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R Markdown

Chapter 12 - E-Book - Applied Predictive Modelling - Exercises pages 327:

Q 12.2

In Exercise 4.4, we described a data set which contained 96 oil samples each from one of seven types of oils (pumpkin, sunflower, peanut, olive, soybean, rapeseed, and corn). Gas chromatography was performed on each sample and the percentage of each type of 7 fatty acids was determined. We would like to use these data to build a model that predicts the type of oil based on a sample's fatty acid percentages.

Q 12.2 a

- a. Like the hepatic injury data, these data suffer from extreme imbalance. Given this imbalance, should the data be split into training and test sets?

Answer (12.2 a)

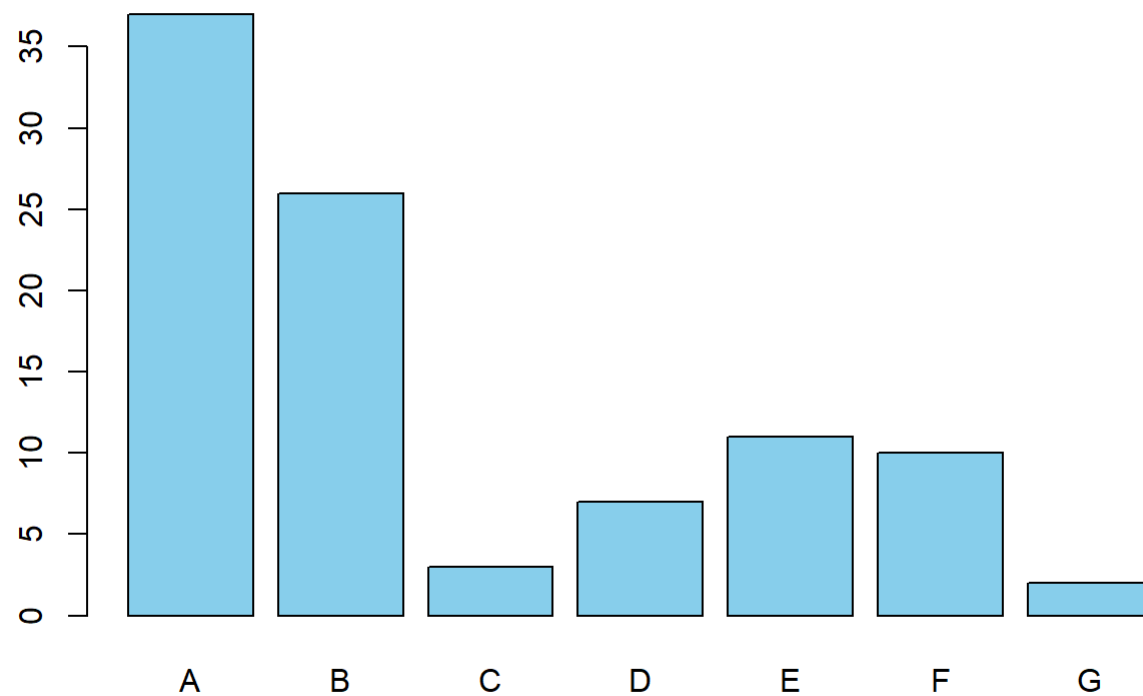
Yes, we would still split the data into training and test data sets.

```
data(oil)

library(MASS)
set.seed(123)

barplot(table(oilType), col=c("skyblue"), main="Class Distribution")
```

Class Distribution



```
# Identifying predictors with zero-variance  
nzv = nearZeroVar(fattyAcids,saveMetrics =TRUE)  
nzv
```

```
##          freqRatio percentUnique zeroVar  nzv
## Palmitic   1.333333      46.87500  FALSE FALSE
## Stearic    1.500000      42.70833  FALSE FALSE
## Oleic      1.000000      78.12500  FALSE FALSE
## Linoleic   1.500000      84.37500  FALSE FALSE
## Linolenic  1.000000      37.50000  FALSE FALSE
## Eicosanoic 1.033333      12.50000  FALSE FALSE
## Eicosenoic 3.176471      14.58333  FALSE FALSE
```

```
#
zv_cols = nearZeroVar(fattyAcids)
print( sprintf("Dropping %d zero variance columns from %d (fraction=%10.6f)", length(zv_cols), dim(fattyAcids)[2], length(zv_cols)/dim(fattyAcids)[2]) );
```

```
## [1] "Dropping 0 zero variance columns from 7 (fraction= 0.000000)"
```

```
X = fattyAcids
```

```
# There are no linearly dependent columns remaining (or to start with)
print( findLinearCombos(X) )
```

```
## $linearCombos
## list()
##
## $remove
## NULL
```

```
# Remove the correlation between the predictors

high.Corr.M<-findCorrelation(cor(fattyAcids),cutoff = .75)
no.high.corr <- fattyAcids[,-high.Corr.M]

# So, after removing the highly correlated predictor, we split the data into 80% training and 20% test (using stratified random sampling)

set.seed(234)
training.Rows = createDataPartition(oilType, p = .80, list= FALSE)

train.FattyAcids <- no.high.corr[ training.Rows, ]
test.FattyAcids <- no.high.corr[-training.Rows, ]

train.OilType <- oilType[training.Rows]
test.OilType <- oilType[-training.Rows]

ctrl <- trainControl(summaryFunction = defaultSummary)
```

Q 12.2 b

b. Which classification statistic would you choose to optimize for this exercise and why?

Answer (12.2 b)

The classification statistic that I have used here is the “**Accuracy**” rate. This is the simplest statistic as it reflects the agreement between the observed and predicted classes and so has the most straight forward interpretation.

Q 12.2 c

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

Answer (12.2 c)

