Code Report Part 1: Model Training

Contents

Data Wrangling	2
.0.1 Introduction to the dataset	. 2
.0.2 Load the dataset (No NA entry)	. 2
.0.3 Factorising variables in character	. 2
.0.4 Catrgorical Random Variables: One-Hot Encoding	. 4
.0.5 Remove Zero Variance or Near-zero variance variable	. 4
.0.6 Remove Correlated predictors	. 5
.0.7 Remove features with linear dependencies:	. 6
.0.8 factorising binary variables:	. 6
Feature Selection	7
.1.1 Train/Test split:	. 7
.1.2 Set up 10-fold-cross-validation	. 7
.1.3 Feature selection by SVM	. 7
1.4 Select features with importance > 40	. 8
Claasifier Training and Testing	
Classifier Training and Testing	9
.2.0 Initialising training settings	
	. 9
.2.0 Initialising training settings	. 9
.2.0 Initialising training settings	. 9 . 10
.2.0 Initialising training settings	. 9 . 10 . 12
.2.0 Initialising training settings	. 9 . 10 . 12 . 14
.2.0 Initialising training settings .2.1 SVM Polynomial	. 9 . 10 . 12 . 14 . 15
2.0 Initialising training settings 2.1 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network	. 9 . 10 . 12 . 14 . 15 . 17
2.0 Initialising training settings 2.1 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network 2.6 Naive Bayes	. 9 . 10 . 12 . 14 . 15 . 17 . 19
2.0 Initialising training settings 2.1 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network 2.6 Naive Bayes 2.7 Logistic Regression	. 9 . 10 . 12 . 14 . 15 . 17 . 20 . 22
2.0 Initialising training settings 2.1 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network 2.6 Naive Bayes 2.7 Logistic Regression 2.8 LDA	. 9 . 10 . 12 . 14 . 15 . 17 . 19 . 20 . 22
2.0 Initialising training settings 2.1 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network 2.6 Naive Bayes 2.7 Logistic Regression 2.8 LDA 2.9 KNN	. 9 . 10 . 12 . 14 . 15 . 17 . 20 . 22 . 23 . 25
2.2 SVM Polynomial 2.2 SVM Radial 2.3 SVM linear 2.4 Random Forest 2.5 Neural Network 2.6 Naive Bayes 2.7 Logistic Regression 2.8 LDA 2.9 KNN 2.10 GBM	9 10 12 14 15 17 20 22 23 25 28

	1.3	3	Review	the	Results	and	Plotting	the	RO	(
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1.4 Combining the models	35
1.4.1 Naive Voting Ensemble (Unweigthed Voting)	36
1.4.2 Train logistic regression on the ensemble data frame (Weighted Voting)	38

33

[Note] The code report for Shiny App, API and other section is included in the second part of the code report with another Table of Contents, since this part is knitted directly from R Markdown file.

```
library(ggplot2)
library(caret)
library(xlsx)
library(pROC)
```

1.0 Data Wrangling

1.0.1 Introduction to the dataset

The data set we used for model training is the Z-Alizadeh Sani Data Set, which is collected for CAD diagnosis and published on the UCI Machine Learning Repository. This data set contains 303 observations and 56 features with no NA or missing value.

1.0.2 Load the dataset (No NA entry)

```
cad <- read.xlsx("DataWrangling/Z-Alizadeh sani dataset.xlsx", 1, header=TRUE)</pre>
```

1.0.3 Factorising variables in character

The categorical features in the original data set is in character format after first reading into R, we need to convert them into factors for the classification.

```
for (i in 1:length(cad)) {
   if (class(cad[,i]) == "character"){
      cad[,i] <- as.factor(cad[,i])
   }
   else if (cad[,i][1] == 0 | cad[,i][1] == 1 ){
      cad[,i] <- as.factor(cad[,i])
   }
}
str(cad)</pre>
```

```
## 'data.frame': 303 obs. of 56 variables:
## $ Age : num 53 67 54 66 50 50 55 72 58 60 ...
## $ Weight : num 90 70 54 67 87 75 80 80 84 71 ...
```

```
## $ Length
                           : num 175 157 164 158 153 175 165 175 163 170 ...
## $ Sex
                          : Factor w/ 2 levels "Fmale", "Male": 2 1 2 1 1 2 2 2 1 2 ...
## $ BMI
                          : num 29.4 28.4 20.1 26.8 37.2 ...
## $ DM
                           : Factor w/ 2 levels "0", "1": 1 1 1 1 1 1 2 1 2 ...
                          : Factor w/ 2 levels "0", "1": 2 2 1 2 2 1 1 1 1 1 ...
##
   $ HTN
##
   $ Current.Smoker
                          : Factor w/ 2 levels "0", "1": 2 1 2 1 1 2 1 2 1 1 ...
  $ EX.Smoker
                          : Factor w/ 2 levels "0"."1": 1 1 1 1 1 1 2 1 1 1 ...
                           : Factor w/ 2 levels "0", "1": 1 1 1 1 1 1 1 1 1 1 ...
## $ FH
##
   $ Obesity
                           : Factor w/ 2 levels "N", "Y": 2 2 1 2 2 1 2 2 1 ...
## $ CRF
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ CVA
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ Airway.disease
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
   $ Thyroid.Disease
## $ CHF
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ DLP
                           : Factor w/ 2 levels "N", "Y": 2 1 1 1 1 1 2 1 1 ...
## $ BP
                           : num 110 140 100 100 110 118 110 130 90 130 ...
## $ PR
                           : num 80 80 100 80 80 70 80 70 50 70 ...
                           : Factor w/ 2 levels "0", "1": 1 2 1 1 1 1 1 1 1 1 ...
##
  $ Edema
## $ Weak.Peripheral.Pulse: Factor w/ 2 levels "N","Y": 1 1 1 1 1 1 1 1 1 1 ...
                          : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
   $ Lung.rales
## $ Systolic.Murmur
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 2 1 2 1 1 1 ...
## $ Diastolic.Murmur
                           : Factor w/ 2 levels "N", "Y": 1 1 1 2 1 1 1 1 1 1 ...
                          : Factor w/ 2 levels "0", "1": 1 2 2 1 1 2 2 2 1 2 ...
## $ Typical.Chest.Pain
   $ Dyspnea
                           : Factor w/ 2 levels "N", "Y": 1 1 1 2 2 1 1 1 2 2 ...
                           : Factor w/ 4 levels "0", "1", "2", "3": 1 1 1 4 3 4 1 1 1 3 ...
## $ Function.Class
## $ Atypical
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ Nonanginal
                           : Factor w/ 2 levels "N", "Y": 1 1 1 2 1 1 1 1 2 1 ...
                           : Factor w/ 1 level "N": 1 1 1 1 1 1 1 1 1 1 ...
   $ Exertional.CP
## $ LowTH.Ang
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
                           : Factor w/ 2 levels "0", "1": 1 1 1 1 1 2 1 1 1 ...
## $ Q.Wave
                           : Factor w/ 2 levels "0", "1": 1 1 1 1 1 2 1 1 1 ...
## $ St.Elevation
   $ St.Depression
                           : Factor w/ 2 levels "0", "1": 2 2 1 2 1 1 1 2 1 1 ...
                           : Factor w/ 2 levels "0", "1": 2 2 1 1 1 1 2 2 1 1 ...
## $ Tinversion
                           : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ LVH
                          : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
##
   $ Poor.R.Progression
                           : Factor w/ 3 levels "LBBB", "N", "RBBB": 2 2 2 2 2 2 2 2 1 ...
##
   $ BBB
## $ FBS
                           : num 90 80 85 78 104 86 80 130 69 209 ...
## $ CR
                           : num 0.7 1 1 1.2 1 1 0.8 0.9 0.6 1.3 ...
##
   $ TG
                                 250 309 103 63 170 139 83 80 79 80 ...
                           : num 155 121 70 55 110 119 85 90 90 90 ...
## $ LDL
## $ HDL
                                 30 36 45 27 50 34 34 55 59 44 ...
                          : num
                           : num 8 30 17 30 16 13 12 19 15 16 ...
## $ BUN
   $ ESR
                          : num 7 26 10 76 27 18 38 4 5 8 ...
## $ HB
                           : num 15.6 13.9 13.5 12.1 13.2 15.6 14.1 16.1 11.6 13.9 ...
## $ K
                                 4.7 4.7 4.7 4.4 4 4.2 4.8 4.3 3.4 4.6 ...
                           : num
                                 141 156 139 142 140 141 139 142 139 140 ...
## $ Na
                           : num
                                 5700 7700 7400 13000 9200 7300 9400 12200 5100 4900 ...
##
   $ WBC
                           : num
## $ Lymph
                           : num 39 38 38 18 55 26 58 25 49 55 ...
## $ Neut
                           : num 52 55 60 72 39 66 33 74 50 42 ...
                                 261 165 230 742 274 194 292 410 370 380 ...
## $ PLT
                           : num
## $ EF.TTE
                          : num 50 40 40 55 50 50 40 45 50 40 ...
                          : Factor w/ 5 levels "0","1","2","3",..: 1 5 3 1 1 1 5 5 1 3 ...
## $ Region.RWMA
                          : Factor w/ 4 levels "mild", "Moderate", ...: 3 3 1 4 4 3 1 1 3 3 ...
## $ VHD
                           : Factor w/ 2 levels "Cad", "Normal": 1 1 1 2 2 1 1 1 2 1 ...
## $ Cath
```

