  0  0  0  0
         B  1  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
         D  0  0  0  2  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  0  0  0  0

Overall Statistics

               Accuracy : 0.9615
                 95% CI : (0.8036, 0.999)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 7.058e-09

                  Kappa : 0.9467

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
Sensitivity            0.9091   1.0000       NA  1.00000   1.0000   1.0000
Specificity            1.0000   0.9474        1  1.00000   1.0000   1.0000
Pos Pred Value         1.0000   0.8750       NA  1.00000   1.0000   1.0000
Neg Pred Value         0.9375   1.0000       NA  1.00000   1.0000   1.0000
Prevalence             0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate         0.3846   0.2692        0  0.07692   0.1154   0.1154
Detection Prevalence   0.3846   0.3077        0  0.07692   0.1154   0.1154
Balanced Accuracy      0.9545   0.9737       NA  1.00000   1.0000   1.0000
                     Class: G
Sensitivity               NA
Specificity                1
Pos Pred Value            NA
Neg Pred Value            NA
Prevalence                 0
Detection Rate             0
```

```
Detection Rate              0
Detection Prevalence        0
Balanced Accuracy          NA
```

kNN:

- Accuracy: 0.9615
- Kappa: 0.9467
- Class A, B, D, E, and F are good
- Class C, and G have no predictions

```
print(svm_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 10  0  0  0  0  0  0
         B  1  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
         D  0  0  0  2  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  0  0  0  0

Overall Statistics

               Accuracy : 0.9615
                 95% CI : (0.8036, 0.999)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 7.058e-09

                  Kappa : 0.9467

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
Sensitivity            0.9091   1.0000       NA  1.00000   1.0000   1.0000
Specificity            1.0000   0.9474        1  1.00000   1.0000   1.0000
Pos Pred Value         1.0000   0.8750       NA  1.00000   1.0000   1.0000
Neg Pred Value         0.9375   1.0000       NA  1.00000   1.0000   1.0000
Prevalence             0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate         0.3846   0.2692        0  0.07692   0.1154   0.1154
Detection Prevalence   0.3846   0.3077        0  0.07692   0.1154   0.1154
Balanced Accuracy      0.9545   0.9737       NA  1.00000   1.0000   1.0000
                     Class: G
Sensitivity               NA
Specificity                1
Pos Pred Value            NA
Neg Pred Value            NA
Prevalence                 0
Detection Rate             0
Detection Prevalence       0
```

```
Detection Prevalence        0
Balanced Accuracy          NA
```

SVM:

- Accuracy: 0.9615
- Kappa: 0.9467
- Class A, B, D, E, and F are predicted well
- Class C and G have no predictions.

```
print(rf_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 11  0  0  0  0  0  0
         B  0  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
         D  0  0  0  2  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  0  0  0  0

Overall Statistics

               Accuracy : 1
                 95% CI : (0.8677, 1)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 1.936e-10

                  Kappa : 1

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
Sensitivity            1.0000   1.0000       NA  1.00000   1.0000   1.0000
Specificity            1.0000   1.0000        1  1.00000   1.0000   1.0000
Pos Pred Value         1.0000   1.0000       NA  1.00000   1.0000   1.0000
Neg Pred Value         1.0000   1.0000       NA  1.00000   1.0000   1.0000
Prevalence             0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate         0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Prevalence   0.4231   0.2692        0  0.07692   0.1154   0.1154
Balanced Accuracy      1.0000   1.0000       NA  1.00000   1.0000   1.0000
                     Class: G
Sensitivity                NA
Specificity                 1
Pos Pred Value             NA
Neg Pred Value             NA
Prevalence                  0
Detection Rate              0
Detection Prevalence        0
Balanced Accuracy          NA
```

```
Balanced Accuracy          NA
```

Random Forest:

- Accuracy: 1.0000
- Kappa: 1.0000
- Class A, B, D, E, F are perfect.

Conclusion:
Random Forest which has perfect accuracy and Kappa. Across all models the most accurate class is A (in terms of class). The least accurate class are Class C and G.

Problem 2 (25 points):

Use the fatty acid data from Problem 1 above.

a. Use the same data splitting approach (if any) and pre-processing steps that you did Problem 1. Using the same classification statistic as before, build models described in Chapter 13: Nonlinear Classification Models for these data. Which model has the best predictive ability? How does this optimal model's performance compare to the best linear model's performance?

```
ctrl <- trainControl(method = "cv", number = 10)

tune_grid <- expand.grid(sigma = c(0.01, 0.05, 0.1, 0.2),
                         C = c(0.25, 0.5, 1, 2, 4, 8, 16, 32, 64, 128))
```

```
set.seed(123)
svm_model <- train(oilType ~ ., data = train_data, method = "svmRadial",
                   trControl = ctrl, tuneGrid = tune_grid)

print(svm_model)
```

```
Support Vector Machines with Radial Basis Function Kernel

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
Resampling results across tuning parameters:

  sigma  C       Accuracy   Kappa
  0.01     0.25  0.3811905  0.0000000
  0.01     0.50  0.4498016  0.1246638
  0.01     1.00  0.7907143  0.7077263
  0.01     2.00  0.9277778  0.9069784
  0.01     4.00  0.9388889  0.9245806
  0.01     8.00  0.9388889  0.9245806
  0.01    16.00  0.9638889  0.9547692
  0.01    32.00  0.9638889  0.9547692
  0.01    64.00  0.9638889  0.9547692
```