Building various models

```
# Build models with this data:
#
##### Logistic Regression Analysis #####
# logistic regression

library(caret)
set.seed(456)
lr.FattyAcids <- train(x=train.FattyAcids,
                      y = train.OilType,
                      method = "multinom",
                      metric = "Accuracy",
                      trControl = ctrl)
```

```
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 33.774638
## iter 20 value 4.872133
## iter 30 value 0.021525
## final value 0.000084
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.182768
## iter 20 value 12.320164
## iter 30 value 9.641936
## iter 40 value 9.541117
## iter 50 value 9.533587
## iter 60 value 9.532916
## iter 70 value 9.532845
## final value 9.532838
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 33.775016
## iter 20 value 4.881610
## iter 30 value 0.180168
## iter 40 value 0.151977
## iter 50 value 0.142520
## iter 60 value 0.133913
## iter 70 value 0.130058
## iter 80 value 0.129193
## iter 90 value 0.127817
## iter 100 value 0.125855
## final value 0.125855
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 51.073659
## iter 20 value 3.868819
## iter 30 value 0.098740
## iter 40 value 0.000605
## final value 0.000076
```

```
## converged
## # weights:  48 (35 variable)
## initial  value 141.548998
## iter   10 value 51.463724
## iter   20 value 10.897481
## iter   30 value  8.302658
## iter   40 value  8.210548
## iter   50 value  8.187258
## iter   60 value  8.179259
## iter   70 value  8.175739
## iter   80 value  8.174449
## final   value  8.174335
## converged
## # weights:  48 (35 variable)
## initial  value 141.548998
## iter   10 value 51.074051
## iter   20 value  3.892800
## iter   30 value  0.207268
## iter   40 value  0.161671
## iter   50 value  0.150492
## iter   60 value  0.136441
## iter   70 value  0.131783
## iter   80 value  0.125323
## iter   90 value  0.118324
## iter  100 value  0.115793
## final   value  0.115793
## stopped after 100 iterations
## # weights:  48 (35 variable)
## initial  value 141.548998
## iter   10 value 19.945112
## iter   20 value  1.771753
## iter   30 value  0.012231
## iter   40 value  0.000145
## final   value  0.000050
## converged
## # weights:  48 (35 variable)
## initial  value 141.548998
## iter   10 value 22.510838
## iter   20 value 10.993928
```

```
## iter 30 value 9.882727
## iter 40 value 9.765650
## iter 50 value 9.729180
## iter 60 value 9.723955
## iter 70 value 9.722478
## iter 80 value 9.722314
## final value 9.722312
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 19.947726
## iter 20 value 1.809113
## iter 30 value 0.276144
## iter 40 value 0.252201
## iter 50 value 0.187651
## iter 60 value 0.174233
## iter 70 value 0.163847
## iter 80 value 0.153294
## iter 90 value 0.149032
## iter 100 value 0.145494
## final value 0.145494
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.294019
## iter 20 value 2.656412
## iter 30 value 0.013691
## iter 40 value 0.000141
## iter 40 value 0.000088
## iter 40 value 0.000040
## final value 0.000040
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 35.778911
## iter 20 value 11.326897
## iter 30 value 9.793150
## iter 40 value 9.714824
## iter 50 value 9.703318
```



```
## iter 60 value 9.699520
## iter 70 value 9.697806
## iter 80 value 9.697734
## final value 9.697729
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.295515
## iter 20 value 2.670047
## iter 30 value 0.199169
## iter 40 value 0.170569
## iter 50 value 0.160670
## iter 60 value 0.145198
## iter 70 value 0.139963
## iter 80 value 0.137289
## iter 90 value 0.135890
## iter 100 value 0.134680
## final value 0.134680
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 29.449743
## iter 20 value 1.257273
## iter 30 value 0.004362
## final value 0.000020
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 30.230615
## iter 20 value 9.382785
## iter 30 value 8.464242
## iter 40 value 8.320560
## iter 50 value 8.299227
## iter 60 value 8.295410
## iter 70 value 8.295003
## iter 80 value 8.294962
## final value 8.294959
## converged
## # weights: 48 (35 variable)
```

```
## initial value 141.548998
## iter 10 value 29.450523
## iter 20 value 1.282222
## iter 30 value 0.149428
## iter 40 value 0.133304
## iter 50 value 0.124125
## iter 60 value 0.116010
## iter 70 value 0.113996
## iter 80 value 0.111558
## iter 90 value 0.108976
## iter 100 value 0.106956
## final value 0.106956
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 26.975726
## iter 20 value 1.730693
## iter 30 value 0.035611
## iter 40 value 0.007637
## iter 50 value 0.001302
## iter 60 value 0.000137
## final value 0.000086
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 30.673762
## iter 20 value 13.146077
## iter 30 value 11.720518
## iter 40 value 11.604553
## iter 50 value 11.571565
## iter 60 value 11.560868
## iter 70 value 11.560240
## iter 80 value 11.560104
## final value 11.560067
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 26.979458
## iter 20 value 1.763946
```

```
## iter 30 value 0.237614
## iter 40 value 0.191283
## iter 50 value 0.176492
## iter 60 value 0.165236
## iter 70 value 0.161341
## iter 80 value 0.157678
## iter 90 value 0.153806
## iter 100 value 0.147464
## final value 0.147464
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 35.178503
## iter 20 value 2.954793
## iter 30 value 0.030551
## final value 0.000055
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 36.969077
## iter 20 value 11.748119
## iter 30 value 7.203886
## iter 40 value 7.008908
## iter 50 value 6.986803
## iter 60 value 6.984883
## iter 70 value 6.984646
## iter 80 value 6.984537
## final value 6.984524
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 35.180314
## iter 20 value 2.965878
## iter 30 value 0.107137
## iter 40 value 0.095150
## iter 50 value 0.084606
## iter 60 value 0.072508
## iter 70 value 0.059575
## iter 80 value 0.056207
```

```
## iter 90 value 0.055349
## iter 100 value 0.053071
## final value 0.053071
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 36.548769
## iter 20 value 8.807080
## iter 30 value 0.127748
## iter 40 value 0.006449
## iter 50 value 0.000324
## final value 0.000034
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 37.798708
## iter 20 value 10.770266
## iter 30 value 8.491106
## iter 40 value 8.277970
## iter 50 value 8.244160
## iter 60 value 8.236133
## iter 70 value 8.235100
## iter 80 value 8.234959
## final value 8.234955
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 36.550028
## iter 20 value 8.848907
## iter 30 value 0.205380
## iter 40 value 0.125465
## iter 50 value 0.115790
## iter 60 value 0.103035
## iter 70 value 0.090301
## iter 80 value 0.086076
## iter 90 value 0.081370
## iter 100 value 0.077920
## final value 0.077920
## stopped after 100 iterations
```

```
## # weights:  56 (42 variable)
## initial  value 153.726902
## iter   10 value 52.249885
## iter   20 value 10.914258
## iter   30 value 0.120758
## iter   40 value 0.000151
## iter   40 value 0.000076
## iter   40 value 0.000072
## final  value 0.000072
## converged
## # weights:  56 (42 variable)
## initial  value 153.726902
## iter   10 value 52.458058
## iter   20 value 16.576746
## iter   30 value 8.165289
## iter   40 value 7.644348
## iter   50 value 7.588415
## iter   60 value 7.556668
## iter   70 value 7.547752
## iter   80 value 7.541614
## iter   90 value 7.540154
## iter  100 value 7.539249
## final  value 7.539249
## stopped after 100 iterations
## # weights:  56 (42 variable)
## initial  value 153.726902
## iter   10 value 52.250094
## iter   20 value 10.924811
## iter   30 value 0.198563
## iter   40 value 0.114267
## iter   50 value 0.105391
## iter   60 value 0.096164
## iter   70 value 0.091426
## iter   80 value 0.087504
## iter   90 value 0.081995
## iter  100 value 0.076734
## final  value 0.076734
## stopped after 100 iterations
## # weights:  56 (42 variable)
```

```
## initial value 153.726902
## iter 10 value 43.943724
## iter 20 value 7.171333
## iter 30 value 0.036433
## iter 40 value 0.000132
## iter 40 value 0.000071
## iter 40 value 0.000067
## final value 0.000067
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 44.604555
## iter 20 value 13.492270
## iter 30 value 8.541689
## iter 40 value 8.372394
## iter 50 value 8.342366
## iter 60 value 8.339582
## iter 70 value 8.339273
## iter 80 value 8.339203
## final value 8.339181
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 43.944389
## iter 20 value 7.178910
## iter 30 value 0.175603
## iter 40 value 0.141547
## iter 50 value 0.116412
## iter 60 value 0.098397
## iter 70 value 0.096145
## iter 80 value 0.086185
## iter 90 value 0.080860
## iter 100 value 0.078996
## final value 0.078996
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 43.987489
## iter 20 value 1.341118
```

```
## iter 30 value 0.008164
## final value 0.000059
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 44.205922
## iter 20 value 9.534398
## iter 30 value 8.205814
## iter 40 value 8.108572
## iter 50 value 8.103823
## iter 60 value 8.102657
## iter 70 value 8.102376
## final value 8.102361
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 43.987707
## iter 20 value 1.370928
## iter 30 value 0.186875
## iter 40 value 0.158170
## iter 50 value 0.144267
## iter 60 value 0.128111
## iter 70 value 0.113659
## iter 80 value 0.109765
## iter 90 value 0.107594
## iter 100 value 0.105170
## final value 0.105170
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 13.989891
## iter 20 value 1.635363
## iter 30 value 0.036504
## iter 40 value 0.005661
## iter 50 value 0.001108
## final value 0.000052
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
```

```
## iter 10 value 16.124110
## iter 20 value 8.826168
## iter 30 value 8.608842
## iter 40 value 8.543402
## iter 50 value 8.537668
## iter 60 value 8.537236
## iter 70 value 8.537229
## final value 8.537228
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 13.992060
## iter 20 value 1.365848
## iter 30 value 0.195606
## iter 40 value 0.156195
## iter 50 value 0.142751
## iter 60 value 0.127753
## iter 70 value 0.124441
## iter 80 value 0.121744
## iter 90 value 0.117968
## iter 100 value 0.114592
## final value 0.114592
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 59.362947
## iter 20 value 12.403577
## iter 30 value 0.088979
## iter 40 value 0.000322
## final value 0.000049
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 59.666592
## iter 20 value 25.151614
## iter 30 value 11.922385
## iter 40 value 11.533296
## iter 50 value 11.498393
## iter 60 value 11.487007
```



```
## iter 70 value 11.483174
## iter 80 value 11.482588
## iter 90 value 11.482533
## final value 11.482504
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 59.363252
## iter 20 value 12.418956
## iter 30 value 0.263417
## iter 40 value 0.223912
## iter 50 value 0.201216
## iter 60 value 0.172529
## iter 70 value 0.155515
## iter 80 value 0.143611
## iter 90 value 0.140029
## iter 100 value 0.132368
## final value 0.132368
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 71.670844
