# ADS-503 Team 4 Modeling

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```
library(readr)
library(data.table)
library(mlbench)
library(ggplot2)
library(tidyr)
library(corrplot)
## corrplot 0.84 loaded
library(e1071)
library(caret)
## Loading required package: lattice
library(naniar)
library(MLmetrics)
## Attaching package: 'MLmetrics'
## The following objects are masked from 'package:caret':
##
##
       MAE, RMSE
## The following object is masked from 'package:base':
##
       Recall
##
library(dplyr)
##
## Attaching package: 'dplyr'
## The following objects are masked from 'package:data.table':
##
##
       between, first, last
## The following objects are masked from 'package:stats':
##
##
       filter, lag
## The following objects are masked from 'package:base':
##
       intersect, setdiff, setequal, union
library(MASS)
```

##

```
## Attaching package: 'MASS'
## The following object is masked from 'package:dplyr':
##
##
       select
library(pROC)
## Type 'citation("pROC")' for a citation.
##
## Attaching package: 'pROC'
## The following objects are masked from 'package:stats':
##
##
       cov, smooth, var
library(gbm)
## Loaded gbm 2.1.8
# Parallel Processing
library(doParallel)
## Loading required package: foreach
## Loading required package: iterators
## Loading required package: parallel
cl <- makePSOCKcluster(5)</pre>
```

## Synthetic Financial Datasets For Fraud Detection

### **Data Preparation**

```
synth_df <- fread('./data/PS_20174392719_1491204439457_log.csv', header = TRUE)
synth_df <- subset(synth_df, select = -c(isFlaggedFraud, nameOrig, nameDest))</pre>
synth_df <- cbind(synth_df, data.frame(hours_intraday = synth_df$step %% 24,
                                             by_day = round(synth_df$step / 24),
                                             day_of_week = round(synth_df$step / 24) %% 7))
{\it \# Log transform (amount, oldbalanceOrg, newbalanceOrig, oldbalanceDest, newbalanceDest)}
cont_vars <- c('amount', 'oldbalanceOrg', 'newbalanceOrig', 'oldbalanceDest', 'newbalanceDest')</pre>
# add small constant to prevent inf values
log_scaled <- sapply(data.frame(synth_df)[, cont_vars], function(x) log(x + 1))</pre>
colnames(log_scaled) <- lapply(cont_vars, function(x) paste('log_', x, sep=''))</pre>
synth_df <- cbind(synth_df, log_scaled)</pre>
synth_df$type <- as.factor(synth_df$type)</pre>
dmy <- dummyVars(" ~ type", data = synth_df, sep = '.', fullRank = TRUE)</pre>
synth_df <- cbind(synth_df, data.frame(predict(dmy, newdata = synth_df)))</pre>
# drop type
synth_df <- subset(synth_df, select = -c(type))</pre>
```

Split Data into Training and Test Datasets using Stratified Random Sampling

```
# split x and y
x <- subset(synth_df, select = -c(isFraud))
y <- synth_df$isFraud

data_part <- createDataPartition(y = y, p = 0.75, list = FALSE)

x_train <- x[data_part, ]
y_train <- y[data_part]
x_test <- x[-data_part, ]
y_test <- y[-data_part]

y_train <- as.factor(y_train)
y_test <- as.factor(y_test)
levels(y_train) <- c('no', 'yes')
levels(y_test) <- c('no', 'yes')</pre>
```

# Modeling

### **Neural Network**