[NOTE] We observe that the feature "Exertional CP" only has one level, so we drop it from the data set, since it contains no useful information and the classifier training with ROC cannot generate probabilities for categorical feature with only one level.

```
cad <- subset(cad, select = -Exertional.CP)</pre>
```

When we train the model with metric ROC, the one-hot encoding process is embedded within the training process, so we need to set up another data set with no one-hot encoding. This data set will also following the same wrangling procedure as the other one to make sure these two data sets are consistent and contain the same features.

```
svm.df <- cad
```

1.0.4 Catrgorical Random Variables: One-Hot Encoding

The data set after one-hot encoding will contain 97 columns.

```
dummy <- dummyVars(" ~ .", data = cad)
cad <- data.frame(predict(dummy, newdata = cad))</pre>
```

1.0.5 Remove Zero Variance or Near-zero variance variable

We first examine the two data set whether they have columns with zero variance or near-zero variance (i.e. imbalanced features).

```
nz <- nearZeroVar(cad, saveMetrics = TRUE)
nz[nz$nzv,]</pre>
```

```
##
                           freqRatio percentUnique zeroVar nzv
## EX.Smoker.0
                            29.30000
                                           0.660066
                                                      FALSE TRUE
## EX.Smoker.1
                            29.30000
                                           0.660066
                                                      FALSE TRUE
## CRF.N
                            49.50000
                                           0.660066
                                                      FALSE TRUE
## CRF.Y
                            49.50000
                                           0.660066
                                                      FALSE TRUE
## CVA.N
                            59.60000
                                           0.660066
                                                      FALSE TRUE
## CVA.Y
                            59.60000
                                           0.660066
                                                      FALSE TRUE
## Airway.disease.N
                            26.54545
                                           0.660066
                                                      FALSE TRUE
## Airway.disease.Y
                                                      FALSE TRUE
                            26.54545
                                           0.660066
## Thyroid.Disease.N
                            42.28571
                                           0.660066
                                                      FALSE TRUE
## Thyroid.Disease.Y
                            42.28571
                                           0.660066
                                                      FALSE TRUE
## CHF.N
                           302.00000
                                           0.660066
                                                      FALSE TRUE
## CHF.Y
                           302.00000
                                           0.660066
                                                      FALSE TRUE
## Edema.0
                                           0.660066
                                                      FALSE TRUE
                            24.25000
## Edema.1
                            24.25000
                                           0.660066
                                                      FALSE TRUE
## Weak.Peripheral.Pulse.N
                            59.60000
                                           0.660066
                                                      FALSE TRUE
## Weak.Peripheral.Pulse.Y
                            59.60000
                                           0.660066
                                                      FALSE TRUE
## Lung.rales.N
                            26.54545
                                           0.660066
                                                      FALSE TRUE
```

```
## Lung.rales.Y
                            26.54545
                                           0.660066
                                                      FALSE TRUE
## Diastolic.Murmur.N
                            32.66667
                                           0.660066
                                                      FALSE TRUE
                                                      FALSE TRUE
## Diastolic.Murmur.Y
                            32.66667
                                           0.660066
## Function.Class.1
                           302.00000
                                           0.660066
                                                      FALSE TRUE
## LowTH.Ang.N
                           150.50000
                                           0.660066
                                                      FALSE TRUE
## LowTH.Ang.Y
                                                     FALSE TRUE
                           150.50000
                                           0.660066
## St.Elevation.0
                                                      FALSE TRUE
                            20.64286
                                           0.660066
## St.Elevation.1
                            20.64286
                                           0.660066
                                                      FALSE TRUE
## Poor.R.Progression.N
                            32.66667
                                           0.660066
                                                      FALSE TRUE
## Poor.R.Progression.Y
                            32.66667
                                           0.660066
                                                      FALSE TRUE
## BBB.LBBB
                            22.30769
                                           0.660066
                                                      FALSE TRUE
## BBB.RBBB
                            36.87500
                                           0.660066
                                                      FALSE TRUE
## Region.RWMA.3
                            20.64286
                                           0.660066
                                                      FALSE TRUE
## Region.RWMA.4
                            20.64286
                                                      FALSE TRUE
                                           0.660066
## VHD.Severe
                            26.54545
                                           0.660066
                                                      FALSE TRUE
```

```
nz.svm <- nearZeroVar(svm.df, saveMetrics = T)
nz.svm[nz.svm$nzv,]</pre>
```

```
##
                         freqRatio percentUnique zeroVar nzv
## EX.Smoker
                          29.30000
                                        0.660066
                                                   FALSE TRUE
## CRF
                          49.50000
                                        0.660066
                                                   FALSE TRUE
## CVA
                          59.60000
                                        0.660066
                                                   FALSE TRUE
## Airway.disease
                          26.54545
                                        0.660066
                                                   FALSE TRUE
## Thyroid.Disease
                                        0.660066
                                                   FALSE TRUE
                          42.28571
## CHF
                         302.00000
                                        0.660066
                                                   FALSE TRUE
## Edema
                          24.25000
                                        0.660066
                                                   FALSE TRUE
## Weak.Peripheral.Pulse 59.60000
                                        0.660066
                                                   FALSE TRUE
## Lung.rales
                          26.54545
                                        0.660066
                                                   FALSE TRUE
## Diastolic.Murmur
                          32.66667
                                        0.660066
                                                   FALSE TRUE
## LowTH.Ang
                                                   FALSE TRUE
                         150.50000
                                        0.660066
## St.Elevation
                          20.64286
                                        0.660066
                                                   FALSE TRUE
## Poor.R.Progression
                          32.66667
                                        0.660066
                                                   FALSE TRUE
## BBB
                          21.69231
                                        0.990099
                                                   FALSE TRUE
```

There are 32 near-zero-variance features which may cause problems when the data are split into cross validation or boostraping samples (lead to samples with features only have one level), we eliminated those features.

```
nzv <- nearZeroVar(cad)
cad <- cad[,-nzv]
nzv.svm <- nearZeroVar(svm.df)
svm.df <- svm.df[,-nzv.svm]</pre>
```

1.0.6 Remove Correlated predictors

```
cad_cor <- cor(cad)
high.cor <- sum(abs(cad_cor[upper.tri(cad_cor)])>0.999)
summary(cad_cor[upper.tri(cad_cor)])
```

```
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## -1.000000 -0.063363 -0.002277 -0.008947 0.060996 0.725005
```

We observed 17 highly correlated features, all of them are generated by one-hot encoding (e.g. for a variable with 3 levels, drop one of the dummies will not lose any information), only one of them (Neut) isn't a column generated by One-Hot Encoding, and it is not having high correlation with "Cath" which is the feature that we want to predict, it has a -0.923 correlation with feature "Lymph". we drop them and the effect of removing those with absolute correlations above 0.75 are shown below:

```
high.cor.feature <- findCorrelation(cad_cor, cutoff = 0.75)
high.cor.feature[1] = 65 #remove the Cath.Normal rather than Cath.cad
cad <- cad[, -high.cor.feature]</pre>
cad_cor2 <- cor(cad)</pre>
summary(cad_cor2[upper.tri(cad_cor2)])
##
       Min. 1st Qu.
                        Median
                                         3rd Qu.
                                                      Max.
                                   Mean
## -0.54585 -0.05229
                      0.01302 0.01417
                                         0.06687 0.72501
# remove the NEUT
svm.df <- svm.df[, -grep("Neut", colnames(svm.df))]</pre>
```

1.0.7 Remove features with linear dependencies:

```
ld <- findLinearCombos(cad)
ld

## $linearCombos
## list()
##
## $remove
## NULL</pre>
```

Nothing observed so we are ok.

1.0.8 factorising binary variables:

One-hot encoding transfers some of the categorical variables into numeric form, we need to convert them back to factor form.

```
for (i in 1:length(cad)) {
  if (cad[,i][1] == 0 | cad[,i][1] == 1 ){
    cad[,i] <- as.factor(cad[,i])
  }
}</pre>
```

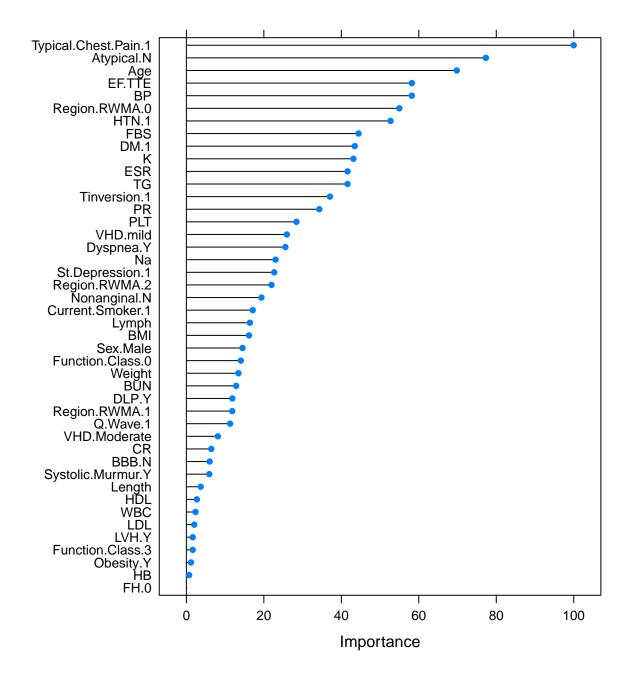
1.1 Feature Selection

The data frame "cad" is used for traing the feature selection SVM.