## iter 20 value 10.605977
## iter 30 value 0.110888
## iter 40 value 0.003531
## iter 50 value 0.000523
## iter 60 value 0.000191
## final value 0.000050
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 47.735745
## iter 20 value 14.071774
## iter 30 value 10.099830
## iter 40 value 9.734830
## iter 50 value 9.677227
## iter 60 value 9.662201
## iter 70 value 9.655346
## iter 80 value 9.653147
```

```
## iter 90 value 9.652196
## iter 100 value 9.651920
## final value 9.651920
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 71.672621
## iter 20 value 10.627082
## iter 30 value 0.225871
## iter 40 value 0.147171
## iter 50 value 0.133213
## iter 60 value 0.127329
## iter 70 value 0.122468
## iter 80 value 0.112722
## iter 90 value 0.107423
## iter 100 value 0.102005
## final value 0.102005
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 38.944571
## iter 20 value 8.074028
## iter 30 value 0.056396
## iter 40 value 0.000570
## final value 0.000055
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 39.390736
## iter 20 value 11.318098
## iter 30 value 8.108949
## iter 40 value 7.998510
## iter 50 value 7.983754
## iter 60 value 7.979945
## iter 70 value 7.979388
## iter 80 value 7.979313
## final value 7.979308
## converged
## # weights: 56 (42 variable)
```

```
## initial value 153.726902
## iter 10 value 38.945016
## iter 20 value 8.088802
## iter 30 value 0.173701
## iter 40 value 0.151142
## iter 50 value 0.132294
## iter 60 value 0.114318
## iter 70 value 0.092336
## iter 80 value 0.073099
## iter 90 value 0.070574
## iter 100 value 0.067382
## final value 0.067382
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.246976
## iter 20 value 3.129732
## iter 30 value 0.014994
## final value 0.000063
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 35.004769
## iter 20 value 10.713633
## iter 30 value 8.611485
## iter 40 value 8.484129
## iter 50 value 8.458486
## iter 60 value 8.446048
## iter 70 value 8.442135
## iter 80 value 8.441803
## iter 90 value 8.441763
## final value 8.441750
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.247741
## iter 20 value 3.146451
## iter 30 value 0.159068
## iter 40 value 0.145749
```

```
## iter 50 value 0.131540
## iter 60 value 0.106770
## iter 70 value 0.097574
## iter 80 value 0.094669
## iter 90 value 0.089187
## iter 100 value 0.084939
## final value 0.084939
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 16.997445
## iter 20 value 0.818301
## iter 30 value 0.017500
## iter 40 value 0.002761
## iter 50 value 0.000307
## final value 0.000023
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 21.407550
## iter 20 value 9.195885
## iter 30 value 8.782977
## iter 40 value 8.681808
## iter 50 value 8.660961
## iter 60 value 8.656798
## iter 70 value 8.654281
## iter 80 value 8.654146
## final value 8.654138
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 17.001971
## iter 20 value 0.856613
## iter 30 value 0.248509
## iter 40 value 0.187528
## iter 50 value 0.151156
## iter 60 value 0.141511
## iter 70 value 0.128400
## iter 80 value 0.124364
```

```
## iter 90 value 0.121915
## iter 100 value 0.121104
## final value 0.121104
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 51.154626
## iter 20 value 5.358411
## iter 30 value 0.021845
## iter 40 value 0.000784
## final value 0.000027
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 52.290418
## iter 20 value 12.835297
## iter 30 value 10.580419
## iter 40 value 10.417425
## iter 50 value 10.383851
## iter 60 value 10.377611
## iter 70 value 10.375046
## iter 80 value 10.374303
## iter 90 value 10.374041
## iter 100 value 10.373819
## final value 10.373819
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 51.155769
## iter 20 value 5.369209
## iter 30 value 0.226549
## iter 40 value 0.188863
## iter 50 value 0.164981
## iter 60 value 0.159444
## iter 70 value 0.145893
## iter 80 value 0.141674
## iter 90 value 0.137021
## iter 100 value 0.132393
## final value 0.132393
```

```
## stopped after 100 iterations
## # weights:  40 (28 variable)
## initial  value 127.145595
## iter   10 value 32.807826
## iter   20 value 0.769667
## iter   30 value 0.001656
## final  value 0.000052
## converged
## # weights:  40 (28 variable)
## initial  value 127.145595
## iter   10 value 33.497478
## iter   20 value 7.110354
## iter   30 value 6.746339
## iter   40 value 6.564488
## iter   50 value 6.548644
## iter   60 value 6.536083
## iter   70 value 6.522318
## final  value 6.522317
## converged
## # weights:  40 (28 variable)
## initial  value 127.145595
## iter   10 value 32.808526
## iter   20 value 0.797600
## iter   30 value 0.154865
## iter   40 value 0.123289
## iter   50 value 0.097058
## iter   60 value 0.087226
## iter   70 value 0.079771
## iter   80 value 0.077196
## iter   90 value 0.074960
## iter  100 value 0.067176
## final  value 0.067176
## stopped after 100 iterations
## # weights:  48 (35 variable)
## initial  value 141.548998
## iter   10 value 56.162320
## iter   20 value 3.237015
## iter   30 value 0.058886
## iter   40 value 0.004859
```

```
## iter 50 value 0.001388
## final value 0.000076
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 37.006711
## iter 20 value 10.005032
## iter 30 value 8.432321
## iter 40 value 8.338280
## iter 50 value 8.319770
## iter 60 value 8.316393
## iter 70 value 8.315619
## iter 80 value 8.315259
## final value 8.315237
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 56.164370
## iter 20 value 3.249091
## iter 30 value 0.238977
## iter 40 value 0.175146
## iter 50 value 0.157407
## iter 60 value 0.148771
## iter 70 value 0.138645
## iter 80 value 0.133566
## iter 90 value 0.128546
## iter 100 value 0.124754
## final value 0.124754
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 10.695706
## iter 20 value 0.340744
## iter 30 value 0.006566
## iter 40 value 0.000905
## final value 0.000069
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
```

```
## iter 10 value 13.280168
## iter 20 value 8.936366
## iter 30 value 8.346602
## iter 40 value 8.297244
## iter 50 value 8.289910
## iter 60 value 8.289539
## iter 70 value 8.289368
## iter 70 value 8.289367
## iter 70 value 8.289367
## final value 8.289367
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 10.698322
## iter 20 value 0.404135
## iter 30 value 0.178476
## iter 40 value 0.164870
## iter 50 value 0.148268
## iter 60 value 0.135913
## iter 70 value 0.128346
## iter 80 value 0.120697
## iter 90 value 0.114981
## iter 100 value 0.113369
## final value 0.113369
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 51.995007
## iter 20 value 7.529170
## iter 30 value 0.044836
## final value 0.000037
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 52.469232
## iter 20 value 13.335203
## iter 30 value 9.465995
## iter 40 value 9.318174
## iter 50 value 9.295935
```



```
## iter 60 value 9.291938
## iter 70 value 9.291218
## iter 80 value 9.291090
## final value 9.291066
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 51.995484
## iter 20 value 7.541295
## iter 30 value 0.227916
## iter 40 value 0.195094
## iter 50 value 0.159839
## iter 60 value 0.141458
## iter 70 value 0.132195
## iter 80 value 0.128237
## iter 90 value 0.116466
## iter 100 value 0.112507
## final value 0.112507
## stopped after 100 iterations
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 26.814274
## iter 20 value 3.337491
## iter 30 value 0.026058
## final value 0.000051
## converged
## # weights: 48 (35 variable)
## initial value 141.548998
## iter 10 value 28.179253
## iter 20 value 8.194786
## iter 30 value 6.927215
## iter 40 value 6.901047
## iter 50 value 6.873601
## iter 60 value 6.858475
## iter 70 value 6.855689
## iter 80 value 6.854679
## final value 6.854626
## converged
## # weights: 48 (35 variable)
```

```
## initial value 141.548998
## iter 10 value 26.815655
## iter 20 value 3.347469
## iter 30 value 0.158008
## iter 40 value 0.139610
## iter 50 value 0.108112
## iter 60 value 0.093077
## iter 70 value 0.074678
## iter 80 value 0.069742
## iter 90 value 0.066699
## iter 100 value 0.061804
## final value 0.061804
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 31.838450
## iter 20 value 1.507277
## iter 30 value 0.040427
## iter 40 value 0.002707
## iter 50 value 0.000836
## final value 0.000085
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 34.900601
## iter 20 value 11.864816
## iter 30 value 10.792848
## iter 40 value 10.695758
## iter 50 value 10.687698
## iter 60 value 10.686885
## iter 70 value 10.686761
## final value 10.686753
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 31.841555
## iter 20 value 1.540988
## iter 30 value 0.309636
## iter 40 value 0.196821
```

```
## iter 50 value 0.160429
## iter 60 value 0.151257
## iter 70 value 0.142794
## iter 80 value 0.132554
## iter 90 value 0.128000
## iter 100 value 0.123995
## final value 0.123995
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 23.900110
## iter 20 value 1.447643
## iter 30 value 0.007902
## final value 0.000078
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 25.003954
## iter 20 value 7.495253
## iter 30 value 6.532706
## iter 40 value 6.476606
## iter 50 value 6.474762
## iter 60 value 6.474685
## iter 70 value 6.474670
## iter 80 value 6.474668
## iter 80 value 6.474668
## iter 80 value 6.474668
## final value 6.474668
## converged
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 23.901196
## iter 20 value 1.461418
## iter 30 value 0.099445
## iter 40 value 0.088551
## iter 50 value 0.079829
## iter 60 value 0.069404
## iter 70 value 0.059109
## iter 80 value 0.045252
```

```
## iter 90 value 0.044396
## iter 100 value 0.042700
## final value 0.042700
## stopped after 100 iterations
## # weights: 56 (42 variable)
## initial value 153.726902
## iter 10 value 38.701008
## iter 20 value 11.445468
## iter 30 value 10.395524
## iter 40 value 10.316670
## iter 50 value 10.313653
## iter 60 value 10.313589
## iter 70 value 10.313569
## final value 10.313567
## converged
```

```
prediction.LR.FattyAcids<-predict(lr.FattyAcids,test.FattyAcids)
```

```
confusionMatrix(data =prediction.LR.FattyAcids,
                  reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 1 0 0 0 0 0

B 2 4 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8235

95% CI : (0.5657, 0.962)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 0.0006427

##

Kappa : 0.7548

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 0.8000 NA 1.0000 1.0000 1.0000

Specificity 0.9000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 0.8333 0.6667 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8182 0.9091 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2353 0 0.05882 0.1176 0.1176

Detection Prevalence 0.3529 0.3529 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8071 0.8167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

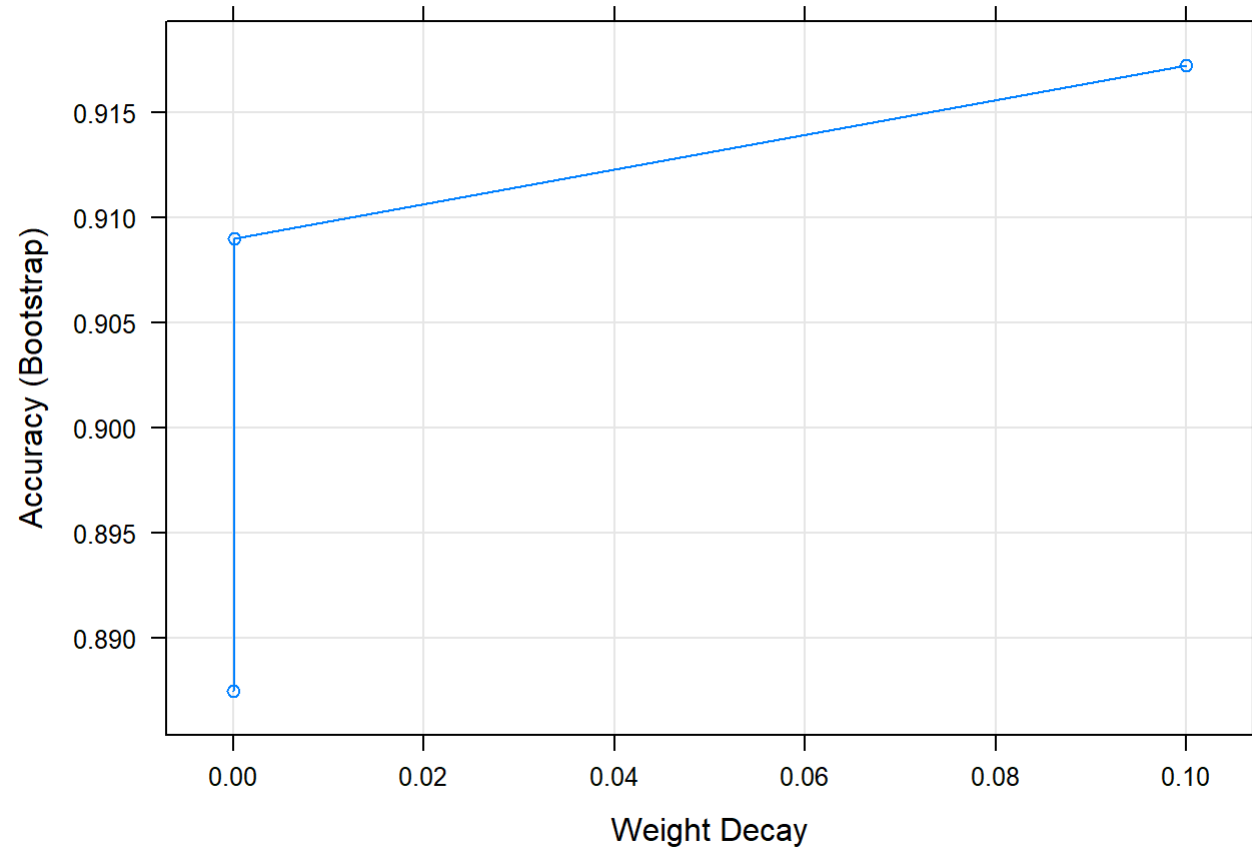
Specificity 1

Pos Pred Value NA

Neg Pred Value NA

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