```
nnetModel
## Neural Network
##
## 4771965 samples
        18 predictor
##
        2 classes: 'no', 'yes'
##
##
## Pre-processing: scaled (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817571, 3817572, 3817572, 3817573
## Resampling results across tuning parameters:
##
##
                              Precision Recall
     size
          decay AUC
##
          0.01
                  0.03841136 0.9991485 0.9998995 0.9995237
     1
##
     1
          0.05
                  0.08480826
                             0.9995132 0.9999060
                                                   0.9997095
##
          0.10
                 0.05056086 0.9991267 0.9999748
                                                   0.9995505
     1
##
     2
          0.01
                 0.00000000 0.9987188 1.0000000
                                                   0.9993590
##
          0.05
                 0.46270579 0.9993290 0.9999692 0.9996489
     2
##
     2
          0.10
                 0.20514610 0.9991269 0.9999287
                                                   0.9995275
          0.01
##
    3
                 0.15922016  0.9987188  1.0000000  0.9993590
##
    3
          0.05
                 0.11514449 0.9989077 0.9999973 0.9994522
##
          0.10
                 0.07911778 0.9989279 0.9999914 0.9994593
     3
          0.01
                 0.00000000 0.9987188 1.0000000 0.9993590
##
     4
          0.05
##
     4
                 0.03219574 0.9987188 1.0000000 0.9993590
##
     4
          0.10
                 0.00000000 0.9987188 1.0000000 0.9993590
##
     5
          0.01
                 0.00000000 0.9987188 1.0000000 0.9993590
     5
          0.05
##
                  0.10122763 0.9988911 0.9999713 0.9994309
##
          0.10
                  0.00000000 0.9987188 1.0000000 0.9993590
##
## AUC was used to select the optimal model using the largest value.
## The final values used for the model were size = 2 and decay = 0.05.
Neural Network Prediction on Test Data
nnetPred <- readRDS('rds_files/nnet_pred.rds')</pre>
nnetCFM <- confusionMatrix(nnetPred, y_test, positive = 'yes')</pre>
nnetCFM
## Confusion Matrix and Statistics
##
##
            Reference
## Prediction
                  no
                         yes
##
         no 1588556
                         2099
##
         yes
                   0
                            0
##
##
                  Accuracy : 0.9987
##
                    95% CI: (0.9986, 0.9987)
      No Information Rate: 0.9987
##
##
       P-Value [Acc > NIR] : 0.5058
##
##
                     Kappa: 0
##
   Mcnemar's Test P-Value : <2e-16
##
##
```

```
##
               Sensitivity: 0.00000
##
               Specificity: 1.00000
##
            Pos Pred Value :
##
            Neg Pred Value: 0.99868
##
                Prevalence: 0.00132
##
            Detection Rate: 0.00000
##
      Detection Prevalence: 0.00000
         Balanced Accuracy: 0.50000
##
##
##
          'Positive' Class : yes
##
```

#### Neural Network Variable Importance

```
varImp(nnetModel)
```

```
## nnet variable importance
##
##
                      Overall
## newbalanceOrig
                      100.000
## oldbalanceOrg
                       94.576
## type.DEBIT
                       55.842
## oldbalanceDest
                       45.186
## log_newbalanceOrig 43.786
## log_oldbalanceDest 41.047
## type.CASH_OUT
                       39.638
## log_oldbalanceOrg
                       32.570
## log_newbalanceDest 31.992
## type.TRANSFER
                       26.864
## type.PAYMENT
                       25.894
## newbalanceDest
                       23.269
## log_amount
                       20.260
## amount
                       19.157
## day_of_week
                       18.376
## by_day
                       13.672
## step
                        5.901
## hours_intraday
                        0.000
```

### Linear Discriminant Analysis

```
}
ldaModel
## Linear Discriminant Analysis
##
## 4771965 samples
##
        18 predictor
         2 classes: 'no', 'yes'
##
##
## Pre-processing: scaled (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817571, 3817572, 3817572, 3817573
## Resampling results:
##
##
     AUC
                   Precision Recall
##
     0.0005841567
                   0.9992177 0.9999041 0.9995608
LDA Prediction on Test Data
ldaPred <- readRDS('rds_files/lda_pred.rds')</pre>
ldaCFM <- confusionMatrix(ldaPred, y_test, positive = 'yes')</pre>
ldaCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                          yes
          no 1588403
##
                          1253
##
          yes
                  153
                          846
##
##
                  Accuracy : 0.9991
##
                    95% CI : (0.9991, 0.9992)
##
       No Information Rate: 0.9987
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 0.5458
##
    Mcnemar's Test P-Value : < 2.2e-16
##
##
##
               Sensitivity: 0.4030491
               Specificity: 0.9999037
##
##
            Pos Pred Value : 0.8468468
            Neg Pred Value: 0.9992118
##
##
                Prevalence : 0.0013196
##
            Detection Rate: 0.0005319
##
      Detection Prevalence: 0.0006280
##
         Balanced Accuracy: 0.7014764
##
##
          'Positive' Class : yes
LDA Variable Importance
varImp(ldaModel)
```