1.1.1 Train/Test split:

1.1.2 Set up 10-fold-cross-validation

1.1.3 Feature selection by SVM



1.1.4 Select features with importance > 40

Selecting feature with importance grater than 40 left with 12 predictors

```
important <- c(feature.rank$importance$X0>40, TRUE)
im <- cad[,important]
str(im)</pre>
```

'data.frame': 303 obs. of 13 variables:

```
: num 53 67 54 66 50 50 55 72 58 60 ...
## $ Age
## $ DM.1
                         : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 2 1 2 ...
## $ HTN.1
                        : Factor w/ 2 levels "0", "1": 2 2 1 2 2 1 1 1 1 1 ...
## $ BP
                          : num 110 140 100 100 110 118 110 130 90 130 ...
## $ Typical.Chest.Pain.1: Factor w/ 2 levels "0","1": 1 2 2 1 1 2 2 2 1 2 ...
## $ Atypical.N : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ FBS
                         : num 90 80 85 78 104 86 80 130 69 209 ...
## $ TG
                         : num 250 309 103 63 170 139 83 80 79 80 ...
## $ ESR
                         : num 7 26 10 76 27 18 38 4 5 8 ...
## $ K
                         : num 4.7 4.7 4.7 4.4 4 4.2 4.8 4.3 3.4 4.6 ...
## $ EF.TTE
                         : num 50 40 40 55 50 50 40 45 50 40 ...
## $ Region.RWMA.0 : Factor w/ 2 levels "0","1": 2 1 1 2 2 2 1 1 2 1 ...
## $ Cath Cad : Factor w/ 2 levels "0","1": 2 2 2 1 1 2 2 2 1 2
## $ Cath.Cad
                         : Factor w/ 2 levels "0","1": 2 2 2 1 1 2 2 2 1 2 ...
# train/test split
im.train <- im[train.index,]</pre>
im.test <- im[-train.index,]</pre>
# to keep two data set consistent
svm.df <- subset(svm.df, select = c(Age, DM, HTN, BP, Typical.Chest.Pain,</pre>
                                    Atypical, FBS, TG, ESR, K, EF.TTE,
                                     Region.RWMA, Cath))
str(svm.df)
## 'data.frame':
                    303 obs. of 13 variables:
                        : num 53 67 54 66 50 50 55 72 58 60 ...
## $ Age
## $ DM
                        : Factor w/ 2 levels "0", "1": 1 1 1 1 1 1 1 2 1 2 ...
## $ HTN
                        : Factor w/ 2 levels "0", "1": 2 2 1 2 2 1 1 1 1 1 ...
## $ BP
                        : num 110 140 100 100 110 118 110 130 90 130 ...
## $ Typical.Chest.Pain: Factor w/ 2 levels "0","1": 1 2 2 1 1 2 2 2 1 2 ...
## $ Atypical : Factor w/ 2 levels "N", "Y": 1 1 1 1 1 1 1 1 1 1 ...
## $ FBS
                       : num 90 80 85 78 104 86 80 130 69 209 ...
## $ TG
                        : num 250 309 103 63 170 139 83 80 79 80 ...
## $ ESR
                      : num 7 26 10 76 27 18 38 4 5 8 ...
## $ K
                       : num 4.7 4.7 4.7 4.4 4 4.2 4.8 4.3 3.4 4.6 ...
## $ EF.TTE : num 50 40 40 55 50 50 40 45 50 40 ...
## $ Region.RWMA : Factor w/ 5 levels "0","1","2","3",..: 1 5 3 1 1 1 5 5 1 3 ...
## $ Cath
                       : Factor w/ 2 levels "Cad", "Normal": 1 1 1 2 2 1 1 1 2 1 ...
```

1.2 Classifier Training and Testing

1.2.0 Initialising training settings

```
Training_ROC = 0:12,
Testing_Accuracy = 0:12,
Test_AUC = 0:12)
```

1.2.1 SVM Polynomial

We want to test if training with ROC will help us to achieve a better performed model, so we trained one without ROC to compare.

```
## degree scale C Accuracy Kappa AccuracySD KappaSD ## 1 1 1 0.8643667 0.6612775 0.06272514 0.1605093 ## 2 1 2 3 0.8622500 0.6564865 0.06229360 0.1579216
```

```
# Test SVM polynomial with ROC
svm.poly.predict = predict(svm.poly, svm.test)
# confusion matrix
cm.svm.poly <- confusionMatrix(svm.poly.predict, svm.test$Cath)</pre>
print(cm.svm.poly)
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction Cad Normal
##
       Cad
               40
                      5
##
       Normal
              3
                      12
##
##
                  Accuracy : 0.8667
##
                    95% CI: (0.7541, 0.9406)
##
       No Information Rate: 0.7167
       P-Value [Acc > NIR] : 0.004937
##
##
##
                     Kappa: 0.6596
##
   Mcnemar's Test P-Value: 0.723674
##
##
##
               Sensitivity: 0.9302
               Specificity: 0.7059
##
##
            Pos Pred Value: 0.8889
            Neg Pred Value: 0.8000
##
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6667
##
      Detection Prevalence : 0.7500
##
         Balanced Accuracy: 0.8181
##
##
          'Positive' Class : Cad
##
# Test SVM polynomial without ROC
svm.predict = predict(SVM, im.test)
# confusion matrix
cm.svm <- confusionMatrix(svm.predict, im.test$Cath.Cad)</pre>
print(cm.svm)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction 0 1
##
            0 13 8
            1 4 35
##
##
##
                  Accuracy: 0.8
                    95% CI : (0.6767, 0.8922)
##
##
       No Information Rate: 0.7167
##
       P-Value [Acc > NIR] : 0.09575
##
##
                     Kappa: 0.5402
```

```
##
   Mcnemar's Test P-Value: 0.38648
##
##
##
              Sensitivity: 0.7647
##
               Specificity: 0.8140
           Pos Pred Value: 0.6190
##
            Neg Pred Value: 0.8974
##
                Prevalence: 0.2833
##
##
           Detection Rate: 0.2167
##
     Detection Prevalence: 0.3500
##
         Balanced Accuracy: 0.7893
##
          'Positive' Class: 0
##
##
```

We notice that training classifier with ROC as metric yields higher testing accuracy, thus, we'll train the left classifiers with ROC.

1.2.2 SVM Radial

```
## sigma C ROC Sens Spec ROCSD SensSD
## 1 0.0622846 0.25 0.9048553 0.9100000 0.7085714 0.06768556 0.06919869
## 2 0.0622846 0.50 0.9000047 0.9202288 0.6371429 0.07110917 0.06684309
## 3 0.0622846 1.00 0.8957423 0.9283660 0.6271429 0.07244670 0.05976535
```

```
2.00 0.8927358 0.9168954 0.6414286 0.07541720 0.06588594
## 4 0.0622846
8.00 0.8802708 0.9057190 0.6214286 0.07787928 0.06998145
## 6 0.0622846
## 7 0.0622846 16.00 0.8840056 0.9085948 0.6142857 0.07712949 0.07069320
## 9 0.0622846 64.00 0.8471615 0.9109804 0.5457143 0.08502766 0.07488678
## 10 0.0622846 128.00 0.8317414 0.9118627 0.5071429 0.08819426 0.07386473
##
       SpecSD
## 1 0.1721965
## 2 0.1820880
## 3 0.1780526
## 4 0.1630656
## 5 0.1680278
## 6 0.1678990
## 7 0.1498986
## 8 0.1471155
## 9 0.1641806
## 10 0.1641743
# Test SVM Radial
svm.rad.predict = predict(svm.rad, svm.test)
# confusion matrix
cm.svm.rad <- confusionMatrix(svm.rad.predict, svm.test$Cath)</pre>
print(cm.svm.rad)
## Confusion Matrix and Statistics
##
##
           Reference
## Prediction Cad Normal
##
      Cad
             40
##
      Normal
            3
                   10
##
##
                Accuracy: 0.8333
##
                 95% CI: (0.7148, 0.9171)
##
      No Information Rate: 0.7167
##
      P-Value [Acc > NIR] : 0.02687
##
##
                  Kappa: 0.5582
##
##
   Mcnemar's Test P-Value: 0.34278
##
##
             Sensitivity: 0.9302
##
             Specificity: 0.5882
##
          Pos Pred Value: 0.8511
##
          Neg Pred Value: 0.7692
##
              Prevalence: 0.7167
##
          Detection Rate: 0.6667
##
     Detection Prevalence: 0.7833
##
       Balanced Accuracy: 0.7592
##
         'Positive' Class : Cad
##
##
```