```
plot(lr.FattyAcids)
```



```
##### Linear Discriminant Analysis #####
```

```
# LDA Analysis
```

```
library(MASS)
```

```
set.seed(678)
```

```
lda.FattyAcids <- train(x = train.FattyAcids,  
                        y = train.OilType,  
                        method = "lda",  
                        metric = "Accuracy",  
                        trControl = ctrl)
```

```
prediction.LDA.FattyAcids <- predict(lda.FattyAcids, test.FattyAcids)  
confusionMatrix(data = prediction.LDA.FattyAcids,  
                 reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA


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

Partial Least Squares Discriminant Analysis

```
library(MASS)
set.seed(123)
pls.FattyAcids <- train(x = train.FattyAcids,
                        y = train.OilType,
                        method = "pls",
                        tuneGrid = expand.grid(.ncomp = 1:4),
                        metric = "Accuracy",
                        trControl = ctrl)

prediction.PLS.FattyAcids <- predict(pls.FattyAcids, test.FattyAcids)
confusionMatrix(data = prediction.PLS.FattyAcids,
                 reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

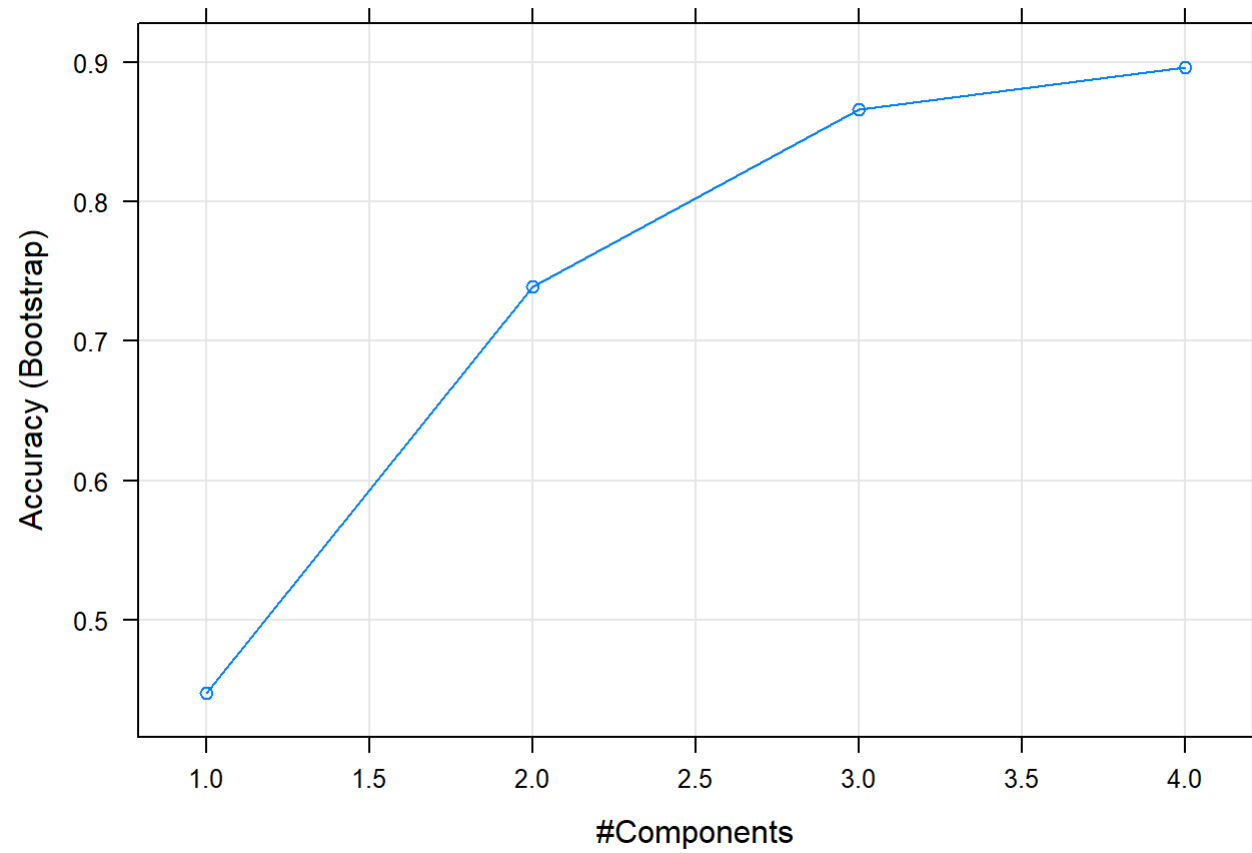
Specificity 1

Pos Pred Value NA

Neg Pred Value NA

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

```
plot(pls.FattyAcids)
```



```
##### Penalized Models #####
```

```
##### Penalized Models for Logistic Regression #####
```

```
glmGrid <- expand.grid(.alpha = c(0, .1, .2, .4, .6, .8, 1),  
                      .lambda = seq(.01, .2, length = 10))
```

```
set.seed(123)
```

```
glm.Tuned.LR.FattyAcids<- train(x=train.FattyAcids,  
                                y =train.OilType,  
                                method = "glmnet",  
                                tuneGrid = glmGrid,  
                                metric = "Accuracy",  
                                trControl = ctrl)
```

```
prediction.Glmnet.FattyAcids <- predict(glm.Tuned.LR.FattyAcids,test.FattyAcids)  
confusionMatrix(data =prediction.Glmnet.FattyAcids,reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

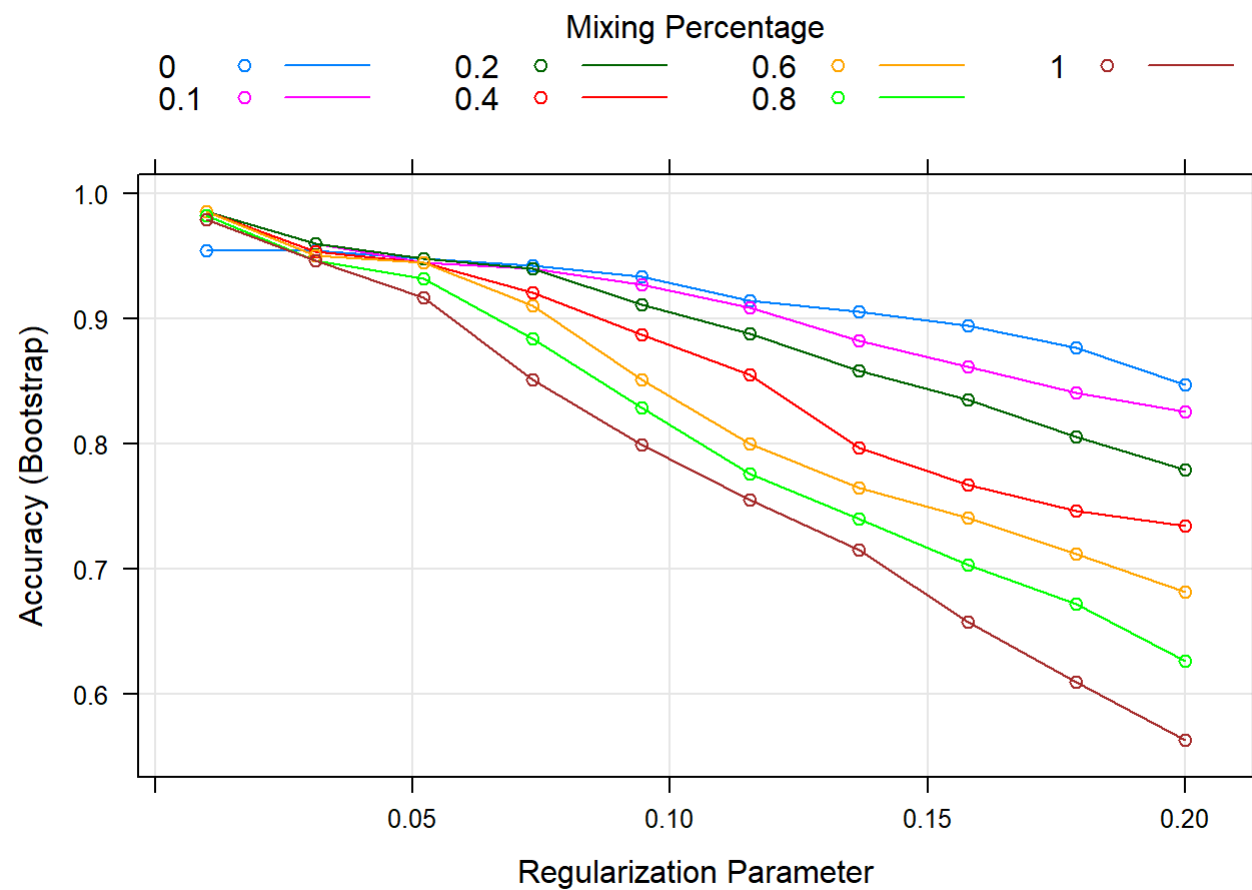
Specificity 1

Pos Pred Value NA

Neg Pred Value NA

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

```
plot(glmn.Tuned.LR.FattyAcids)
```



Penalized Models for LDA

```
library(sparseLDA)
set.seed(123)
sparse.Lda.ModelFattyAcids <- sda(x=train.FattyAcids,
                                y =train.OilType,
                                lambda = 0.01,
                                stop = -7)
## the ridge parameter called lambda.

prediction.Sparse.LDA.FattyAcids <- predict(sparse.Lda.ModelFattyAcids,test.FattyAcids)
confusionMatrix(data =prediction.Sparse.LDA.FattyAcids$class, reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 0 2 0 0 0 0 0

B 0 0 0 0 0 0 0

C 0 0 0 0 0 0 0

D 7 3 0 1 2 2 0

E 0 0 0 0 0 0 0

F 0 0 0 0 0 0 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.0588

95% CI : (0.0015, 0.2869)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 0.9999

##

Kappa : -0.0462

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.0000 0.0000 NA 1.00000 0.0000 0.0000

Specificity 0.8000 1.0000 1 0.12500 1.0000 1.0000

Pos Pred Value 0.0000 NaN NA 0.06667 NaN NaN

Neg Pred Value 0.5333 0.7059 NA 1.00000 0.8824 0.8824

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.0000 0.0000 0 0.05882 0.0000 0.0000

Detection Prevalence 0.1176 0.0000 0 0.88235 0.0000 0.0000

Balanced Accuracy 0.4000 0.5000 NA 0.56250 0.5000 0.5000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA


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

Nearest Shrunken Centroids

```
library(pamr)
nsc.Grid.FattyAcids <- data.frame(.threshold = seq(0,4, by=0.1))
set.seed(123)
nsc.Tuned.FattyAcids <- train(x = train.FattyAcids,
                             y = train.OilType,
                             method = "pam",
                             tuneGrid = nsc.Grid.FattyAcids,
                             metric = "Accuracy",
                             trControl = ctrl)
```