```
##
##
                      Importance
                          100.00
## log_oldbalanceOrg
                          100.00
## oldbalanceOrg
## log_amount
                           93.07
## amount
                           93.07
## type.TRANSFER
                           66.00
## newbalanceOrig
                           65.53
## log_newbalanceOrig
                           65.53
## type.PAYMENT
                           54.10
## step
                           54.00
## by_day
                           52.76
## hours_intraday
                           49.38
## log_oldbalanceDest
                           41.67
## oldbalanceDest
                           41.67
## type.CASH_OUT
                           23.98
## day_of_week
                           15.74
## newbalanceDest
                           11.49
## log_newbalanceDest
                           11.49
## type.DEBIT
                            0.00
```

### Quadratic Discriminant Analysis

#### Training

#### qdaModel

```
## Quadratic Discriminant Analysis
##
## 4771965 samples
##
        18 predictor
         2 classes: 'no', 'yes'
##
##
## Pre-processing: principal component signal extraction (18), scaled
## (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817571, 3817572, 3817572, 3817573
## Resampling results:
##
##
     AUC
                                      F
                Precision Recall
##
    0.2011124 0.9997956 0.9934996 0.9966375
```

#### QDA Prediction on Test Data

```
qdaPred <- readRDS('rds_files/qda_pred.rds')</pre>
qdaCFM <- confusionMatrix(qdaPred, y_test, positive = 'yes')</pre>
qdaCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                           yes
##
          no 1578607
                           295
##
          yes
                 9949
                          1804
##
##
                  Accuracy : 0.9936
##
                    95% CI: (0.9934, 0.9937)
##
       No Information Rate: 0.9987
##
       P-Value [Acc > NIR] : 1
##
##
                     Kappa: 0.2588
##
    Mcnemar's Test P-Value : <2e-16
##
##
##
               Sensitivity: 0.859457
##
               Specificity: 0.993737
##
            Pos Pred Value: 0.153493
            Neg Pred Value: 0.999813
##
##
                Prevalence: 0.001320
##
            Detection Rate: 0.001134
##
      Detection Prevalence: 0.007389
##
         Balanced Accuracy: 0.926597
##
##
          'Positive' Class : yes
##
```

#### **QDA** Variable Importance

varImp(qdaModel)

```
## ROC curve variable importance
##
##
                       Importance
## log_oldbalanceOrg
                           100.00
## oldbalanceOrg
                           100.00
## log_amount
                           93.07
## amount
                            93.07
## type.TRANSFER
                            66.00
## newbalanceOrig
                            65.53
## log newbalanceOrig
                            65.53
## type.PAYMENT
                           54.10
## step
                           54.00
## by_day
                           52.76
## hours_intraday
                            49.38
## log_oldbalanceDest
                           41.67
## oldbalanceDest
                            41.67
## type.CASH_OUT
                            23.98
## day_of_week
                            15.74
```

```
## newbalanceDest 11.49
## log_newbalanceDest 11.49
## type.DEBIT 0.00
```

### Logistic Regression

##

Mcnemar's Test P-Value : < 2.2e-16

```
Training
if (TRAIN) {
  ctrl <- trainControl(summaryFunction = prSummary, classProbs = TRUE)</pre>
  lrModel <- train(x_train, y= y_train, method = 'glm',</pre>
                   preProcess = c('center', 'scale'),
                   metric = 'AUC', trControl = ctrl)
  saveRDS(lrModel, "rds_files/lr_model.rds")
} else {
  lrModel <- readRDS('rds_files/lr_model.rds')</pre>
}
lrModel
## Generalized Linear Model
## 4771965 samples
        18 predictor
##
         2 classes: 'no', 'yes'
##
## Pre-processing: centered (18), scaled (18)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 4771965, 4771965, 4771965, 4771965, 4771965, 4771965, ...
## Resampling results:
##
##
     AUC
                Precision Recall
     0.1244624 0.9993675 0.9999007 0.999634
##
Logistic Regression Prediction on Test Data
lrPred <- readRDS('rds_files/lr_pred.rds')</pre>
lrCFM <- confusionMatrix(lrPred, y_test, positive = 'yes')</pre>
lrCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                           yes
##
          no 1588485
                           565
                          1534
##
                   71
          yes
##
##
                  Accuracy : 0.9996
##
                     95% CI: (0.9996, 0.9996)
##
       No Information Rate: 0.9987
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                      Kappa: 0.8281
```