1.2.3 SVM linear

```
set.seed(3164)
# Train SVM linear
svm.l= train(Cath ~ ., data = svm.train,
           method = "svmLinear",
            trControl = control,
            tuneLength = 10,
            preProcess = c("pca", "scale", "center"),
            metric = "ROC",
            na.action = na.omit)
print(svm.l$results)
             ROC
                      Sens
                                Spec
                                           ROCSD
                                                   SensSD
                                                             SpecSD
## 1 1 0.9152148 0.9245098 0.6885714 0.05763243 0.062564 0.1666729
# Test SVM linear
svm.l.predict = predict(svm.l, svm.test)
# confusion matrix
cm.svm.l <- confusionMatrix(svm.l.predict, svm.test$Cath)</pre>
print(cm.svm.l)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               42
                       5
##
       Normal
              1
                      12
##
                  Accuracy: 0.9
##
##
                    95% CI: (0.7949, 0.9624)
##
       No Information Rate: 0.7167
       P-Value [Acc > NIR] : 0.0005383
##
##
```

```
##
                     Kappa: 0.7349
##
##
   Mcnemar's Test P-Value: 0.2206714
##
##
               Sensitivity: 0.9767
               Specificity: 0.7059
##
##
            Pos Pred Value: 0.8936
            Neg Pred Value: 0.9231
##
##
                Prevalence: 0.7167
            Detection Rate: 0.7000
##
##
      Detection Prevalence: 0.7833
##
         Balanced Accuracy: 0.8413
##
##
          'Positive' Class : Cad
##
# Store the training ROC and the Testing accuracy to the result table
result$Training_ROC[3] = max(svm.l$results$ROC)
result$Testing_Accuracy[3] = cm.svm.l$overall[1]
# predict in probabilities
svm.l.probs = predict(svm.l,svm.test[,!names(svm.test) %in% c("Cath")],
                      type = "prob")
# store the testing ROC values for plotting later
svm.l.ROC = roc(response = svm.test$Cath,
              predictor = svm.l.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
#store the testing AUC
result$Test_AUC[3] = svm.1.ROC$auc
```

1.2.4 Random Forest

```
# train the random forest
rf <- train(Cath ~., data = svm.train,</pre>
                 method = "rf",
                 trControl = control,
                 preProc = c("center", "scale"),
                 tuneLength = 10,
                 metric = "ROC")
print(rf)
## Random Forest
##
## 243 samples
  12 predictor
    2 classes: 'Cad', 'Normal'
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 218, 219, 218, 219, 218, ...
```

```
## Resampling results across tuning parameters:
##
##
     mtry ROC
                     Sens
                                 Spec
##
          0.9215780 0.9130392 0.6971429
     2
##
      3
          0.9158310 0.9068301 0.7214286
##
          0.9125934 0.9009804 0.7214286
##
          0.9118511 0.8916993 0.7342857
      6
##
          0.9117787 0.8923529 0.7371429
     7
##
     9
          0.9102171 0.8934967 0.7414286
##
     10
          ##
     12
          0.9074416 0.8901307 0.7400000
##
     13
          0.9060224 0.8848693 0.7442857
##
          0.9042554 0.8871895 0.7528571
##
\ensuremath{\mbox{\#\#}} ROC was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 2.
# Test the random forest
rf.predict = predict(rf, svm.test)
# confusion matrix
cm.rf <- confusionMatrix(rf.predict, svm.test$Cath)</pre>
print(cm.rf)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
      Cad
              40
##
      Normal
              3
                      12
##
##
                  Accuracy : 0.8667
##
                    95% CI: (0.7541, 0.9406)
##
      No Information Rate: 0.7167
##
      P-Value [Acc > NIR] : 0.004937
##
##
                     Kappa: 0.6596
##
   Mcnemar's Test P-Value: 0.723674
##
##
##
               Sensitivity: 0.9302
##
               Specificity: 0.7059
##
            Pos Pred Value: 0.8889
##
            Neg Pred Value: 0.8000
##
                Prevalence: 0.7167
##
           Detection Rate: 0.6667
##
     Detection Prevalence: 0.7500
##
        Balanced Accuracy: 0.8181
##
##
          'Positive' Class : Cad
##
# store the training ROC and Testing accuracy to the results table
result$Training_ROC[4] = max(rf$results$ROC)
```

1.2.5 Neural Network

```
##
## 243 samples
## 12 predictor
   2 classes: 'Cad', 'Normal'
##
##
## Pre-processing: scaled (7), centered (7), ignore (5)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 218, 219, 218, 219, 219, 219, ...
## Resampling results across tuning parameters:
##
##
    size decay ROC
                            Sens
                                       Spec
          0e+00 0.8444935 0.8625817 0.7971429
##
##
    1
          1e-04 0.8717110 0.8568301 0.7857143
          1e-03 0.8980252 0.8647386 0.7871429
##
    1
          1e-02 0.9149253 0.8681373 0.7914286
##
    1
##
          1e-01 0.9207843 0.8879085 0.7614286
          0e+00 0.8070215 0.8605882 0.7028571
##
    3
##
    3
          1e-04 0.8328735 0.8534641 0.7442857
##
    3
          1e-03 0.8578618 0.8758497 0.7200000
##
    3
          1e-02 0.8530439 0.8589542 0.6800000
          1e-01 0.9024697 0.8878105 0.7185714
##
    3
##
    5
          0e+00 0.7889052 0.8517647 0.6571429
##
    5
         1e-04 0.8278175 0.8631699 0.6600000
##
    5
          1e-03 0.8374510 0.8638562 0.6528571
```

```
##
          1e-02 0.8569328 0.8715033 0.6157143
##
          1e-01 0.9035434 0.9028431 0.6857143
     5
          0e+00 0.7809687 0.8523203 0.6571429
##
     7
##
    7
          1e-04 0.8320121 0.8742484 0.6142857
##
     7
          1e-03 0.8449090 0.8684314 0.5957143
##
    7
          1e-02 0.8593931 0.8778758 0.6357143
     7
          1e-01 0.8979458 0.9022549 0.6871429
##
##
     9
          0e+00 0.7843044 0.8584967 0.6385714
##
     9
          1e-04 0.8561064 0.8838562 0.6471429
##
     9
          1e-03 0.8666270 0.8763072 0.6571429
##
     9
          1e-02 0.8732610 0.8784967 0.6385714
##
     9
           1e-01 0.8984687 0.8993464 0.6842857
##
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were size = 1 and decay = 0.1.
# testing the neural network
nn.predict = predict(nn, svm.test)
# confusion matrix
cm.nn <- confusionMatrix(nn.predict, svm.test$Cath)</pre>
print(cm.nn)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
              37
      Cad
##
       Normal
                      13
##
##
                  Accuracy : 0.8333
                    95% CI: (0.7148, 0.9171)
##
##
      No Information Rate: 0.7167
      P-Value [Acc > NIR] : 0.02687
##
##
##
                     Kappa: 0.6037
##
##
   Mcnemar's Test P-Value: 0.75183
##
##
               Sensitivity: 0.8605
##
               Specificity: 0.7647
##
            Pos Pred Value: 0.9024
##
            Neg Pred Value: 0.6842
##
                Prevalence: 0.7167
##
           Detection Rate: 0.6167
##
      Detection Prevalence: 0.6833
##
         Balanced Accuracy: 0.8126
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training ROC[5] = max(nn$results$ROC)
result$Testing_Accuracy[5] = cm.nn$overall[1]
```

1.2.6 Naive Bayes

```
set.seed(3164)
# train Naive Bayes
nb <- train(Cath ~., data = svm.train,</pre>
                 method = "nb",
                 trControl = control,
                 preProc = c("center", "scale"),
                 tuneGrid = data.frame(fL = 0, usekernel = T, adjust = 1),
                 metric = "ROC")
print(nb)
## Naive Bayes
##
## 243 samples
## 12 predictor
   2 classes: 'Cad', 'Normal'
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results:
##
##
    ROC
                Sens
                           Spec
##
    0.8881139 0.5108497 0.9428571
## Tuning parameter 'fL' was held constant at a value of 0
## Tuning
## parameter 'usekernel' was held constant at a value of TRUE
## Tuning
## parameter 'adjust' was held constant at a value of 1
# Test the Naive Bayes
nb.predict = predict(nb, svm.test)
# confusion matrix
cm.nb <- confusionMatrix(nb.predict, svm.test$Cath)</pre>
print(cm.nb)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
```

```
##
       Cad
##
       Normal 19
##
##
                  Accuracy : 0.6667
##
                    95% CI: (0.5331, 0.7831)
##
       No Information Rate: 0.7167
##
       P-Value [Acc > NIR] : 0.8421385
##
##
                     Kappa: 0.3782
##
##
    Mcnemar's Test P-Value: 0.0001439
##
               Sensitivity: 0.5581
##
##
               Specificity: 0.9412
            Pos Pred Value : 0.9600
##
##
            Neg Pred Value: 0.4571
##
                Prevalence: 0.7167
##
            Detection Rate: 0.4000
##
      Detection Prevalence: 0.4167
##
         Balanced Accuracy: 0.7497
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[6] = max(nb$results$ROC)
result$Testing_Accuracy[6] = cm.nb$overall[1]
# Save the testing ROC for plotting later
nb.probs = predict(nb,svm.test[,!names(svm.test) %in% c("Cath")],type = "prob")
nb.ROC = roc(response = svm.test$Cath,
              predictor = nb.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[6] = nb.ROC$auc
```