```
## 11Warning: a class contains only 1 sample1Warning: a class contains only 1 sample11Warning: a class contains only 1 samp
le111Warning: a class contains only 1 sample1Warning: a class contains only 1 sample111111Warning: a class contains only 1
sample1Warning: a class contains only 1 sample1Warning: a class contains only 1 sample111Warning: a class contains only 1 sa
mple1Warning: a class contains only 1 sample1Warning: a class contains only 1 sample11
```

```
prediction.NSC.FattyAcids <-predict(nsc.Tuned.FattyAcids,test.FattyAcids)
confusionMatrix(data =prediction.NSC.FattyAcids, reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

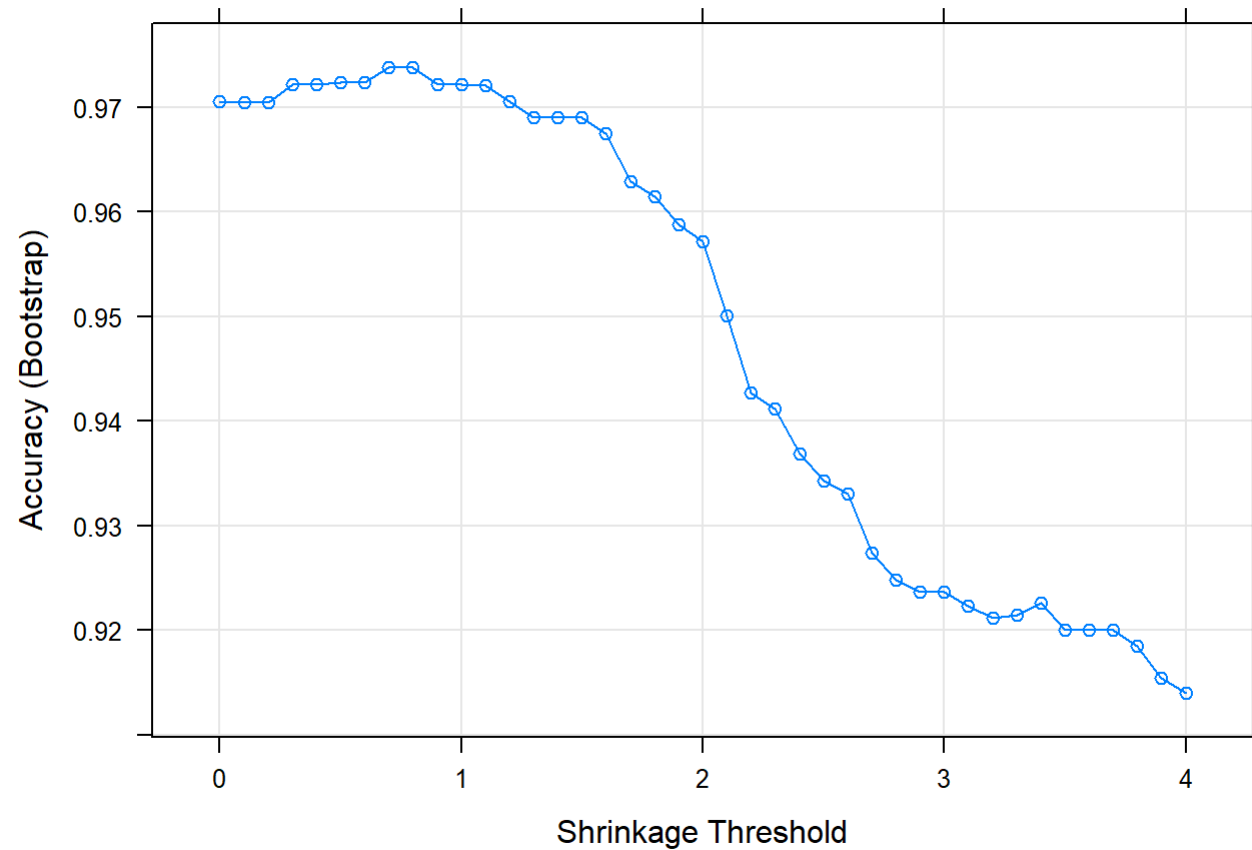
Specificity 1

Pos Pred Value NA

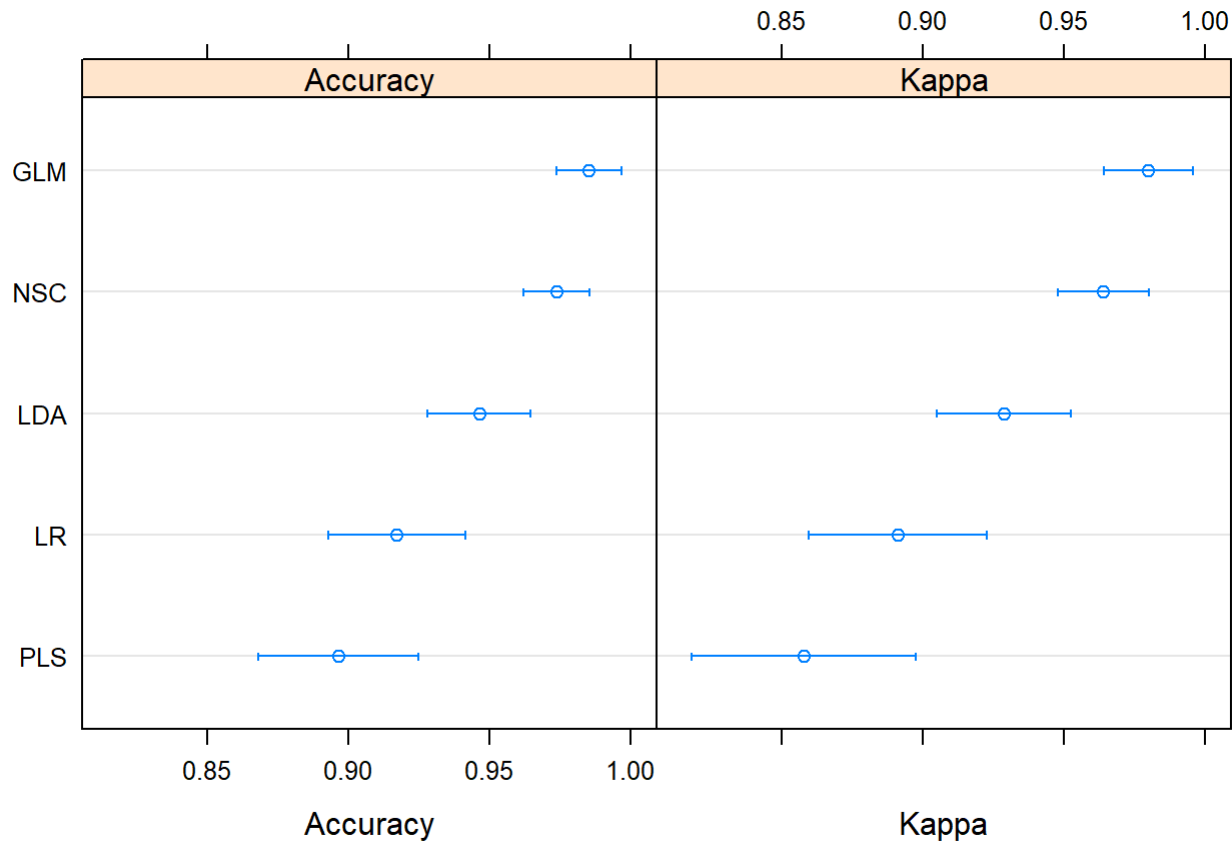
Neg Pred Value NA

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

```
plot(nsc.Tuned.FattyAcids)
```



```
# Combining the models from Question 12
res12 = resamples(list(LR=lr.FattyAcids,LDA=lda.FattyAcids,PLS=pls.FattyAcids,GLM=glm.Tuned.LR.FattyAcids,NSC=nsc.Tuned.FattyAcids ))
dotplot(res12)
```



Confidence Level: 0.95

Based on the output of the resamples function on the training data and using the classification statistic “**Accuracy**”, and also matching with the Confusion Matrix data for test data, we can say that **GLM (Penalized Model for Logistic Regression)** is the best model as far as accuracy of prediction is concerned.

And from the data, we can also see that **PLS (Partial Least Square Discriminant Analysis)** is the model with the least accurate prediction.

Chapter 13 - E-Book - Applied Predictive Modelling - Exercises pages 367:

Q 13.2

Use the fatty acid data from the previous exercise set (Exercise 12.2).

Q 13.2 a

- a. Use the same data splitting approach (if any) and pre-processing steps that you did in the previous chapter. Using the same classification statistic as before, build models described in this chapter for these data. Which model has the best predictive ability? How does this optimal model's performance compare to the best linear model's performance? Would you infer that the data have nonlinear separation boundaries based on this comparison?

Answer (13.2 a)