```
  0.01   64.00  0.9638889  0.9547692
  0.01   128.00  0.9638889  0.9547692
  0.05     0.25  0.7379365  0.6237136
  0.05     0.50  0.9152778  0.8903510
  0.05     1.00  0.9388889  0.9240000
  0.05     2.00  0.9388889  0.9240000
  0.05     4.00  0.9750000  0.9686154
  0.05     8.00  0.9638889  0.9550595
  0.05    16.00  0.9638889  0.9550595
  0.05    32.00  0.9638889  0.9550595
  0.05    64.00  0.9638889  0.9550595
  0.05   128.00  0.9638889  0.9550595
  0.10     0.25  0.8573810  0.8067221
  0.10     0.50  0.9263889  0.9070702
  0.10     1.00  0.9500000  0.9378462
  0.10     2.00  0.9750000  0.9686154
  0.10     4.00  0.9638889  0.9550595
  0.10     8.00  0.9638889  0.9550595
  0.10    16.00  0.9638889  0.9550595
  0.10    32.00  0.9638889  0.9550595
  0.10    64.00  0.9638889  0.9550595
  0.10   128.00  0.9638889  0.9550595
  0.20     0.25  0.8916667  0.8580089
  0.20     0.50  0.9250000  0.9042889
  0.20     1.00  0.9375000  0.9209163
  0.20     2.00  0.9513889  0.9384427
  0.20     4.00  0.9513889  0.9384427
  0.20     8.00  0.9513889  0.9387330
  0.20    16.00  0.9513889  0.9387330
  0.20    32.00  0.9513889  0.9387330
  0.20    64.00  0.9513889  0.9387330
  0.20   128.00  0.9513889  0.9387330

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were sigma = 0.1 and C = 2.
```

Support Vector Machines (SVM):

- sigma = 0.1
- C = 2
- Accuracy: 0.9277778
- Kappa: 0.9069784

```r
svm_pred <- predict(svm_model, test_data)

svm_cm <- confusionMatrix(svm_pred, test_data$oilType)
print(svm_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 10  0  0  0  0  0  0
         B  1  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
```

```
         C  0  0  0  0  0  0  0
         D  0  0  0  2  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  0  0  0  0

Overall Statistics

               Accuracy : 0.9615
                 95% CI : (0.8036, 0.999)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 7.058e-09

                  Kappa : 0.9467

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
Sensitivity            0.9091   1.0000       NA  1.00000   1.0000   1.0000
Specificity            1.0000   0.9474        1  1.00000   1.0000   1.0000
Pos Pred Value         1.0000   0.8750       NA  1.00000   1.0000   1.0000
Neg Pred Value         0.9375   1.0000       NA  1.00000   1.0000   1.0000
Prevalence             0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate         0.3846   0.2692        0  0.07692   0.1154   0.1154
Detection Prevalence   0.3846   0.3077        0  0.07692   0.1154   0.1154
Balanced Accuracy      0.9545   0.9737       NA  1.00000   1.0000   1.0000
                     Class: G
Sensitivity                NA
Specificity                 1
Pos Pred Value             NA
Neg Pred Value             NA
Prevalence                  0
Detection Rate              0
Detection Prevalence        0
Balanced Accuracy          NA
```

SVM Matrix: - Accuracy : 0.9615
- Kappa : 0.9467 - High accuracy for classes A, B, D, E, and F. - Classes C, G are not predictable.

```r
set.seed(123) # for reproducibility
gbm_model <- train(oilType ~ ., data = train_data, method = "gbm",
                   trControl = ctrl, verbose = FALSE)
print(gbm_model)
```

```
Stochastic Gradient Boosting

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
```

```
Resampling results across tuning parameters:

  interaction.depth  n.trees  Accuracy  Kappa
  1                   50      0.9425    0.9248248
  1                  100      0.9425    0.9251265
  1                  150      0.9425    0.9251265
  2                   50      0.9425    0.9248248
  2                  100      0.9425    0.9251265
  2                  150      0.9425    0.9251265
  3                   50      0.9300    0.9087999
  3                  100      0.9425    0.9251265
  3                  150      0.9425    0.9251265

Tuning parameter 'shrinkage' was held constant at a value of 0.1

Tuning parameter 'n.minobsinnode' was held constant at a value of 10
Accuracy was used to select the optimal model using the largest value.
The final values used for the model were n.trees = 50, interaction.depth =
 1, shrinkage = 0.1 and n.minobsinnode = 10.
```

GBM Model: - n.trees = 50 - interaction.depth = 1 - shrinkage = 0.1 - n.minobsinnode = 10 - Accuracy: 0.9425 - Kappa: 0.9248248

```
gbm_pred <- predict(gbm_model, test_data)
gbm_cm <- confusionMatrix(gbm_pred, test_data$oilType)
print(gbm_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 11  0  0  0  0  0  0
         B  0  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
         D  0  0  0  2  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  0  0  0  0

Overall Statistics

               Accuracy : 1
                 95% CI : (0.8677, 1)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 1.936e-10

                  Kappa : 1

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
Sensitivity            1.0000   1.0000       NA  1.00000   1.0000   1.0000
```

```
Specificity             1.0000   1.0000        1  1.00000   1.0000   1.0000
Pos Pred Value          1.0000   1.0000       NA  1.00000   1.0000   1.0000
Neg Pred Value          1.0000   1.0000       NA  1.00000   1.0000   1.0000
Prevalence              0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate          0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Prevalence    0.4231   0.2692        0  0.07692   0.1154   0.1154
Balanced Accuracy       1.0000   1.0000       NA  1.00000   1.0000   1.0000
                     Class: G
Sensitivity                NA
Specificity                 1
Pos Pred Value             NA
Neg Pred Value             NA
Prevalence                  0
Detection Rate              0
Detection Prevalence        0
Balanced Accuracy          NA
```

GBM Matrix:

- Accuracy : 1
- Kappa : 1
- High accuracy for classes A, B, D, E, and F.
- Classes C, G are not predictable.