1.2.7 Logistic Regression

Generalized Linear Model

##

```
## 243 samples
## 12 predictor
    2 classes: 'Cad', 'Normal'
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results:
##
##
     ROC
                Sens
                          Spec
##
     0.9166153 0.905915 0.74
# Test the logistic regression
lr.predict = predict(lr, svm.test)
# confusion matrix
cm.lr <- confusionMatrix(lr.predict, svm.test$Cath)</pre>
print(cm.lr)
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction Cad Normal
##
       Cad
               39
##
       Normal
                4
                      13
##
##
                  Accuracy : 0.8667
##
                    95% CI: (0.7541, 0.9406)
##
       No Information Rate: 0.7167
##
       P-Value [Acc > NIR] : 0.004937
##
##
                     Kappa: 0.6717
##
##
   Mcnemar's Test P-Value: 1.000000
##
               Sensitivity: 0.9070
##
               Specificity: 0.7647
##
##
            Pos Pred Value: 0.9070
##
            Neg Pred Value: 0.7647
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6500
##
      Detection Prevalence: 0.7167
##
         Balanced Accuracy: 0.8358
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[7] = max(lr$results$ROC)
result$Testing_Accuracy[7] = cm.lr$overall[1]
# Save the testing ROC for plotting later
lr.probs = predict(lr,svm.test[,!names(svm.test) %in% c("Cath")],type = "prob")
lr.ROC = roc(response = svm.test$Cath,
```

1.2.8 LDA

```
set.seed(3164)
# train the LDA
lda <- train(Cath ~., data = svm.train,</pre>
                method = "lda",
                 trControl = control,
                 preProc = c("center", "scale"),
                 tuneLength = 10,
                 metric = "ROC")
print(lda)
## Linear Discriminant Analysis
##
## 243 samples
## 12 predictor
   2 classes: 'Cad', 'Normal'
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results:
##
##
    ROC
               Sens
                          Spec
##
    # Test the lda
lda.predict = predict(lda, svm.test)
# confusion matrix
cm.lda <- confusionMatrix(lda.predict, svm.test$Cath)</pre>
print(cm.lda)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
               39
##
       Cad
##
       Normal
                     13
##
##
                  Accuracy : 0.8667
##
                    95% CI: (0.7541, 0.9406)
##
       No Information Rate: 0.7167
       P-Value [Acc > NIR] : 0.004937
##
##
##
                     Kappa : 0.6717
```

```
##
   Mcnemar's Test P-Value: 1.000000
##
##
               Sensitivity: 0.9070
##
##
               Specificity: 0.7647
            Pos Pred Value: 0.9070
##
##
            Neg Pred Value: 0.7647
                Prevalence: 0.7167
##
##
            Detection Rate: 0.6500
##
     Detection Prevalence: 0.7167
##
         Balanced Accuracy: 0.8358
##
          'Positive' Class : Cad
##
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[8] = max(lda$results$ROC)
result$Testing_Accuracy[8] = cm.lda$overall[1]
# Save the testing ROC for plotting later
lda.probs = predict(lda,svm.test[,!names(svm.test) %in% c("Cath")],type = "prob")
lda.ROC = roc(response = svm.test$Cath,
              predictor = lda.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[8] = lda.ROC$auc
```

1.2.9 KNN

##

k

ROC

Sens

Spec

```
set.seed(3164)
# train the KNN
knn <- train(Cath ~., data = svm.train,
                 method = "knn",
                 trControl = control,
                 preProc = c("center", "scale"),
                 tuneLength = 10,
                 metric = "ROC")
print(knn)
## k-Nearest Neighbors
##
## 243 samples
  12 predictor
     2 classes: 'Cad', 'Normal'
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results across tuning parameters:
##
```

```
##
      5 0.8788235 0.8977451 0.6814286
##
     7 0.8883380 0.9076144 0.7185714
##
     9 0.8888025 0.9065686 0.7485714
##
     11 0.8864169 0.9006536 0.7600000
##
     13 0.8926471 0.9012092 0.7700000
##
     15 0.8988049 0.9041503 0.7542857
##
     17 0.8996615 0.9006863 0.7371429
##
     19 0.8984757 0.9008170 0.7314286
##
     21 0.9008730 0.9019608 0.7100000
##
     23 0.8997946 0.9025490 0.7085714
##
## ROC was used to select the optimal model using the largest value.
## The final value used for the model was k = 21.
# Test the knn
knn.predict = predict(knn, svm.test)
# confusion matrix
cm.knn <- confusionMatrix(knn.predict, svm.test$Cath)</pre>
print(cm.knn)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               39
                      6
##
       Normal
                      11
##
##
                  Accuracy: 0.8333
##
                    95% CI: (0.7148, 0.9171)
##
      No Information Rate: 0.7167
      P-Value [Acc > NIR] : 0.02687
##
##
##
                     Kappa: 0.5745
##
   Mcnemar's Test P-Value : 0.75183
##
##
##
               Sensitivity: 0.9070
##
               Specificity: 0.6471
##
            Pos Pred Value: 0.8667
##
            Neg Pred Value: 0.7333
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6500
##
      Detection Prevalence: 0.7500
##
        Balanced Accuracy: 0.7770
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[9] = max(knn$results$ROC)
result$Testing_Accuracy[9] = cm.knn$overall[1]
# Save the testing ROC for plotting later
```

1.2.10 GBM

```
## Stochastic Gradient Boosting
##
## 243 samples
## 12 predictor
    2 classes: 'Cad', 'Normal'
##
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results across tuning parameters:
##
##
     interaction.depth n.trees ROC
                                           Sens
                                                      Spec
##
     1
                        50
                                0.9198413 0.9299673 0.6685714
##
                        100
                                0.9258497 0.9248366 0.7242857
     1
##
     1
                        150
                                0.9243371 0.9143791 0.7300000
##
                        200
                                0.9221849 0.9069281 0.7285714
     1
##
      1
                        250
                                0.9213725 0.9085948 0.7257143
##
      1
                        300
                                0.9184407 0.9022222 0.7300000
##
                                0.9167554 0.8992157 0.7157143
      1
                        350
##
      1
                        400
                                0.9154155 0.8986928 0.7157143
##
      1
                        450
                                0.9134314 0.8963399 0.7128571
##
                       500
                                0.9109104 0.8934641 0.7100000
     1
##
      2
                        50
                                0.9195985 0.9214052 0.7085714
##
     2
                       100
                                0.9158777 0.9167320 0.7128571
##
     2
                       150
                                0.9127218 0.9107843 0.7057143
                                0.9088936 0.9022549 0.7128571
##
     2
                       200
##
     2
                        250
                                0.9083987 0.9028431 0.7042857
     2
##
                       300
                                0.9044164 0.9046732 0.6957143
##
      2
                        350
                                0.9045285 0.9017320 0.6885714
##
      2
                        400
                                0.9046359 0.8987908 0.6928571
```