So, the classification statistic that I will be using here is the same as the one I used in the previous question which is "Accuracy" rate. This is the simplest statistic as it reflects the agreement between the observed and predicted classes and so has the most straight forward interpretation.

```
### Create a control function that will be used across models.
#set.seed(100)

ctrl <- trainControl(summaryFunction = defaultSummary, classProbs = TRUE)

##### Regularized discriminant analysis (RDA) #####

set.seed(476)
library(klaR)

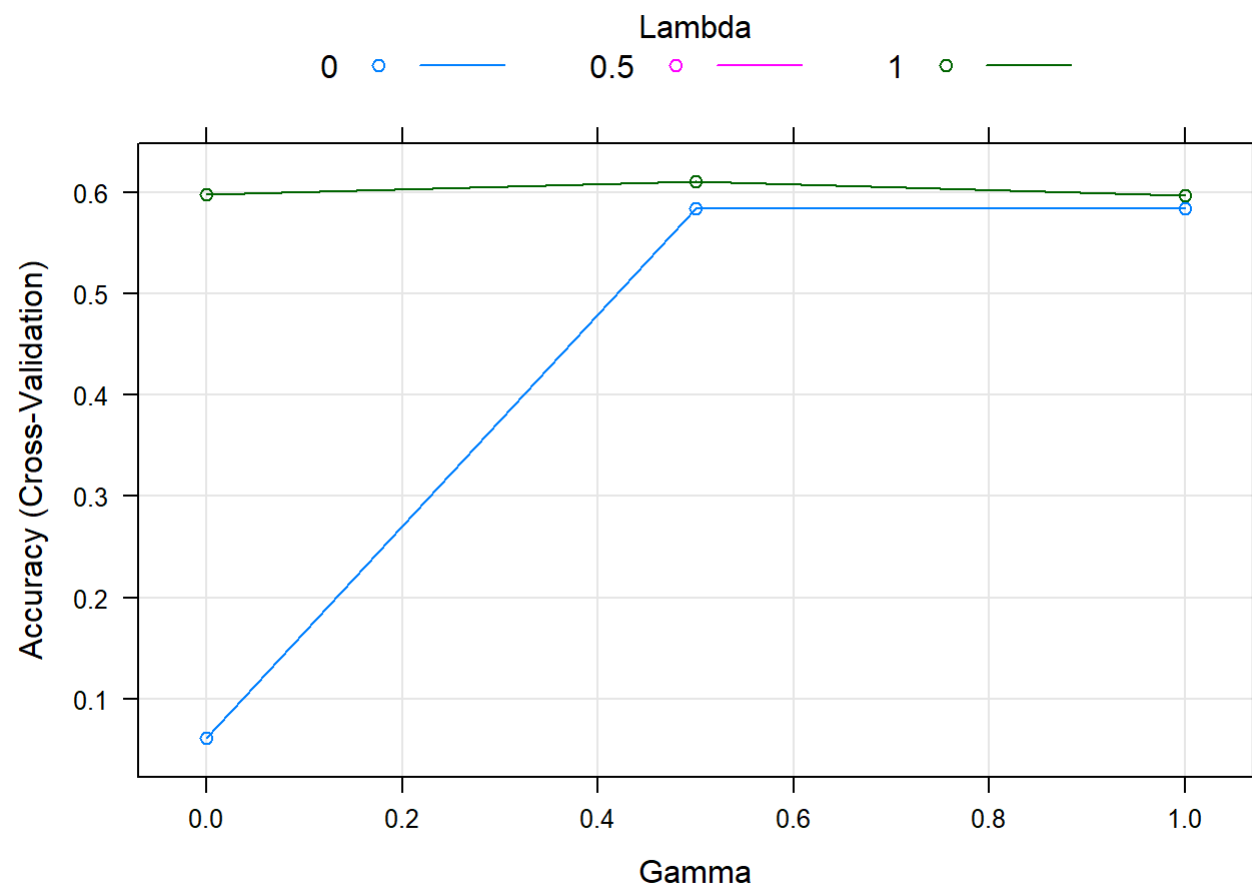
rda_grid = trainControl(method = "cv", number = 5)

RDATune <- train(x=train.FattyAcids,
y = train.OilType,
method = "rda",
metric = "Accuracy",
trControl = rda_grid)

RDATune
```

```
## Regularized Discriminant Analysis
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 63, 64, 64, 62, 63
## Resampling results across tuning parameters:
##
##  gamma  lambda  Accuracy    Kappa
##  0.0    0.0    0.06066176 0.0000000
##  0.0    0.5    0.59843137 0.5653438
##  0.0    1.0    0.59843137 0.5657895
##  0.5    0.0    0.58509804 0.5469163
##  0.5    0.5    0.61093137 0.5824561
##  0.5    1.0    0.61093137 0.5824561
##  1.0    0.0    0.58509804 0.5469163
##  1.0    0.5    0.59759804 0.5639376
##  1.0    1.0    0.59759804 0.5653179
##
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were gamma = 0.5 and lambda = 1.
```

```
plot(RDATune)
```



```
##### Mixture discriminant analysis (MDA) #####
```

```
set.seed(476)
```

```
library(mda)
```

```
MDATune <- train(as.matrix(train.FattyAcids),
```

```
y = train.OilType,
```

```
method = "mda",
```

```
tuneGrid = expand.grid(.subclasses = 3:10),
```

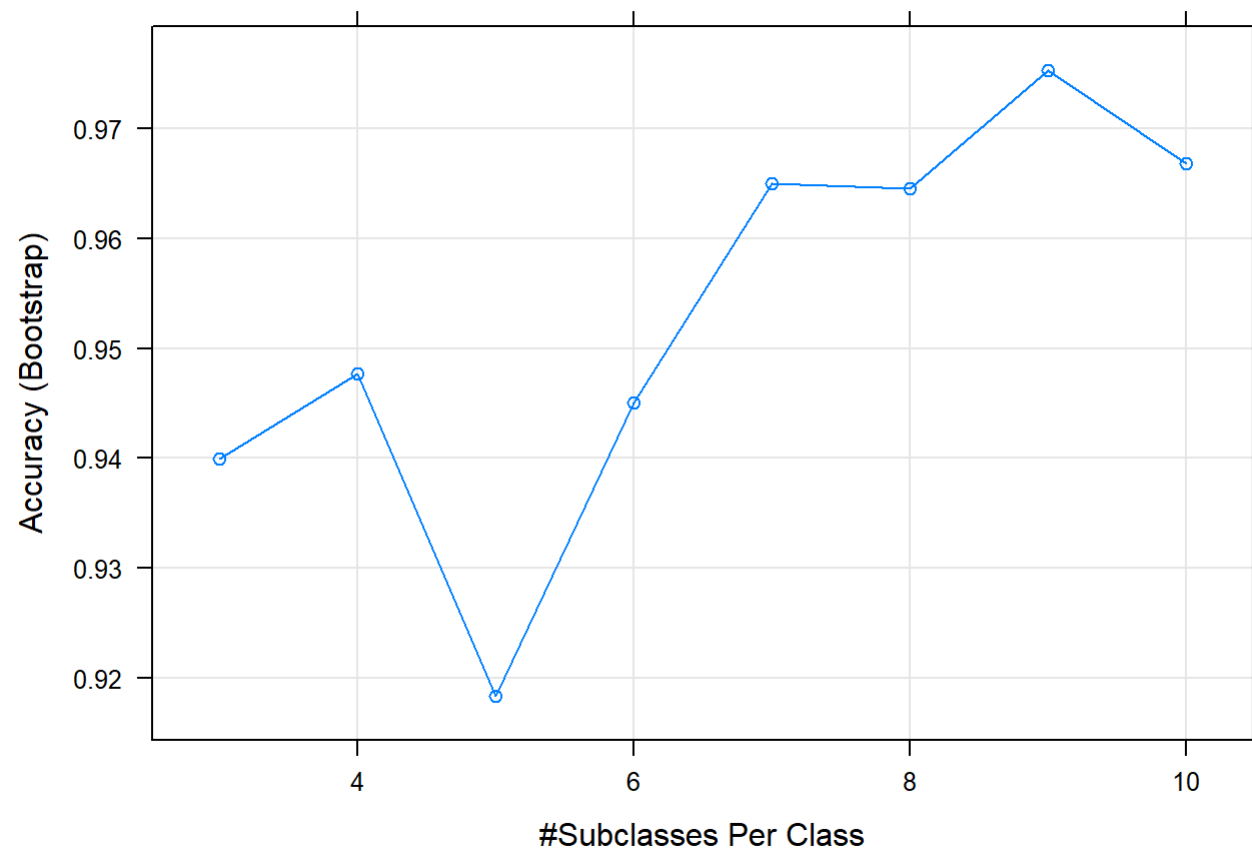
```
metric = "Accuracy",
```

```
trControl = ctrl)
```

```
MDATune
```

```
## Mixture Discriminant Analysis
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## No pre-processing
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
## subclasses Accuracy Kappa
## 3 0.9399608 0.9177847
## 4 0.9477165 0.9277604
## 5 0.9183273 0.8860572
## 6 0.9450660 0.9227933
## 7 0.9649807 0.9533588
## 8 0.9645560 0.9535669
## 9 0.9753166 0.9665862
## 10 0.9668271 0.9544511
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was subclasses = 9.
```

```
plot(MDATune)
```

```
##### Naïve Bayes (NB) #####
```

```
set.seed(476)
```

```
NBTune <- train(x = as.matrix(train.FattyAcids),  
y = train.OilType,  
method = "nb",  
preProc = c('center', 'scale'),  
metric = "Accuracy",  
trControl = ctrl)
```

```
NBTune
```

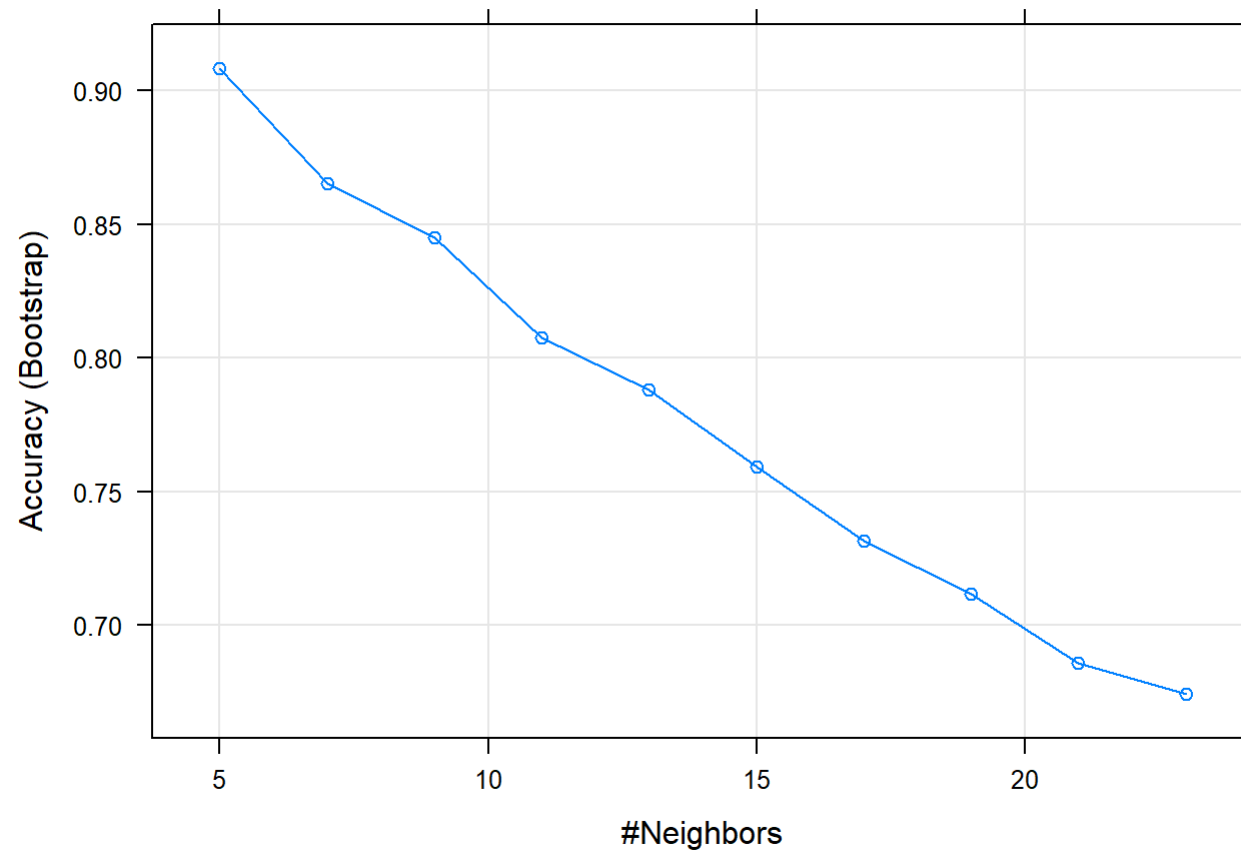
```
## Naive Bayes
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## Pre-processing: centered (6), scaled (6)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
##   usekernel  Accuracy  Kappa
##   FALSE      NaN      NaN
##   TRUE       0.9317812  0.9070348
##
## Tuning parameter 'fL' was held constant at a value of 0
## Tuning
## parameter 'adjust' was held constant at a value of 1
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were fL = 0, usekernel = TRUE and adjust
## = 1.
```