```
##
##
               Sensitivity: 0.7308242
##
               Specificity: 0.9999553
            Pos Pred Value : 0.9557632
##
##
            Neg Pred Value: 0.9996444
##
                Prevalence : 0.0013196
##
            Detection Rate: 0.0009644
##
      Detection Prevalence: 0.0010090
##
         Balanced Accuracy: 0.8653898
##
##
          'Positive' Class : yes
##
```

#### Logistic Regression Variable Importance

```
varImp(lrModel)
```

```
## glm variable importance
##
##
                        Overall
## log_newbalanceDest 1.000e+02
## log_amount
                      7.269e+01
## log_oldbalanceOrg 6.838e+01
## log_newbalanceOrig 6.382e+01
## hours_intraday
                      6.361e+01
## oldbalanceOrg
                      5.883e+01
## newbalanceOrig
                      5.532e+01
## amount
                      2.922e+01
## day_of_week
                      1.648e+01
## oldbalanceDest
                      1.479e+01
## newbalanceDest
                      1.457e+01
## log_oldbalanceDest 5.659e+00
## step
                      3.498e+00
## type.TRANSFER
                      6.534e-01
## type.CASH_OUT
                      6.514e-01
## type.PAYMENT
                      1.366e-01
## type.DEBIT
                      7.362e-03
## by_day
                      0.000e+00
```

### Partial Least Squares Discriminant Analysis

```
plsdaModel
## Partial Least Squares
##
## 4771965 samples
##
        18 predictor
##
         2 classes: 'no', 'yes'
##
## Pre-processing: centered (18), scaled (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817572, 3817572, 3817572
## Resampling results across tuning parameters:
##
##
                       Precision Recall F
     ncomp AUC
##
            0.9998824 0.9987188 1
     1
                                           0.999359
##
            0.9998644 0.9987188 1
                                           0.999359
##
     3
            0.9999250 0.9987188 1
                                           0.999359
##
     4
            0.9999585 0.9987188 1
                                           0.999359
##
            0.9999605 0.9987188 1
                                           0.999359
##
## AUC was used to select the optimal model using the largest value.
## The final value used for the model was ncomp = 5.
PLSDA on Test Data
plsdaPred <- readRDS('rds_files/plsda_pred.rds')</pre>
plsdaCFM <- confusionMatrix(plsdaPred, y_test, positive = 'yes')</pre>
plsdaCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                          yes
##
          no 1588556
                         2099
##
                            0
          yes
##
                  Accuracy : 0.9987
##
##
                    95% CI: (0.9986, 0.9987)
       No Information Rate: 0.9987
##
##
       P-Value [Acc > NIR] : 0.5058
##
##
                     Kappa: 0
##
##
    Mcnemar's Test P-Value : <2e-16
##
##
               Sensitivity: 0.00000
##
               Specificity: 1.00000
##
            Pos Pred Value :
##
            Neg Pred Value: 0.99868
##
                Prevalence: 0.00132
##
            Detection Rate: 0.00000
##
      Detection Prevalence: 0.00000
##
         Balanced Accuracy: 0.50000
##
##
          'Positive' Class : yes
```

##

#### PLSDA Variable Importance

```
varImp(plsdaModel)
##
## Attaching package: 'pls'
## The following object is masked from 'package:caret':
##
##
## The following object is masked from 'package:corrplot':
##
##
       corrplot
## The following object is masked from 'package:stats':
##
##
       loadings
## pls variable importance
##
##
                      Overall
## amount
                      100.000
## log_oldbalanceOrg
                      78.252
## type.TRANSFER
                       61.690
## log_newbalanceOrig 55.866
## log_newbalanceDest 49.261
## type.PAYMENT
                       47.320
## log_amount
                       44.899
## hours_intraday
                       42.615
                       40.622
## step
## log_oldbalanceDest 40.594
                       39.698
## by_day
## oldbalanceOrg
                       35.692
## type.CASH_OUT
                       33.679
## oldbalanceDest
                       22.278
## newbalanceOrig
                       14.196
## newbalanceDest
                        6.730
## type.DEBIT
                        2.192
## day_of_week
                        0.000
```

### Support Vector Machines