##	2	450	0.9033894	0.8959150	0.700000
##	2	500	0.9010131	0.8970915	0.6928571
##	3	50	0.9132213	0.9133660	0.7014286
##	3	100	0.9062325	0.9041503	0.6928571
##	3	150	0.9006863	0.9024837	0.6857143
##	3	200	0.8991690	0.8964706	0.6928571
##	3	250	0.8976657	0.8959477	0.6900000
##	3	300	0.8961625	0.8942484	0.6942857
##	3	350	0.8962792	0.8914052	0.6928571
##	3	400	0.8937628	0.8948366	0.6957143
##	3	450	0.8930812	0.8913725	0.6957143
##	3	500	0.8922782	0.8907516	0.6957143
##	4	50	0.9087162	0.9138889	0.6900000
##	4	100	0.9031746	0.9001307	0.6885714
##	4	150	0.8989356	0.8948366	0.6971429
##	4	200	0.8956022	0.8872876	0.6971429
##	4	250	0.8958870	0.8862418	0.700000
##	4	300	0.8934500	0.8896078	0.6928571
##	4	350	0.8911251	0.8855882	0.6914286
##	4	400	0.8908450	0.8843791	0.6971429
##	4	450	0.8893184	0.8826797	0.6900000
##	4	500	0.8908310	0.8832680	0.6928571
##	5	50	0.9092810	0.9161111	0.7100000
##	5	100	0.9019468	0.8999020	0.7042857
##	5	150	0.8982446	0.8964706	0.6942857
##	5	200	0.8957516	0.8930065	0.7000000
##	5	250	0.8915033	0.8924183	0.6928571
##	5	300	0.8907563	0.8879085	0.6928571
##	5	350	0.8892764	0.8850000	0.6900000
##	5	400	0.8869608	0.8809477	0.6871429
##	5	450	0.8871382	0.8768627	0.6828571
##	5	500	0.8848880	0.8774183	0.6871429
##	6	50	0.9030019	0.9075490	0.6885714
##	6	100	0.8936181	0.8925163	0.6914286
##	6	150	0.8908777	0.8900654	0.6828571
##	6	200	0.8903688	0.8894771	0.6842857
##	6	250	0.8872782	0.8842484	0.6871429
##	6	300	0.8870962	0.8831046	0.6842857
##	6	350	0.8877591	0.8837908	0.6842857
##	6	400	0.8865453	0.8826471	0.6928571
##	6	450	0.8862792	0.8769935	0.6942857
##	6	500	0.8840289	0.8768627	0.6914286
##	7	50	0.9033707	0.9052614	0.7057143
##	7	100	0.8953455	0.8929739	0.6914286
##	7	150	0.8906162	0.8877778	0.6900000
##	7	200	0.8892390	0.8854248	0.6871429
##	7	250	0.8888329	0.8792157	0.6871429
##	7	300	0.8866387	0.8808170	0.6885714
##	7	350	0.8864939	0.8784967	0.6814286
##	7	400	0.8846545	0.8784967	0.6857143
##	7	450	0.8831979	0.8756863	0.6900000
##	7	500	0.8836461	0.8720261	0.6885714
##	8	50	0.9052007	0.9046405	0.6914286
##	8	100	0.8976797	0.8983007	0.6885714

```
##
     8
                       150
                                0.8928478 0.8919935 0.6928571
##
     8
                       200
                                0.8912885 0.8889869 0.7071429
                                                     0.7000000
##
     8
                       250
                                0.8907843 0.8866340
##
     8
                       300
                                0.8889683 0.8849346 0.7014286
##
     8
                       350
                                0.8888002 0.8831046
                                                     0.7014286
##
     8
                       400
                                0.8885247 0.8790523 0.7028571
##
     8
                       450
                                0.8875163 0.8791176 0.6885714
##
                       500
     8
                                0.8868861 0.8768301 0.6885714
##
     9
                        50
                                0.9036835 0.9035621 0.7028571
##
     9
                       100
                                0.8968347 0.8884641
                                                     0.6771429
                                0.8947059 0.8845098 0.6800000
##
     9
                       150
                       200
##
     9
                                0.8913632 0.8797386
                                                     0.6814286
##
     9
                       250
                                0.8891923 0.8774183
                                                     0.6957143
##
     9
                       300
                                0.8860831 0.8750654
                                                     0.6914286
##
     9
                       350
                                0.8869141 0.8733987
                                                     0.6985714
##
     9
                       400
                                0.8839683 0.8728105
                                                     0.7000000
##
     9
                       450
                                0.8834827 0.8721895
                                                     0.6957143
##
     9
                       500
                                0.8831373 0.8726797
                                                     0.6942857
##
    10
                        50
                                0.9031232 0.9000000 0.7042857
##
    10
                       100
                                0.9006956 0.8936928 0.7028571
##
    10
                       150
                                0.8959244 0.8885621 0.7014286
##
    10
                       200
                                ##
    10
                       250
                                ##
    10
                       300
                                0.8890009 0.8868301
                                                     0.6900000
##
    10
                       350
                                0.8884127 0.8844444
                                                     0.7000000
##
    10
                       400
                                0.8873716 0.8815686
                                                     0.6871429
##
    10
                       450
                                0.8868908 0.8785948
                                                     0.6900000
##
                       500
                                0.8875724 0.8843464 0.6900000
    10
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were n.trees = 100, interaction.depth =
  1, shrinkage = 0.1 and n.minobsinnode = 10.
# Test the gbm
gbm.predict = predict(gbm, svm.test)
# confusion matrix
cm.gbm <- confusionMatrix(gbm.predict, svm.test$Cath)</pre>
print(cm.gbm)
## Confusion Matrix and Statistics
##
##
            Reference
## Prediction Cad Normal
##
      Cad
              38
                      4
##
      Normal
               5
                     13
##
##
                 Accuracy: 0.85
##
                   95% CI: (0.7343, 0.929)
##
      No Information Rate: 0.7167
##
      P-Value [Acc > NIR] : 0.01221
##
```

```
##
                     Kappa: 0.6371
##
##
   Mcnemar's Test P-Value: 1.00000
##
##
               Sensitivity: 0.8837
##
               Specificity: 0.7647
            Pos Pred Value: 0.9048
##
            Neg Pred Value: 0.7222
##
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6333
##
      Detection Prevalence: 0.7000
##
         Balanced Accuracy: 0.8242
##
          'Positive' Class : Cad
##
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[10] = max(gbm$results$ROC)
result$Testing_Accuracy[10] = cm.gbm$overall[1]
# Save the testing ROC for plotting later
gbm.probs = predict(gbm,svm.test[,!names(svm.test) %in% c("Cath")],
                    type = "prob")
gbm.ROC = roc(response = svm.test$Cath,
              predictor = gbm.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[10] = gbm.ROC$auc
```

1.2.11 Decision Tree

```
set.seed(3164)
# train the decision tree
dt <- train(Cath ~., data = svm.train,</pre>
                 method = "C5.0",
                 trControl = control,
                 verbose = FALSE,
                 preProc = c("center", "scale"),
                 tuneLength = 10,
                 metric = "ROC")
print(dt)
## C5.0
##
## 243 samples
## 12 predictor
    2 classes: 'Cad', 'Normal'
##
##
## Pre-processing: centered (15), scaled (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
```

Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...

```
## Resampling results across tuning parameters:
##
                   trials
##
     model
            winnow
                             ROC
                                         Sens
                                                    Spec
##
            FALSE
                                        0.8885294
                                                    0.6857143
     rules
                      1
                             0.8246032
##
     rules
            FALSE
                     10
                             0.8984174
                                        0.9158497
                                                    0.6685714
##
     rules FALSE
                     20
                             0.9100373
                                        0.9163072
                                                    0.7014286
##
     rules FALSE
                     30
                             0.9118254
                                        0.9144444
                                                    0.7100000
##
     rules FALSE
                     40
                             0.9131839
                                        0.9144771
                                                    0.7085714
##
     rules FALSE
                     50
                             0.9132586
                                        0.9157190
                                                    0.7057143
##
     rules FALSE
                     60
                             0.9143184
                                        0.9157190
                                                    0.7171429
##
     rules FALSE
                     70
                             0.9135481
                                        0.9157516
                                                    0.7171429
##
            FALSE
     rules
                     80
                             0.9142157
                                        0.9162745
                                                    0.7114286
##
     rules
           FALSE
                     90
                             0.9149813
                                        0.9156536
                                                    0.7157143
     rules
##
             TRUE
                      1
                             0.8276517
                                        0.8772876
                                                    0.6785714
##
             TRUE
                                        0.9000000
     rules
                     10
                             0.8701774
                                                    0.6714286
##
     rules
             TRUE
                     20
                             0.8764776
                                        0.8902614
                                                    0.6900000
##
                     30
             TRUE
                             0.8781816
                                        0.8884967
                                                    0.6900000
     rules
##
     rules
             TRUE
                     40
                             0.8780182
                                        0.8885621
                                                    0.6957143
##
             TRUE
     rules
                     50
                             0.8793347
                                        0.8896078
                                                    0.6957143
##
     rules
             TRUE
                     60
                             0.8799977
                                        0.8879085
                                                    0.6957143
##
     rules
             TRUE
                     70
                             0.8799276
                                        0.8890850
                                                    0.6971429
##
             TRUE
                                        0.8884967
     rules
                     80
                             0.8818231
                                                    0.6957143
             TRUE
##
     rules
                     90
                             0.8813329
                                        0.8884967
                                                    0.6985714
                                        0.8884967
##
     tree
            FALSE
                     1
                             0.8182493
                                                    0.6771429
##
     tree
            FALSE
                     10
                             0.8977848
                                        0.9040850
                                                    0.6871429
##
     tree
            FALSE
                     20
                             0.9047806
                                        0.9086928
                                                    0.7100000
##
            FALSE
                     30
                                        0.9064052
     tree
                             0.9068161
                                                    0.7071429
##
            FALSE
                     40
                             0.9090803
                                        0.9041503
                                                    0.7171429
     tree
##
            FALSE
     tree
                     50
                             0.9114099
                                        0.9063725
                                                    0.7171429
##
            FALSE
                     60
                             0.9103315
                                        0.9064706
                                                    0.7100000
     tree
##
     tree
            FALSE
                     70
                             0.9117507
                                        0.9064706
                                                    0.7142857
##
            FALSE
                     80
                             0.9124416
                                        0.9094444
                                                    0.7200000
     tree
##
            FALSE
                     90
                             0.9126284
                                        0.9065033
                                                    0.7157143
     tree
##
             TRUE
                             0.8200980
                                        0.8756209
                                                    0.6814286
                      1
     tree
##
             TRUE
                     10
                             0.8711438
                                        0.8913725
                                                    0.6914286
     tree
##
             TRUE
     tree
                     20
                             0.8765033
                                        0.8872876
                                                    0.7000000
##
     tree
             TRUE
                     30
                             0.8789309
                                        0.8872876
                                                    0.7071429
##
             TRUE
                                        0.8843791
                                                    0.7085714
                     40
                             0.8789799
     tree
##
             TRUE
                     50
                                        0.8837582
                                                    0.7100000
     tree
                             0.8785341
##
             TRUE
                     60
                                        0.8837908
                                                    0.7085714
     tree
                             0.8787068
##
     tree
             TRUE
                     70
                             0.8796125
                                        0.8826471
                                                    0.7057143
##
             TRUE
                     80
                                        0.8832353
                                                    0.7057143
     tree
                             0.8797899
##
     tree
             TRUE
                     90
                             0.8795472
                                        0.8849346
                                                    0.7100000
##
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were trials = 90, model = rules and
    winnow = FALSE.
# Test the decision tree
dt.predict = predict(dt, svm.test)
# confusion matrix
cm.dt <- confusionMatrix(dt.predict, svm.test$Cath)</pre>
print(cm.dt)
```

```
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               39
                4
                      14
##
       Normal
##
##
                  Accuracy : 0.8833
                    95% CI : (0.7743, 0.9518)
##
       No Information Rate: 0.7167
##
##
       P-Value [Acc > NIR] : 0.001754
##
                     Kappa: 0.7177
##
##
##
   Mcnemar's Test P-Value : 1.000000
##
##
               Sensitivity: 0.9070
##
               Specificity: 0.8235
##
            Pos Pred Value: 0.9286
##
            Neg Pred Value: 0.7778
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6500
##
      Detection Prevalence: 0.7000
         Balanced Accuracy: 0.8653
##
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[11] = max(dt$results$ROC)
result$Testing_Accuracy[11] = cm.dt$overall[1]
# Save the testing ROC for plotting later
dt.probs = predict(dt,svm.test[,!names(svm.test) %in% c("Cath")],type = "prob")
dt.ROC = roc(response = svm.test$Cath,
              predictor = dt.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[11] = dt.ROC$auc
```