K-nearest neighbors (KNN)

```
set.seed(1)
KNNTune = train(x=train.FattyAcids, y=train.OilType, method="knn", metric = "Accuracy",preProcess=c("center","scale"), tuneL
ength=10)
KNNTune
```

```
## k-Nearest Neighbors
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## Pre-processing: centered (6), scaled (6)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
##  k    Accuracy    Kappa
##   5  0.9085544  0.8781189
##   7  0.8653627  0.8216568
##   9  0.8449985  0.7938198
##  11  0.8076641  0.7417653
##  13  0.7881356  0.7134347
##  15  0.7593568  0.6698862
##  17  0.7314335  0.6275864
##  19  0.7116438  0.5961364
##  21  0.6856207  0.5549648
##  23  0.6740550  0.5377973
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was k = 5.
```

```
plot(KNNTune)
```



```
##### Neural networks (NN) #####  
set.seed(476)  
  
nnetGrid <- expand.grid(.size = 1:10,  
  .decay = c(0, .1, 1, 2))  
maxSize <- max(nnetGrid$.size)  
numWts <- 200  
  
NNTune <- train(x = as.matrix(train.FattyAcids),  
  y = train.OilType,  
  method = "nnet",  
  metric = "Accuracy",  
  preProc = c("center", "scale", "spatialSign"),  
  tuneGrid = nnetGrid,  
  trace = FALSE,  
  maxit = 2000,  
  MaxNWts = numWts,  
  trControl = ctrl)  
  
NNTune
```

```

## Neural Network
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## Pre-processing: centered (6), scaled (6), spatial sign transformation (6)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
##   size  decay  Accuracy   Kappa
##   1    0.0    0.7538554  0.65573062
##   1    0.1    0.6668914  0.51397841
##   1    1.0    0.6332390  0.44049879
##   1    2.0    0.4093663  0.08997442
##   2    0.0    0.8037841  0.73740077
##   2    0.1    0.8258184  0.75985316
##   2    1.0    0.6800462  0.51411136
##   2    2.0    0.5207266  0.25701899
##   3    0.0    0.8680357  0.82080082
##   3    0.1    0.9098924  0.87692567
##   3    1.0    0.6965723  0.54180210
##   3    2.0    0.5682829  0.33650389
##   4    0.0    0.8874056  0.84721102
##   4    0.1    0.9217128  0.89361252
##   4    1.0    0.7131944  0.57107632
##   4    2.0    0.5745016  0.34335711
##   5    0.0    0.9075085  0.87678433
##   5    0.1    0.9206029  0.89198672
##   5    1.0    0.7276461  0.59302754
##   5    2.0    0.5767849  0.34907932
##   6    0.0    0.9073718  0.87539184
##   6    0.1    0.9206459  0.89191039
##   6    1.0    0.7233038  0.58726371
##   6    2.0    0.5868525  0.36141344
##   7    0.0    0.9241425  0.89731282
##   7    0.1    0.9206459  0.89190913
##   7    1.0    0.7341276  0.60370926

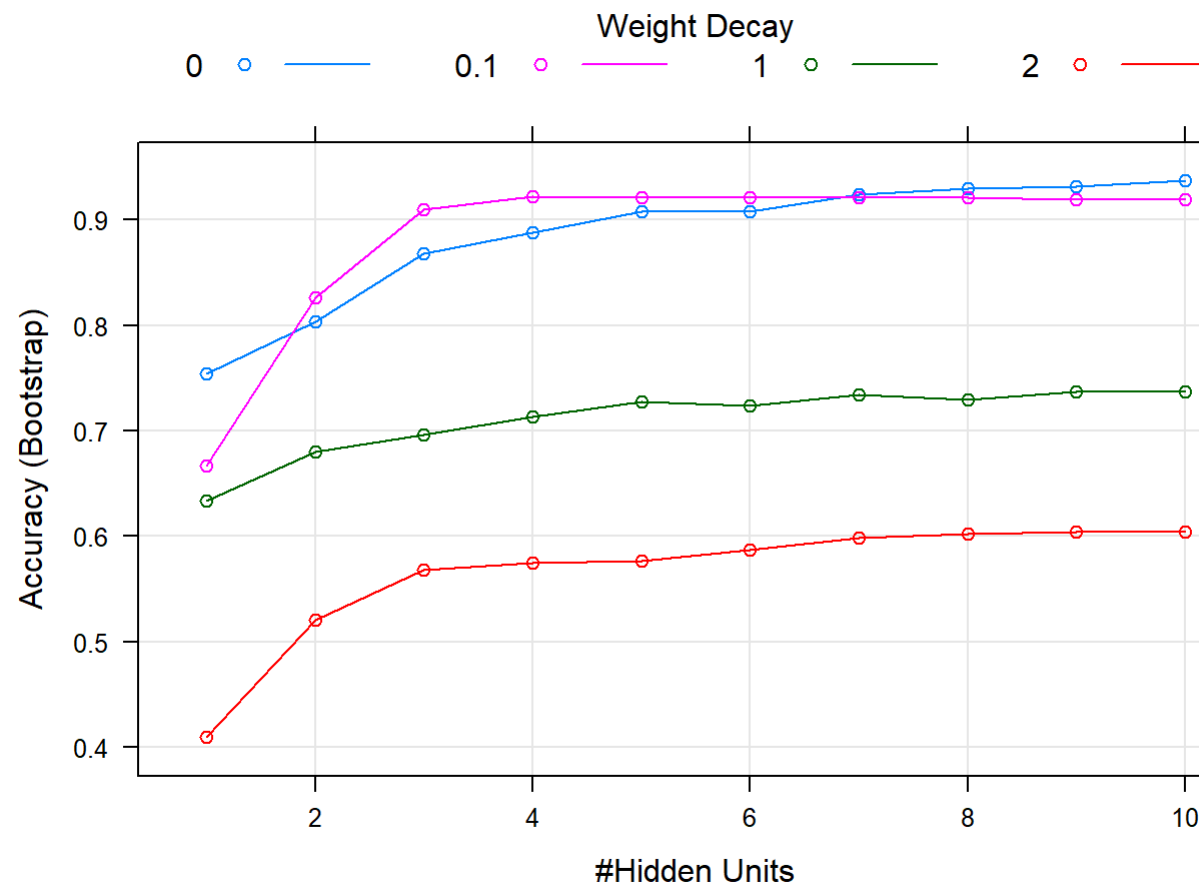
```

```
##      7      2.0      0.5987207  0.37874697
##      8      0.0      0.9294742  0.90538081
##      8      0.1      0.9206918  0.89223841
##      8      1.0      0.7293657  0.59787680
##      8      2.0      0.6018021  0.38402564
##      9      0.0      0.9317742  0.90813314
##      9      0.1      0.9193125  0.89015029
##      9      1.0      0.7371736  0.60977713
##      9      2.0      0.6044586  0.38798309
##     10      0.0      0.9367121  0.91421819
##     10      0.1      0.9193125  0.89033655
##     10      1.0      0.7369355  0.60990750
##     10      2.0      0.6045608  0.38853294
##
```

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

The final values used for the model were size = 10 and decay = 0.

```
plot(NNTune)
```




```
##### Flexible discriminant analysis (FDA) #####
```

```
set.seed(476)
```

```
library(mda)
```

```
FDATune <- train(as.matrix(train.FattyAcids),
```

```
y = train.OilType,
```

```
method = "fda",
```

```
tuneGrid = expand.grid(.nprune = 2:30,.degree = 1:2),
```

```
metric = "Accuracy",
```

```
trControl = ctrl)
```

```
FDATune
```