```r
set.seed(123)
nn_model <- train(oilType ~ ., data = train_data, method = "nnet",
                  trControl = ctrl, tuneLength = 5, linout = TRUE, trace = FALSE)
print(nn_model)
```

```
Neural Network

70 samples
 7 predictor
 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 62, 61, 62, 65, 63, 62, ...
Resampling results across tuning parameters:

  size  decay  Accuracy   Kappa
  1     0e+00  0.7385317  0.6383084
  1     1e-04  0.7191667  0.6065154
  1     1e-03  0.7701587  0.6728330
  1     1e-02  0.7396032  0.6430604
  1     1e-01  0.6308730  0.4573382
  3     0e+00  0.8877778  0.8516943
  3     1e-04  0.9388889  0.9233333
  3     1e-03  0.9763889  0.9699375
  3     1e-02  0.9638889  0.9547692
  3     1e-01  0.9513889  0.9400000
  5     0e+00  0.9750000  0.9679487
  5     1e-04  0.9563889  0.9429915
  5     1e-03  0.9638889  0.9550595
```

```
  5     1e-02  0.9638889  0.9547692
  5     1e-01  0.9513889  0.9387813
  7     0e+00  0.9638889  0.9534872
  7     1e-04  0.9638889  0.9541026
  7     1e-03  0.9763889  0.9707692
  7     1e-02  0.9763889  0.9707692
  7     1e-01  0.9763889  0.9707692
  9     0e+00  0.9300000  0.9105798
  9     1e-04  0.9763889  0.9710595
  9     1e-03  0.9763889  0.9710595
  9     1e-02  0.9763889  0.9707692
  9     1e-01  0.9763889  0.9710595

Accuracy was used to select the optimal model using the largest value.
The final values used for the model were size = 3 and decay = 0.001.
```

Neural Network (NN):

- size = 3
- decay = 0.001
- Accuracy: 0.9638889
  -Kappa: 0.9547692

```r
nn_pred <- predict(nn_model, test_data)

nn_cm <- confusionMatrix(nn_pred, test_data$oilType)
print(nn_cm)
```

```
Confusion Matrix and Statistics

          Reference
Prediction  A  B  C  D  E  F  G
         A 11  0  0  0  0  0  0
         B  0  7  0  0  0  0  0
         C  0  0  0  0  0  0  0
         D  0  0  0  1  0  0  0
         E  0  0  0  0  3  0  0
         F  0  0  0  0  0  3  0
         G  0  0  0  1  0  0  0

Overall Statistics

               Accuracy : 0.9615
                 95% CI : (0.8036, 0.999)
    No Information Rate : 0.4231
    P-Value [Acc > NIR] : 7.058e-09

                  Kappa : 0.9465

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: A Class: B Class: C Class: D Class: E Class: F
```

```
Sensitivity            1.0000   1.0000       NA  0.50000   1.0000   1.0000
Specificity            1.0000   1.0000        1  1.00000   1.0000   1.0000
Pos Pred Value         1.0000   1.0000       NA  1.00000   1.0000   1.0000
Neg Pred Value         1.0000   1.0000       NA  0.96000   1.0000   1.0000
Prevalence             0.4231   0.2692        0  0.07692   0.1154   0.1154
Detection Rate         0.4231   0.2692        0  0.03846   0.1154   0.1154
Detection Prevalence   0.4231   0.2692        0  0.03846   0.1154   0.1154
Balanced Accuracy      1.0000   1.0000       NA  0.75000   1.0000   1.0000
                     Class: G
Sensitivity                NA
Specificity           0.96154
Pos Pred Value             NA
Neg Pred Value             NA
Prevalence            0.00000
Detection Rate        0.00000
Detection Prevalence  0.03846
Balanced Accuracy          NA
```

Nueral Network Matrix: - Accuracy : 0.9615 - Kappa : 0.9465 - High accuracy for classes A, B, D, E, and F. - Classes C, and G do not perform well.

Conclusion: The Random forest model outperforms all the other models, almost having a perfect score; however, SVM is the best model.

b. Would you infer that the data have nonlinear separation boundaries based on this comparison?

Model performance and the confusion matrices suggests that the data has nonlinear separation boundaries due to the fact that the random forest model has a perfect accuracy and kappa, and nonlinear models performed well.

c. Which oil type does the optimal model most accurately predict? Least accurately predict?

Stochastic Gradient Boosting had perfect classification, but missing class predictions (C and G). Support Vector Machines (SVM) and Neural Network both achieved high accuracy. SVM and Neural Network have a more realistic performance reflecting slight misclassification.

Problem 3 (25 points):

The “churn” data set was developed to predict telecom customer churn based on information about their account. The data files state that the data are “artificial based on claims similar to real world.” The data consist of 19 predictors related to the customer account, such as the number of customer service calls, the area code, and the number of minutes. The outcome is whether the customer churned:

a. Start R and use these commands to load the data