1.2.12 AdaBoost Classification tree

Since the training using ROC to select the optimal model with tuneLength equal to 10 for this particular boosted model takes more than a whole night to run. We therefore adopted another approach to train this classifier, which customizing the tune grid and selecting the optimal model using accuracy.

```
na.action = na.omit)
print(adaB)
## AdaBoost.M1
## 243 samples
  12 predictor
     2 classes: 'Cad', 'Normal'
##
##
## Pre-processing: scaled (15), centered (15)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 243, 243, 243, 243, 243, 243, ...
## Resampling results across tuning parameters:
##
     coeflearn mfinal Accuracy
##
                                   Kappa
##
     Breiman
                5
                        0.8049827 0.5145849
##
    Freund
                10
                        0.7937542 0.4847262
##
     Zhu
                15
                        0.7944090 0.4817667
##
## Tuning parameter 'maxdepth' was held constant at a value of 5
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were mfinal = 5, maxdepth = 5 and
## coeflearn = Breiman.
# Testing AdaBoost Classification tree
adab.tree.predict = predict(adaB, svm.test)
# confusion matrix
cm.adab.tree <- confusionMatrix(adab.tree.predict, svm.test$Cath)</pre>
print(cm.adab.tree)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               38
##
       Normal
              5
                      13
##
##
                  Accuracy: 0.85
                    95% CI: (0.7343, 0.929)
##
##
       No Information Rate: 0.7167
##
       P-Value [Acc > NIR] : 0.01221
##
##
                     Kappa: 0.6371
##
##
   Mcnemar's Test P-Value : 1.00000
##
               Sensitivity: 0.8837
##
##
               Specificity: 0.7647
##
            Pos Pred Value: 0.9048
##
            Neg Pred Value: 0.7222
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6333
##
      Detection Prevalence: 0.7000
```

```
##
         Balanced Accuracy: 0.8242
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[12] = paste(as.character(max(adaB$results$Accuracy)),
                                "(Accuracy)", sep = " ")
result$Testing_Accuracy[12] = cm.adab.tree$overall[1]
# Save the testing ROC for plotting later
adab.probs = predict(adaB,svm.test[,!names(svm.test) %in% c("Cath")],
                     type = "prob")
adab.ROC = roc(response = svm.test$Cath,
              predictor = adab.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[12] = adab.ROC$auc
```

1.2.13 Boosted Logistic Regression

##

50

```
set.seed(3164)
# train Boosted Logistic Regression
blr = train(Cath ~ ., data = svm.train,
           method = "LogitBoost",
            tuneGrid = data.frame(nIter = c(5,10,20,50)),
            trControl = control,
           preProcess = c("scale", "center"),
           metric = "ROC",
            na.action = na.omit)
print(blr)
## Boosted Logistic Regression
##
## 243 samples
## 12 predictor
   2 classes: 'Cad', 'Normal'
##
## Pre-processing: scaled (15), centered (15)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 219, 219, 218, 219, 219, 218, ...
## Resampling results across tuning parameters:
##
##
    nIter ROC
                       Sens
                                  Spec
##
     5
           0.8263515 0.8718301 0.6014286
           0.8794748 0.9193723 0.7221429
##
     10
##
    20
           0.8829342 0.9162630 0.7043571
```

0.8844981 0.9043243 0.6862381

The final value used for the model was nIter = 50.

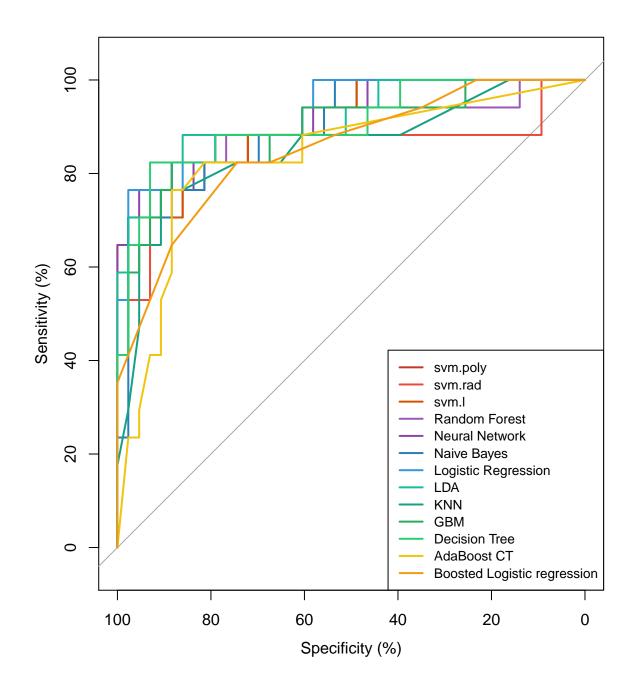
ROC was used to select the optimal model using the largest value.

```
# Testing Boosted logistic regression
blr.predict = predict(blr, svm.test)
# confusion matrix
cm.blr <- confusionMatrix(blr.predict, svm.test$Cath)</pre>
print(cm.blr)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               34
##
       Normal 5
                      11
##
##
                  Accuracy : 0.8333
##
                    95% CI : (0.7071, 0.9208)
##
       No Information Rate: 0.7222
##
       P-Value [Acc > NIR] : 0.04242
##
##
                     Kappa : 0.593
##
##
   Mcnemar's Test P-Value : 1.00000
##
               Sensitivity: 0.8718
##
##
               Specificity: 0.7333
##
            Pos Pred Value: 0.8947
            Neg Pred Value: 0.6875
##
##
                Prevalence: 0.7222
##
            Detection Rate: 0.6296
##
      Detection Prevalence: 0.7037
##
         Balanced Accuracy: 0.8026
##
##
          'Positive' Class : Cad
##
# store the ROC and Testing accuracy to the results table
result$Training_ROC[13] = max(blr$results$ROC)
result$Testing_Accuracy[13] = cm.blr$overall[1]
# Save the testing ROC for plotting later
blr.probs = predict(blr,svm.test[,!names(svm.test) %in% c("Cath")],
                    type = "prob")
blr.ROC = roc(response = svm.test$Cath,
              predictor = blr.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
result$Test_AUC[13] = blr.ROC$auc
```