```
fit = FALSE)
  saveRDS(svmModel, 'rds_files/svm_model.rds')
} else {
  svmModel <- readRDS('rds_files/svm_model.rds')</pre>
svmModel
## Support Vector Machines with Radial Basis Function Kernel
## 4771965 samples
##
        18 predictor
         2 classes: 'no', 'yes'
##
## Pre-processing: scaled (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817572, 3817572, 3817572
## Resampling results:
##
##
     ROC
                Sens
                           Spec
##
     0.9956985 0.9999631 0.7440299
##
## Tuning parameter 'sigma' was held constant at a value of 0.01837413
## Tuning parameter 'C' was held constant at a value of 1
SVM on Test Data
svmPred <- readRDS('rds_files/svm_pred.rds')</pre>
svmCFM <- confusionMatrix(svmPred, y_test, positive = 'yes')</pre>
svmCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   nο
                          yes
##
         no 1588494
                          500
                         1599
##
                   62
         yes
##
##
                  Accuracy: 0.9996
##
                    95% CI: (0.9996, 0.9997)
       No Information Rate: 0.9987
##
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 0.8504
##
   Mcnemar's Test P-Value : < 2.2e-16
##
##
##
               Sensitivity: 0.761791
               Specificity: 0.999961
##
##
            Pos Pred Value: 0.962673
            Neg Pred Value: 0.999685
##
##
                Prevalence: 0.001320
##
            Detection Rate: 0.001005
##
      Detection Prevalence: 0.001044
```

##

Balanced Accuracy: 0.880876

```
##
## 'Positive' Class : yes
##
```

#### SVM Variable Importance

```
varImp(svmModel)
```

```
## ROC curve variable importance
##
##
                     Importance
## oldbalanceOrg
                        100.00
## log_oldbalanceOrg
                        100.00
## log_amount
                         93.07
## amount
                          93.07
## type.TRANSFER
                          66.00
## newbalanceOrig
                          65.53
## log_newbalanceOrig
                          65.53
## type.PAYMENT
                          54.10
## step
                          54.00
## by_day
                          52.76
## hours_intraday
                          49.38
## log_oldbalanceDest
                          41.67
## oldbalanceDest
                          41.67
## type.CASH_OUT
                          23.98
## day_of_week
                          15.74
## newbalanceDest
                          11.49
## log_newbalanceDest
                          11.49
## type.DEBIT
                           0.00
```

#### Nearest Shrunken Centroids

#### Training

nscModel

```
## Nearest Shrunken Centroids
##
## 4771965 samples
## 18 predictor
## 2 classes: 'no', 'yes'
##
```

```
## Pre-processing: scaled (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817573, 3817571, 3817572, 3817572
## Resampling results across tuning parameters:
##
##
     threshold ROC
                           Sens
                                      Spec
##
                0.9323871 0.9987912 0.06934934
##
      1
                0.9317410 0.9988023 0.06885847
##
      2
                0.9310041 0.9988073
                                      0.06738601
##
      3
                0.9301870 0.9988122 0.06526009
##
      4
                0.9292877
                           0.9988178 0.06411537
##
      5
                0.9282892
                           0.9988246 0.06280671
##
      6
                0.9272498
                           0.9988323 0.06100758
      7
##
                           0.9988430 0.05904506
                0.9262361
##
      8
                0.9252065
                           0.9988539 0.05708241
##
      9
                0.9242789
                           0.9988726
                                     0.05593755
##
     10
                           0.9988883 0.05381123
                0.9232327
##
     11
                0.9220452
                          0.9989064 0.05135784
##
     12
                0.9210972 0.9989223 0.05004931
##
     13
                0.9203243 0.9989395
                                     0.04841372
##
     14
                0.9194647
                           0.9989557
                                      0.04759579
##
                0.9185028 0.9989775 0.04514241
##
## ROC was used to select the optimal model using the largest value.
## The final value used for the model was threshold = 0.
NSC on Test Data
nscPred <- readRDS('rds_files/nsc_pred.rds')</pre>
nscCFM <- confusionMatrix(nscPred, y_test, positive = 'yes')</pre>
nscCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                          ves
##
                         1947
          no 1586646
##
          ves
                 1910
                          152
##
##
                  Accuracy : 0.9976
##
                    95% CI: (0.9975, 0.9977)
##
       No Information Rate: 0.9987
       P-Value [Acc > NIR] : 1.0000
##
##
##
                     Kappa: 0.0718
##
   Mcnemar's Test P-Value: 0.5621
##
##
##
               Sensitivity: 7.242e-02
##
               Specificity: 9.988e-01
##
            Pos Pred Value: 7.371e-02
##
            Neg Pred Value: 9.988e-01
##
                Prevalence: 1.320e-03
##
            Detection Rate: 9.556e-05
##
      Detection Prevalence: 1.296e-03
```