```
data(mlc_churn)
str(mlc_churn)
```

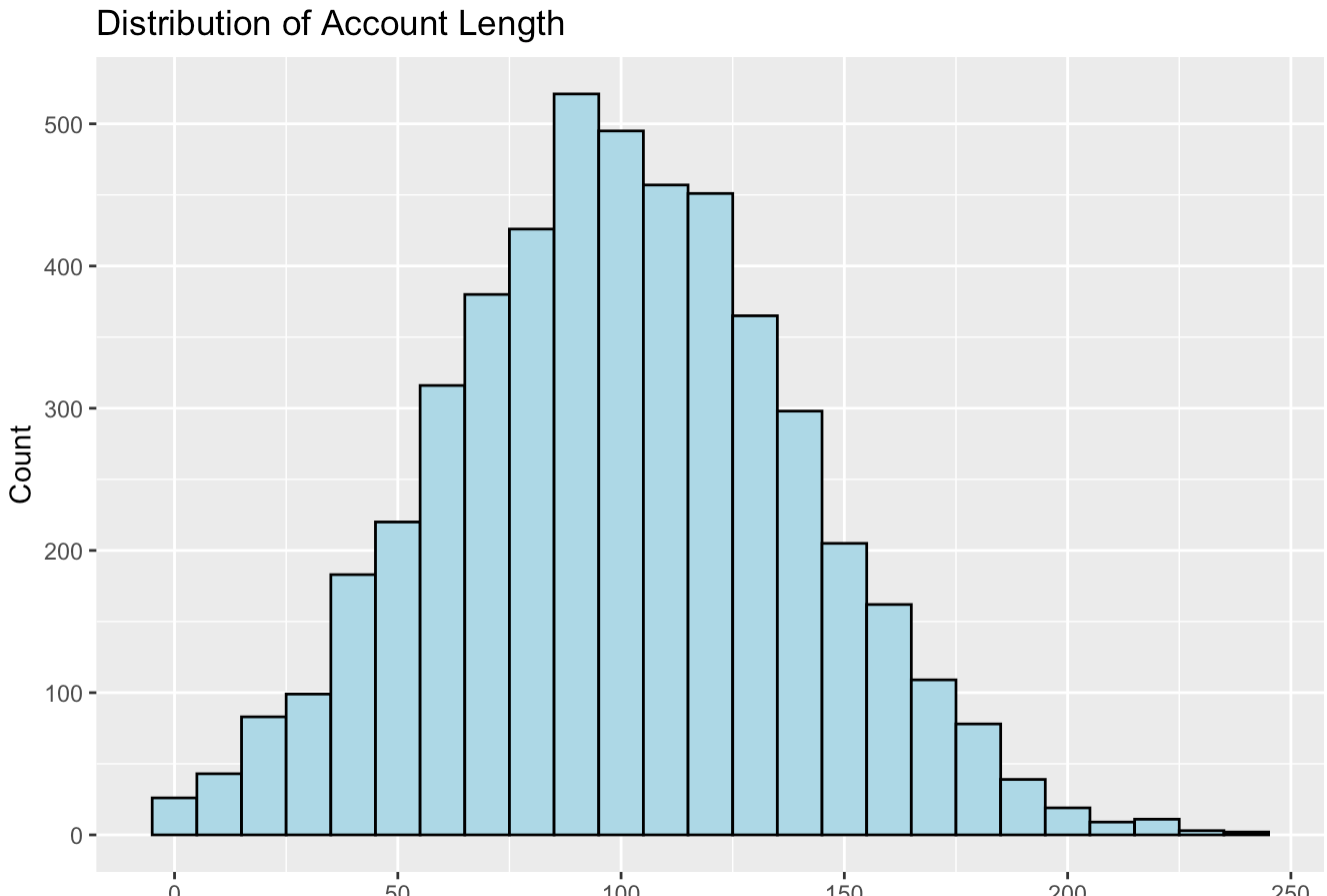
```
tibble [5,000 × 20] (S3: tbl_df/tbl/data.frame)
 $ state                     : Factor w/ 51 levels "AK","AL","AR",..: 17 36 32 36 37 2 20
25 19 50 ...
 $ account_length            : int [1:5000] 128 107 137 84 75 118 121 147 117 141 ...
 $ area_code                 : Factor w/ 3 levels "area_code_408",..: 2 2 2 1 2 3 3 2 1 2
```