1.3 Review the Results and Plotting the ROC

```
# view the results
print(result)
##
                        Classifier
                                                    Training ROC Testing Accuracy
## 1
                          SVM.Poly
                                               0.915214752567694
                                                                        0.8666667
## 2
                        SVM.Radial
                                               0.904855275443511
                                                                        0.8333333
## 3
                        SVM.Linear
                                               0.915214752567694
                                                                        0.900000
## 4
                     Random Forest
                                               0.921577964519141
                                                                        0.866667
## 5
                   Neurual Network
                                               0.92078431372549
                                                                        0.8333333
## 6
                       Naive Bayes
                                               0.888113912231559
                                                                        0.6666667
## 7
               Logistic Regression
                                               0.916615312791783
                                                                        0.8666667
## 8
                               LDA
                                               0.923487394957983
                                                                        0.8666667
## 9
                               KNN
                                               0.900873015873016
                                                                        0.8333333
                               GBM
## 10
                                               0.925849673202614
                                                                        0.8500000
## 11
                     Decision Tree
                                               0.914981325863679
                                                                        0.8833333
## 12 AdaBoost Classification Tree 0.804982729619275 (Accuracy)
                                                                        0.8500000
## 13 Boosted Logistic Regression
                                               0.884498132586368
                                                                        0.8333333
##
      Test AUC
## 1 90.69767
## 2 85.36252
## 3 90.69767
## 4 89.60328
## 5 91.79207
## 6 90.01368
## 7 92.61286
## 8 91.51847
## 9 85.49932
## 10 89.05609
## 11 90.42408
## 12 83.51573
## 13 85.22572
# ploting the ROC
plot(svm.poly.ROC,type = "S",col = "#C0392B")
plot(svm.rad.ROC,add = TRUE,col = "#E74C3C")
plot(svm.1.ROC,add = TRUE,col = "#D35400")
plot(rf.ROC,add = TRUE,col = "#9B59B6")
plot(nn.ROC,add = TRUE,col = "#8E44AD")
plot(nb.ROC,add = TRUE,col = "#2980B9")
plot(lr.ROC,add = TRUE,col = "#3498DB")
plot(lda.ROC,add = TRUE,col = "#1ABC9C")
plot(knn.ROC,add = TRUE,col = "#16A085")
plot(gbm.ROC,add = TRUE,col = "#27AE60")
plot(dt.ROC,add = TRUE,col = "#2ECC71")
plot(adab.ROC,add = TRUE,col = "#F1C40F")
plot(blr.ROC,add = TRUE,col = "#F39C12")
legend("bottomright", legend = c("svm.poly", "svm.rad", "svm.l", "Random Forest",
                                 "Neural Network", "Naive Bayes",
                                 "Logistic Regression", "LDA", "KNN", "GBM",
                                 "Decision Tree", "AdaBoost CT",
                                 "Boosted Logistic regression"),
       col = c("#C0392B", "#E74C3C", "#D35400", "#9B59B6", "#8E44AD",
```

```
"#2980B9", "#3498DB", "#1ABC9C", "#16A085", "#27AE60", "#2ECC71", "#F1C40F", "#F39C12"), lwd = 2, cex = 0.8)
```



1.4 Combining the models

We try to combine the classifiers we have trained to obtain a more robust ensemble model. We combine 12 classifiers we have trained, excluding the Naive Bayes classifier since its testing accuracy is only 63%.

```
# generate a dataframe that contains the prediction results of all models
generate_ensemble_df <- function(caddataset){</pre>
  #Input: caddataset - the training dataset
  #Output: a data frame of size (nrow x 12). Each feature (column) is comprised
          of the predictions made by that specific model, in probabilities.
  #Runtime: Linear
  aggregate_pred.df <- as.data.frame(caddataset$Cath)</pre>
  colnames(aggregate_pred.df)=c("Cath")
  #attach predictions
  aggregate_pred.df$knnres <- predict(knn, caddataset, type = "prob")$Cad
  aggregate_pred.df$ldares <- predict(lda, caddataset, type = "prob")$Cad
  aggregate_pred.df$1rres <- predict(lr, caddataset, type = "prob")$Cad</pre>
  aggregate_pred.df$rfres <- predict(rf, caddataset, type = "prob")$Cad
  aggregate_pred.df$svmLres <- predict(svm.1, caddataset, type = "prob")$Cad
  aggregate_pred.df$svmPres <- predict(svm.poly, caddataset, type = "prob")$Cad
  aggregate_pred.df$svmRres <- predict(svm.rad, caddataset, type = "prob")$Cad
  aggregate_pred.df$NNres <- predict(nn, caddataset, type = "prob")$Cad</pre>
  aggregate_pred.df$GBMres <- predict(gbm, caddataset, type = "prob")$Cad</pre>
  aggregate_pred.df$AdaBres <- predict(adaB, caddataset, type = "prob")$Cad
  aggregate_pred.df$dtres <- predict(dt, caddataset, type = "prob")$Cad
  aggregate_pred.df$blrres <- predict(blr, caddataset, type = "prob")$Cad
  return(aggregate_pred.df)
```

1.4.1 Naive Voting Ensemble (Unweighted Voting)

```
vote_ensemble <- function(dataset, label="Cath"){</pre>
  #Input: dataset - the output dataframe from the generate_ensemble_df functino.
  #Input label - A column name to predict values for.
  #Output: a vector containing the average value of all features for each
          input row.
  #Converts Y or N in input df to 1 and 0 respectively.
  #To be used to take a unweighted vote of columns, aka. vote ensembling
  #when combined with generate ensemble df
  df = dataset[,names(dataset) != c(label)]
  num = dim(df)[2]
  vote = apply(df, 1, function(x) sum(as.numeric(x)))/num
  return(as.factor(ifelse(round(vote) == 0, "Normal", "Cad")))
# compute the Confusion matrix on the training data set
ensem_result <- vote_ensemble(generate_ensemble_df(svm.train))</pre>
confusionMatrix(ensem_result,svm.train$Cath)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
      Cad 163
##
```

```
##
       Normal 10
                      62
##
##
                  Accuracy: 0.9259
##
                    95% CI: (0.8855, 0.9555)
##
       No Information Rate: 0.7119
##
       P-Value [Acc > NIR] : <2e-16
##
##
                     Kappa: 0.8209
##
    Mcnemar's Test P-Value: 0.8137
##
##
##
               Sensitivity: 0.9422
               Specificity: 0.8857
##
##
            Pos Pred Value: 0.9532
##
            Neg Pred Value: 0.8611
##
                Prevalence: 0.7119
##
            Detection Rate: 0.6708
##
      Detection Prevalence: 0.7037
##
         Balanced Accuracy: 0.9140
##
##
          'Positive' Class : Cad
##
# compute the Confusion matrix on the testing data set
ensem_result_test <- vote_ensemble(generate_ensemble_df(svm.test))</pre>
confusionMatrix(ensem_result_test,svm.test$Cath)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cad Normal
##
       Cad
               39
                      13
##
       Normal
                4
##
##
                  Accuracy : 0.8667
                    95% CI: (0.7541, 0.9406)
##
##
       No Information Rate: 0.7167
##
       P-Value [Acc > NIR] : 0.004937
##
##
                     Kappa: 0.6717
##
##
    Mcnemar's Test P-Value : 1.000000
##
##
               Sensitivity: 0.9070
               Specificity: 0.7647
##
##
            Pos Pred Value: 0.9070
##
            Neg Pred Value: 0.7647
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6500
##
      Detection Prevalence: 0.7167
##
         Balanced Accuracy: 0.8358
##
##
          'Positive' Class : Cad
##
```

1.4.2 Train logistic regression on the ensemble data frame (Weighted Voting)

```
set.seed(3164)
ensem_train <- generate_ensemble_df(svm.train)</pre>
ensem_test <- generate_ensemble_df(svm.test)</pre>
# set up 10 cross validation
control <- trainControl(method="repeatedcv",</pre>
                        number=10,
                         classProbs = TRUE,
                         summaryFunction = twoClassSummary)
# train logistic regression on result
lr_ensem<-train(Cath ~., data = ensem_train,</pre>
                method="glm",
                family = "binomial",
                trControl=control,
                metric = "ROC")
# testing the logistic regression model
ensem_lr_test=predict(lr_ensem, ensem_test)
cm.lr_ensem = confusionMatrix(ensem_lr_test, svm.test$Cath)
cm.lr_ensem
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction Cad Normal
##
       Cad
               39
       Normal
                      14
##
##
##
                  Accuracy : 0.8833
##
                    95% CI: (0.7743, 0.9518)
##
       No Information Rate: 0.7167
       P-Value [Acc > NIR] : 0.001754
##
##
##
                     Kappa: 0.7177
##
##
    Mcnemar's Test P-Value: 1.000000
##
##
               Sensitivity: 0.9070
               Specificity: 0.8235
##
            Pos Pred Value: 0.9286
##
##
            Neg Pred Value: 0.7778
##
                Prevalence: 0.7167
##
            Detection Rate: 0.6500
      Detection Prevalence: 0.7000
##
##
         Balanced Accuracy: 0.8653
##
##
          'Positive' Class : Cad
##
```

```
# Save the testing ROC for plotting later
lr.ensem.probs = predict(lr_ensem, ensem_test[,2:length(ensem_test)],
                         type = "prob")
lr.ensem.ROC = roc(response = svm.test$Cath,
              predictor = lr.ensem.probs$Cad,
              levels = levels(svm.test$Cath),
              percent = T)
# display the training ROC and Testing accuracy
cat("The training ROC is:", lr_ensem$results$ROC,"\n")
## The training ROC is: 1
cat("The Testing Accuracy is:", cm.lr_ensem$overall[1], "\n")
## The Testing Accuracy is: 0.8833333
# display the testing AUC
cat("The test AUC is: ", as.character(lr.ensem.ROC$auc))
## The test AUC is: 88.8508891928865
# Plot the Testing ROC curve
\# and compare it with the besting performing non-ensemble classifier
plot(lr.ensem.ROC,type = "S",col = "#2980B9")
plot(svm.1.ROC,add = TRUE,col = "#D35400")
legend("bottomright",
       legend= c("SVM Linear", "Weighted Voting with Logistic Regression"),
       col = c("\#D35400", "\#2980B9"), lwd = 2, cex = 0.8)
```