```
## Balanced Accuracy : 5.356e-01
##
## 'Positive' Class : yes
##
```

#### NSC Variable Importance

```
varImp(nscModel)
```

```
## pam variable importance
##
##
                     Importance
## amount
                       0.127151
## type.TRANSFER
                       0.088481
## log_amount
                       0.066681
## log_oldbalanceOrg
                       0.056623
## step
                       0.051994
## by_day
                       0.050711
## hours_intraday
                       0.050355
## log_newbalanceOrig
                       0.047248
## type.PAYMENT
                       0.041969
## log_oldbalanceDest
                       0.027505
## type.CASH_OUT
                       0.018248
## oldbalanceOrg
                       0.015725
## newbalanceOrig
                       0.012498
## log_newbalanceDest
                       0.011205
## day_of_week
                       0.008764
## oldbalanceDest
                       0.008650
## type.DEBIT
                       0.003743
## newbalanceDest
                       0.000000
```

### Gradient Boosting Model

```
## Stochastic Gradient Boosting
##
## 4771965 samples
## 18 predictor
## 2 classes: 'no', 'yes'
##
```

```
## Pre-processing: principal component signal extraction (18), scaled
## (18), centered (18)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 3817572, 3817572, 3817572, 3817572, 3817572
## Resampling results:
##
##
    ROC
               Sens
                          Spec
     0.975896 0.9999442 0.6234864
##
##
## Tuning parameter 'n.trees' was held constant at a value of 500
## Tuning
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.01
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 5
GBM Prediction on Test Data
gbmPred <- readRDS('rds_files/gbm_pred.rds')</pre>
gbmCFM <- confusionMatrix(gbmPred, y_test, positive = 'yes')</pre>
gbmCFM
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                   no
                          yes
          no 1588471
                          781
##
                   85
                         1318
##
          yes
##
##
                  Accuracy: 0.9995
                    95% CI : (0.9994, 0.9995)
##
##
       No Information Rate: 0.9987
       P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 0.7525
##
##
   Mcnemar's Test P-Value : < 2.2e-16
##
               Sensitivity: 0.6279181
##
##
               Specificity: 0.9999465
##
            Pos Pred Value : 0.9394155
##
            Neg Pred Value: 0.9995086
##
                Prevalence: 0.0013196
##
            Detection Rate: 0.0008286
##
      Detection Prevalence: 0.0008820
         Balanced Accuracy: 0.8139323
##
##
##
          'Positive' Class : yes
##
GBM Variable Importance
varImp(gbmModel)
```

## gbm variable importance

##

```
##
        Overall
## PC1 100.000
        45.776
## PC5
## PC11 30.244
## PC2
         19.484
## PC4
        18.358
## PC9
        18.211
## PC10 11.081
         7.499
## PC7
## PC3
         1.025
## PC6
         0.169
## PC8
         0.000
```

# Stop cluster and parallel processing
stopCluster(cl)
registerDoSEQ()

#### Model Metrics on Test Data

```
# ROC values
nnetROC <- roc(y_test, readRDS('rds_files/nnet_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
ldaROC <- roc(y_test, readRDS('rds_files/lda_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
qdaROC <- roc(y_test, readRDS('rds_files/qda_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
lrROC <- roc(y_test, readRDS('rds_files/lr_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
plsdaROC <- roc(y_test, readRDS('rds_files/plsda_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
svmROC <- roc(y_test, readRDS('rds_files/svm_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
nscROC <- roc(y_test, readRDS('rds_files/nsc_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
```