```
...
 $ international_plan           : Factor w/ 2 levels "no","yes": 1 1 1 2 2 2 1 2 1 2 ...
 $ voice_mail_plan              : Factor w/ 2 levels "no","yes": 2 2 1 1 1 1 2 1 1 2 ...
 $ number_vmail_messages        : int [1:5000] 25 26 0 0 0 0 24 0 0 37 ...
 $ total_day_minutes            : num [1:5000] 265 162 243 299 167 ...
 $ total_day_calls              : int [1:5000] 110 123 114 71 113 98 88 79 97 84 ...
 $ total_day_charge             : num [1:5000] 45.1 27.5 41.4 50.9 28.3 ...
 $ total_eve_minutes            : num [1:5000] 197.4 195.5 121.2 61.9 148.3 ...
 $ total_eve_calls              : int [1:5000] 99 103 110 88 122 101 108 94 80 111 ...
 $ total_eve_charge             : num [1:5000] 16.78 16.62 10.3 5.26 12.61 ...
 $ total_night_minutes          : num [1:5000] 245 254 163 197 187 ...
 $ total_night_calls            : int [1:5000] 91 103 104 89 121 118 118 96 90 97 ...
 $ total_night_charge           : num [1:5000] 11.01 11.45 7.32 8.86 8.41 ...
 $ total_intl_minutes           : num [1:5000] 10 13.7 12.2 6.6 10.1 6.3 7.5 7.1 8.7 11.2 ...
 $ total_intl_calls             : int [1:5000] 3 3 5 7 3 6 7 6 4 5 ...
 $ total_intl_charge            : num [1:5000] 2.7 3.7 3.29 1.78 2.73 1.7 2.03 1.92 2.35 3.02
...
 $ number_customer_service_calls: int [1:5000] 1 1 0 2 3 0 3 0 1 0 ...
 $ churn                        : Factor w/ 2 levels "yes","no": 2 2 2 2 2 2 2 2 2 2 ...
```

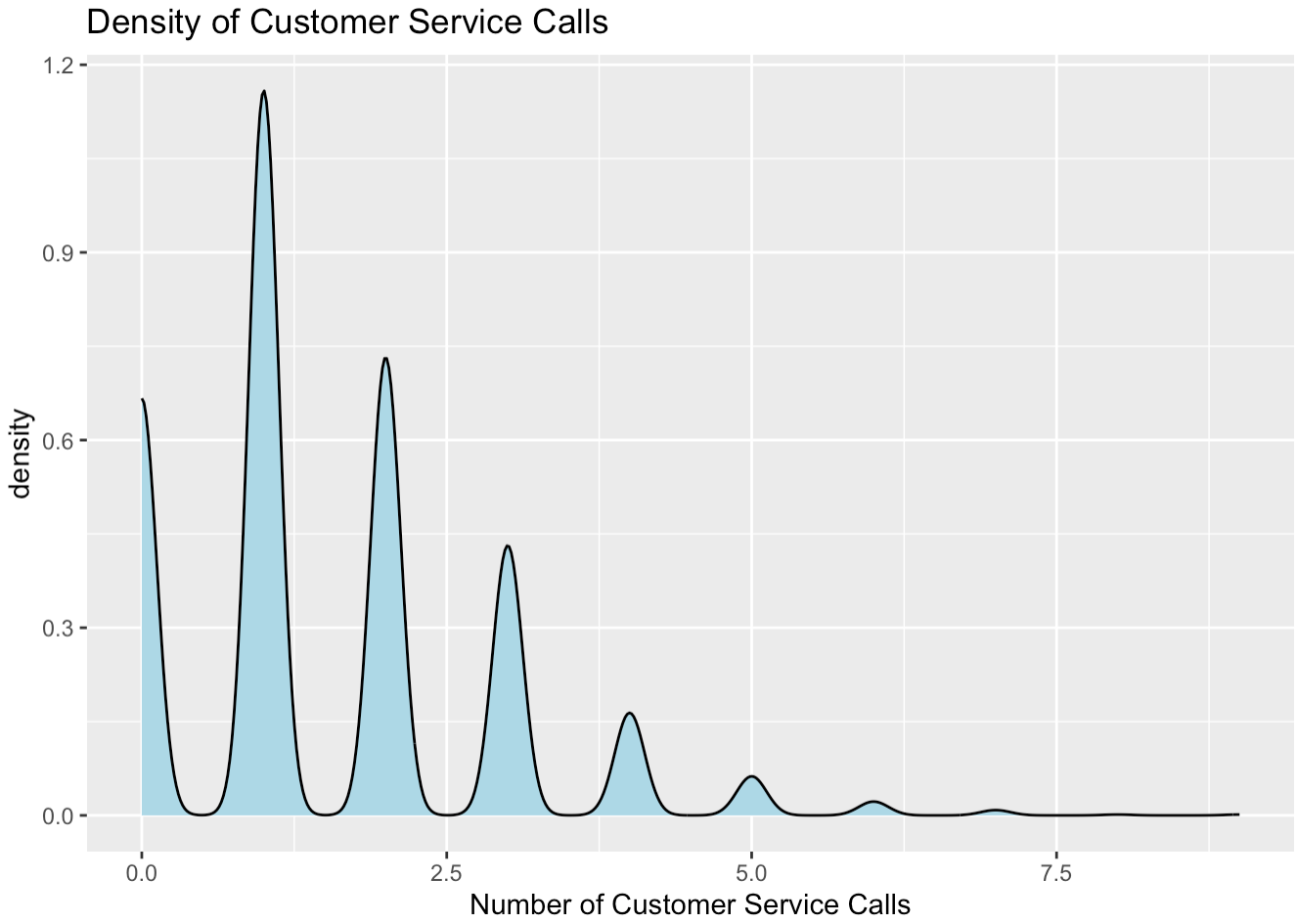
```
?mlc_churn
```

b. Explore the data by visualizing the relationship between the predictors and the outcome. Are there important features of the predictor data themselves, such as between-predictor correlations or degenerate distributions? Can functions of more than one predictor be used to model the data more effectively?

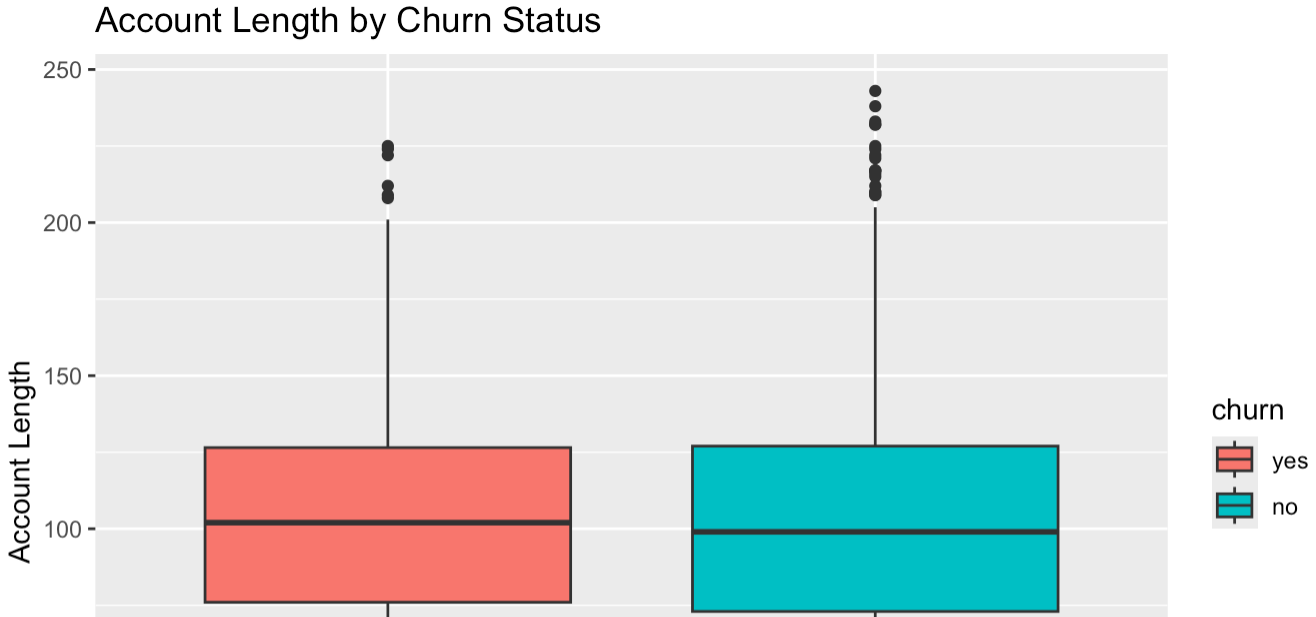
```
ggplot(mlc_churn, aes(x = account_length)) +
  geom_histogram(binwidth = 10, fill = "lightblue", color = "black") +
  labs(title = "Distribution of Account Length", x = "Account Length", y = "Count")
```

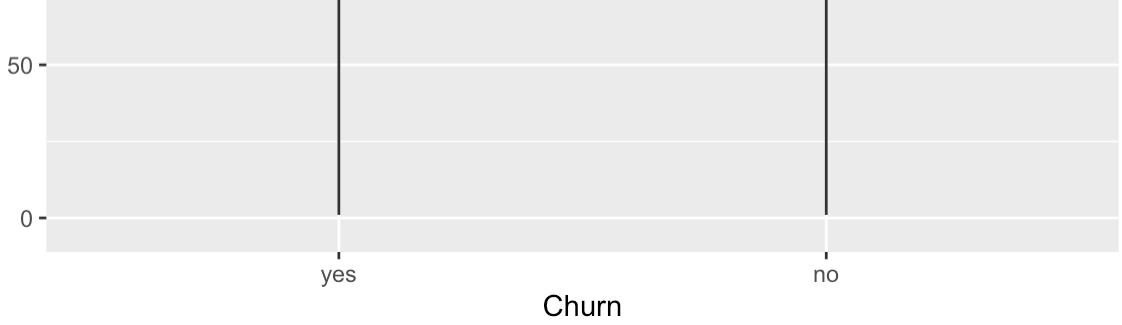



```
ggplot(mlc_churn, aes(x = number_customer_service_calls)) +
  geom_density(fill = "lightblue") +
  labs(title = "Density of Customer Service Calls", x = "Number of Customer Service Calls")
```




```
ggplot(mlc_churn, aes(x = churn, y = account_length, fill = churn)) +
  geom_boxplot() +
  labs(title = "Account Length by Churn Status", x = "Churn", y = "Account Length")
```



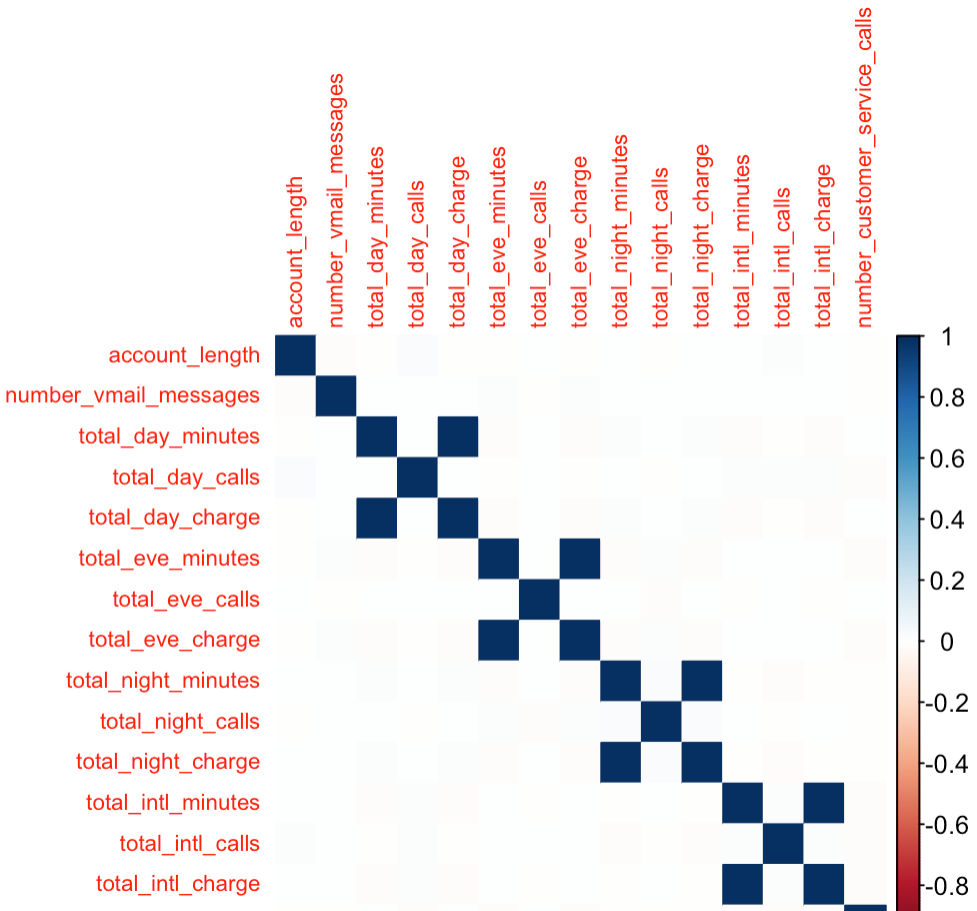