```
gbmROC <- roc(y_test, readRDS('rds_files/gbm_prob.rds')$yes)</pre>
## Setting levels: control = no, case = yes
## Setting direction: controls < cases
#AUC
nnetAUC <- auc(nnetROC)</pre>
ldaAUC <- auc(ldaROC)</pre>
qdaAUC <- auc(qdaROC)
lrAUC <- auc(lrROC)</pre>
plsdaAUC <- auc(plsdaROC)</pre>
svmAUC <- auc(svmROC)</pre>
nscAUC <- auc(nscROC)</pre>
gbmAUC <- auc(gbmROC)</pre>
model names <- c('Neural Network', 'Linear Discriminant Analysis', 'Quadratic Discriminant Analysis',
                  'PLS Discriminant Analysis', 'Logistic Regression', 'Support Vector Machines',
                  'Nearest Shrunken Centroids', 'Gradient Boosting Machine')
metricsdf <- rbind(nnetCFM$byClass, ldaCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, qdaCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, plsdaCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, lrCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, svmCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, nscCFM$byClass)</pre>
metricsdf <- rbind(metricsdf, gbmCFM$byClass)</pre>
metricsdf <- cbind(data.frame("Models" = model names, "AUC" = c(nnetAUC, ldaAUC, qdaAUC,
                                                                   plsdaAUC, lrAUC, svmAUC,
                                                                   nscAUC, gbmAUC)),
                    data.frame(metricsdf))
metricsdf[order(-metricsdf$Sensitivity), ]
##
                               Models
                                             AUC Sensitivity Specificity
## 3 Quadratic Discriminant Analysis 0.9927164 0.85945688
                                                                0.9937371
## 6
             Support Vector Machines 0.9978020 0.76179133
                                                                0.9999610
## 5
                 Logistic Regression 0.9964422 0.73082420
                                                                0.9999553
## 8
           Gradient Boosting Machine 0.9777450 0.62791806
                                                                0.9999465
## 2
        Linear Discriminant Analysis 0.9621525 0.40304907
                                                                0.9999037
## 7
          Nearest Shrunken Centroids 0.9362662 0.07241544
                                                                0.9987977
## 1
                       Neural Network 0.5000000 0.00000000
                                                                1.0000000
## 4
           PLS Discriminant Analysis 0.9771492 0.00000000
                                                                1.0000000
##
     Pos.Pred.Value Neg.Pred.Value Precision
                                                    Recall
                                                                    F1 Prevalence
## 3
                          0.9998132 0.15349273 0.85945688 0.26046780 0.001319582
         0.15349273
## 6
         0.96267309
                          0.9996853 0.96267309 0.76179133 0.85053191 0.001319582
                          0.9996444 0.95576324 0.73082420 0.82829374 0.001319582
## 5
         0.95576324
         0.93941554
## 8
                          0.9995086 0.93941554 0.62791806 0.75271274 0.001319582
## 2
         0.84684685
                          0.9992118 0.84684685 0.40304907 0.54615881 0.001319582
                          0.9987744 0.07371484 0.07241544 0.07305936 0.001319582
## 7
         0.07371484
## 1
                NaN
                          0.9986804
                                             NA 0.00000000
                                                                    NA 0.001319582
## 4
                          0.9986804
                                             NA 0.00000000
                                                                    NA 0.001319582
                NaN
    Detection.Rate Detection.Prevalence Balanced.Accuracy
## 3
       1.134124e-03
                             0.0073887801
                                                   0.9265970
## 6
       1.005246e-03
                             0.0010442239
                                                   0.8808762
```

0.8653898

0.0010090183

## 5

9.643826e-04

## 8	8.285895e-04	0.0008820266	0.8139323	
## 2	5.318564e-04	0.0006280432	0.7014764	
## 7	9.555812e-05	0.0012963213	0.5356065	
## 1	0.000000e+00	0.000000000	0.5000000	
## 4	0.000000e+00	0.000000000	0.5000000	

### **ROC Plots**

#### Model ROC Curves