```
colnames(mlc_churn)
```

```
 [1] "state"                          "account_length"
 [3] "area_code"                      "international_plan"
 [5] "voice_mail_plan"                "number_vmail_messages"
 [7] "total_day_minutes"              "total_day_calls"
 [9] "total_day_charge"               "total_eve_minutes"
[11] "total_eve_calls"                "total_eve_charge"
[13] "total_night_minutes"            "total_night_calls"
[15] "total_night_charge"             "total_intl_minutes"
[17] "total_intl_calls"               "total_intl_charge"
[19] "number_customer_service_calls" "churn"
```

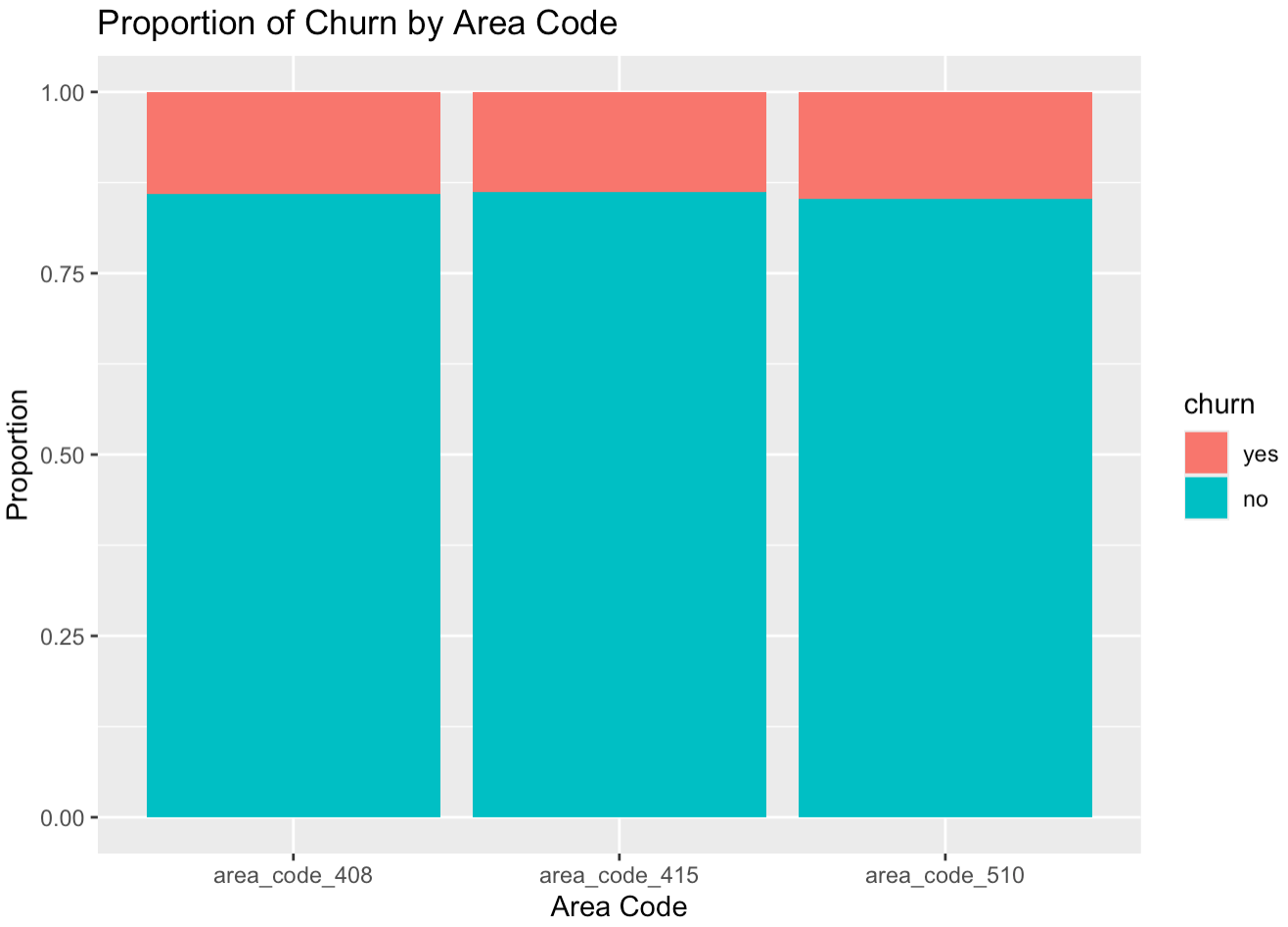
```
num_vars <- mlc_churn %>%
  select(where(is.numeric)) %>%
  select(-one_of("churn")) # Exclude the `churn` column

corr_matrix <- cor(num_vars, use = "pairwise.complete.obs")
corrplot(corr_matrix, method = "color", tl.cex = 0.7)
```



number_customer_service_calls -1

```
ggplot(mlc_churn, aes(x = area_code, fill = churn)) +
  geom_bar(position = "fill") +
  labs(title = "Proportion of Churn by Area Code", x = "Area Code", y = "Proportion")
```



c. Split the data into a training and a testing set, pre-process the data if appropriate.

```
set.seed(123)
split <- initial_split(mlc_churn, prop = 0.7)
train_data <- training(split)
test_data <- testing(split)

recipe <- recipe(churn ~ ., data = train_data) %>%
  step_normalize(all_numeric()) %>%
  step_dummy(all_nominal()) %>%
  prep(training = train_data, retain = TRUE)

train_prepped <- bake(recipe, new_data = train_data)
test_prepped <- bake(recipe, new_data = test_data)
```

d. Try building other models discussed in this chapter. Do any have better predictive performance?

```
tree_model <- rpart(churn_no ~ ., data = train_prepped, method = "class")
tree_preds <- predict(tree_model, newdata = test_prepped, type = "class")
tree_preds <- factor(tree_preds, levels = c("0", "1"))
test_churn <- factor(test_prepped$churn_no, levels = c("0", "1"))
```

```r
tree_metrics <- confusionMatrix(tree_preds, test_churn)
print(tree_metrics)
```

```
Confusion Matrix and Statistics

          Reference
Prediction    0    1
         0  142   22
         1   64 1272

               Accuracy : 0.9427
                 95% CI : (0.9297, 0.9539)
    No Information Rate : 0.8627
    P-Value [Acc > NIR] : < 2.2e-16

                  Kappa : 0.7353

 Mcnemar's Test P-Value : 9.818e-06

            Sensitivity : 0.68932
            Specificity : 0.98300
         Pos Pred Value : 0.86585
         Neg Pred Value : 0.95210
             Prevalence : 0.13733
         Detection Rate : 0.09467
   Detection Prevalence : 0.10933
      Balanced Accuracy : 0.83616

       'Positive' Class : 0
```

```r
rf_model <- ranger(churn_no ~ ., data = train_prepped, classification = TRUE)
rf_preds <- predict(rf_model, data = test_prepped)$predictions
rf_preds <- factor(rf_preds, levels = c("0", "1"))

test_churn <- factor(test_prepped$churn_no, levels = c("0", "1"))

rf_metrics <- confusionMatrix(rf_preds, test_churn)
print(rf_metrics)
```

```
Confusion Matrix and Statistics

          Reference
Prediction    0    1
         0  152    6
         1   54 1288

               Accuracy : 0.96
                 95% CI : (0.9488, 0.9693)
    No Information Rate : 0.8627
    P-Value [Acc > NIR] : < 2.2e-16

                  Kappa : 0.8129
```

```
 Mcnemar's Test P-Value : 1.298e-09

            Sensitivity : 0.7379
            Specificity : 0.9954
         Pos Pred Value : 0.9620
         Neg Pred Value : 0.9598
             Prevalence : 0.1373
         Detection Rate : 0.1013
   Detection Prevalence : 0.1053
      Balanced Accuracy : 0.8666

       'Positive' Class : 0
```

```r
svm_model <- svm(churn_no ~ ., data = train_prepped, kernel = "linear")
svm_preds <- predict(svm_model, newdata = test_prepped)
svm_preds <- factor(svm_preds, levels = c("0", "1"))

test_churn <- factor(test_prepped$churn_no, levels = c("0", "1"))

svm_metrics <- confusionMatrix(svm_preds, test_churn)
print(svm_metrics)
```

```
Confusion Matrix and Statistics

          Reference
Prediction 0 1
         0 0 0
         1 0 0

               Accuracy : NaN
                 95% CI : (NA, NA)
    No Information Rate : NA
    P-Value [Acc > NIR] : NA

                  Kappa : NaN

 Mcnemar's Test P-Value : NA

            Sensitivity :  NA
            Specificity :  NA
         Pos Pred Value :  NA
         Neg Pred Value :  NA
             Prevalence : NaN
         Detection Rate : NaN
   Detection Prevalence : NaN
      Balanced Accuracy :  NA

       'Positive' Class : 0
```

Recommendations: Random Forest: Recommended for predicting customer churn. It has the highest accuracy and balanced accuracy, so it is the most reliable. Decision Tree: Performs well. It could be considered if a

simpler model is preferred. SVM Model: Performed poorly. Might be necessary to experiment with different parameters/tuning.

Problem 4 (25 points):

Use the fatty acid data from Problem 3 above.

a. Use the same data splitting approach (if any) and pre-processing steps that you did in Problem 3.

```
set.seed(123)
split <- initial_split(fattyAcids, prop = 0.7)
train_data <- training(split)
test_data <- testing(split)

recipe <- recipe(Palmitic ~ ., data = train_data) %>%
  step_normalize(all_numeric()) %>%
  prep(training = train_data, retain = TRUE)

train_prepped <- bake(recipe, new_data = train_data)
test_prepped <- bake(recipe, new_data = test_data)
```

b. Fit a few basic trees to the training set.

```
set.seed(123)
tree_model <- train(Palmitic ~ ., data = train_prepped, method = "rpart",
                    trControl = trainControl(method = "cv", number = 10))

print(tree_model)
```

```
CART

67 samples
 6 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 61, 59, 60, 60, 60, 62, ...
Resampling results across tuning parameters:

  cp          RMSE       Rsquared   MAE
  0.01269014  0.4343674  0.8293833  0.3239018
  0.03634568  0.4755753  0.7887882  0.3522876
  0.41822619  0.8435007  0.3796150  0.6447531

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was cp = 0.01269014.
```

Summary of Model Selection:

- cp: 0.01269014
- RMSE: 0.4344
- R-squared: 0.8294
- MAE: 0.3239

- MAE: 0.3239

c. Does bagging improve the performance of the trees? What about boosting?

```
set.seed(123)
bag_model <- train(Palmitic ~ ., data = train_prepped, method = "treebag",
                   trControl = trainControl(method = "cv", number = 10))
print(bag_model)
```

```
Bagged CART

67 samples
 6 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 61, 59, 60, 60, 60, 62, ...
Resampling results:

  RMSE       Rsquared   MAE
  0.4737903  0.8053511  0.3563861
```

```
bag_pred <- predict(bag_model, newdata = test_prepped)
true_values <- test_prepped$Palmitic

bag_rmse <- sqrt(mean((true_values - bag_pred)^2))
bag_mae <- mean(abs(true_values - bag_pred))
bag_r2 <- 1 - (sum((true_values - bag_pred)^2) / sum((true_values - mean(true_values))^2))
```

Reported Bagged CART Metrics:

RMSE: 0.4738 R-squared: 0.8054 MAE: 0.3564

```
set.seed(123)
boost_model <- train(Palmitic ~ ., data = train_prepped, method = "gbm",
                     trControl = trainControl(method = "cv", number = 10),
                     verbose = FALSE)
print(boost_model)
```

```
Stochastic Gradient Boosting

67 samples
 6 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 61, 59, 60, 60, 60, 62, ...
Resampling results across tuning parameters:

  interaction.depth  n.trees  RMSE       Rsquared   MAE
  1                   50      0.6626056  0.6237379  0.5423409
  1                  100      0.6362505  0.6624431  0.5116362
  1                  150      0.6165107  0.6822524  0.5015556
  2                   50      0.6364163  0.6691804  0.5231758
```

```
  2                  100      0.5842062  0.7173840  0.4729791
  2                  150      0.5624239  0.7326215  0.4603205
  3                   50      0.6417222  0.6786888  0.5130903
  3                  100      0.6176002  0.6811174  0.4895127
  3                  150      0.5818666  0.7215028  0.4630890

Tuning parameter 'shrinkage' was held constant at a value of 0.1

Tuning parameter 'n.minobsinnode' was held constant at a value of 10
RMSE was used to select the optimal model using the smallest value.
The final values used for the model were n.trees = 150, interaction.depth =
 2, shrinkage = 0.1 and n.minobsinnode = 10.
```

```r
boost_pred <- predict(boost_model, newdata = test_prepped)
boost_rmse <- sqrt(mean((true_values - boost_pred)^2))
boost_mae <- mean(abs(true_values - boost_pred))
boost_r2 <- 1 - (sum((true_values - boost_pred)^2) / sum((true_values - mean(true_values))^2)
```

Stochastic Gradient Boosting: - (n.trees): 150 - (interaction.depth): 2 - (shrinkage): 0.1 (constant) - (n.minobsinnode): 10 (constant) - RMSE: 0.5819 - R-squared: 0.7215 - MAE: 0.4631

d. Which model has better performance, and what are the corresponding tuning parameters?

The Decision Tree model has the lowest RMSE, indicating the best performance in terms of prediction accuracy.The Boosting model achieves the highest R-squared value, suggesting it explains the variance best.