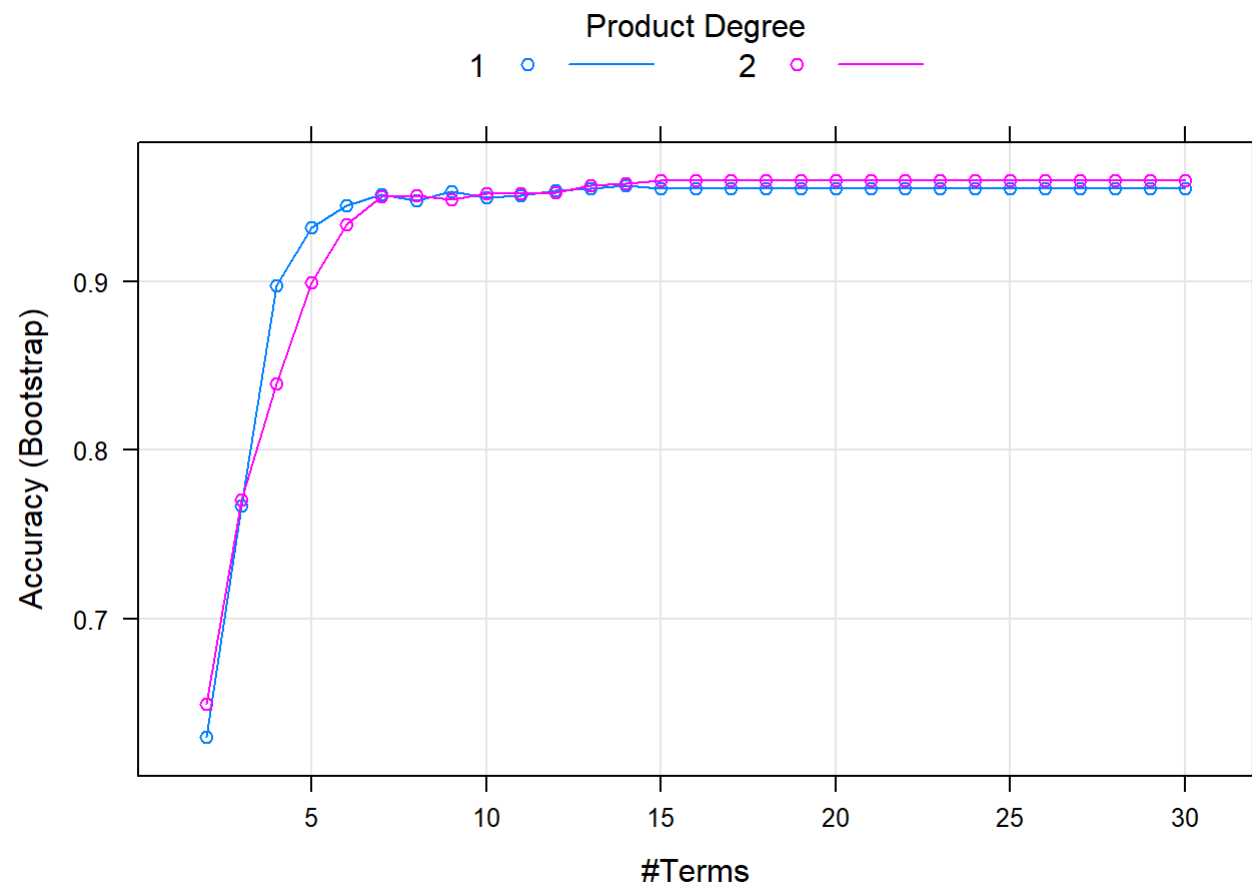
```
## Flexible Discriminant Analysis
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## No pre-processing
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
##  nprune  degree  Accuracy  Kappa
##    2      1      0.6298498  0.4501024
##    2      2      0.6494450  0.4758130
##    3      1      0.7667217  0.6691438
##    3      2      0.7708481  0.6745045
##    4      1      0.8977735  0.8563852
##    4      2      0.8395508  0.7754163
##    5      1      0.9316972  0.9068045
##    5      2      0.8992119  0.8585319
##    6      1      0.9448666  0.9248773
##    6      2      0.9336017  0.9069360
##    7      1      0.9517139  0.9339442
##    7      2      0.9504849  0.9321043
##    8      1      0.9476869  0.9279072
##    8      2      0.9506034  0.9321027
##    9      1      0.9532736  0.9355339
##    9      2      0.9486826  0.9294467
##   10      1      0.9493888  0.9304827
##   10      2      0.9519720  0.9339302
##   11      1      0.9511271  0.9331036
##   11      2      0.9522983  0.9345158
##   12      1      0.9536868  0.9361965
##   12      2      0.9523873  0.9348404
##   13      1      0.9551656  0.9383075
##   13      2      0.9565676  0.9403595
##   14      1      0.9566471  0.9402144
##   14      2      0.9579709  0.9423340
##   15      1      0.9552185  0.9384904
```

##	15	2	0.9595053	0.9440537
##	16	1	0.9552185	0.9384904
##	16	2	0.9595053	0.9441142
##	17	1	0.9552185	0.9384904
##	17	2	0.9595053	0.9442221
##	18	1	0.9552185	0.9384904
##	18	2	0.9595053	0.9442566
##	19	1	0.9552185	0.9384904
##	19	2	0.9595053	0.9442954
##	20	1	0.9552185	0.9384904
##	20	2	0.9595053	0.9442954
##	21	1	0.9552185	0.9384904
##	21	2	0.9595053	0.9442954
##	22	1	0.9552185	0.9384904
##	22	2	0.9595053	0.9442954
##	23	1	0.9552185	0.9384904
##	23	2	0.9595053	0.9442954
##	24	1	0.9552185	0.9384904
##	24	2	0.9595053	0.9442954
##	25	1	0.9552185	0.9384904
##	25	2	0.9595053	0.9442954
##	26	1	0.9552185	0.9384904
##	26	2	0.9595053	0.9442954
##	27	1	0.9552185	0.9384904
##	27	2	0.9595053	0.9442954
##	28	1	0.9552185	0.9384904
##	28	2	0.9595053	0.9442954
##	29	1	0.9552185	0.9384904
##	29	2	0.9595053	0.9442954
##	30	1	0.9552185	0.9384904
##	30	2	0.9595053	0.9442954
##				

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

The final values used for the model were degree = 2 and nprune = 15.

```
plot(FDATune)
```



Support Vector Machines (SVM)

```
set.seed(0)
```

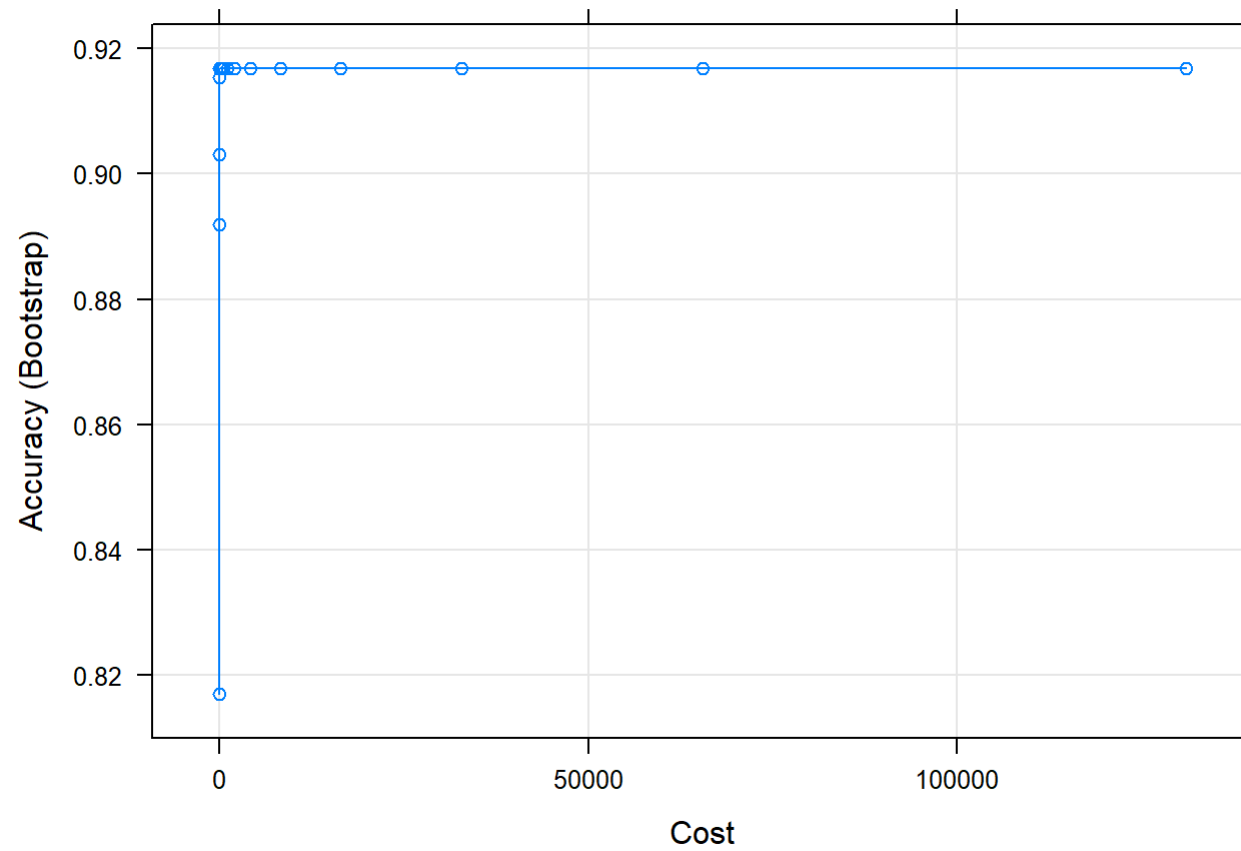
```
library(kernlab)
```

```
SVMTune = train(x=train.FattyAcids, y=train.OilType, method="svmRadial", metric = "Accuracy", preProcess=c("center","scale"), tuneLength=20)
```

```
SVMTune
```

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 79 samples
## 6 predictor
## 7 classes: 'A', 'B', 'C', 'D', 'E', 'F', 'G'
##
## Pre-processing: centered (6), scaled (6)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 79, 79, 79, 79, 79, 79, ...
## Resampling results across tuning parameters:
##
##      C          Accuracy   Kappa
##      0.25  0.8169850  0.7509460
##      0.50  0.8919323  0.8561479
##      1.00  0.9031009  0.8712838
##      2.00  0.9153426  0.8882733
##      4.00  0.9168811  0.8901886
##      8.00  0.9168811  0.8901886
##     16.00  0.9168811  0.8901886
##     32.00  0.9168811  0.8901886
##     64.00  0.9168811  0.8901886
##    128.00  0.9168811  0.8901886
##    256.00  0.9168811  0.8901886
##    512.00  0.9168811  0.8901886
##   1024.00  0.9168811  0.8901886
##   2048.00  0.9168811  0.8901886
##   4096.00  0.9168811  0.8901886
##   8192.00  0.9168811  0.8901886
##  16384.00  0.9168811  0.8901886
##  32768.00  0.9168811  0.8901886
##  65536.00  0.9168811  0.8901886
## 131072.00  0.9168811  0.8901886
##
## Tuning parameter 'sigma' was held constant at a value of 0.2143859
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were sigma = 0.2143859 and C = 4.
```

```
plot(SVMTune)
```



```
### Predict the test set based on eight models
#RDA
pred.rda <- predict(RDATune,test.FattyAcids, type = "prob")[,1]
#MDA
pred.mda <- predict(MDATune,test.FattyAcids, type = "prob")[,1]
#NB
pred.nb <- predict(NBTune,test.FattyAcids, type = "prob")[,1]
#KNN
pred.knn <- predict(KNNTune,test.FattyAcids, type = "prob")[,1]
#NN
pred.nn <- predict(NNTune,test.FattyAcids, type = "prob")[,1]
#FDA
pred.fda <- predict(FDATune, test.FattyAcids, type = "prob")[,1]
#SVM
pred.svm <- predict(SVMTune, test.FattyAcids, type = "prob")[,1]

#####Create the confusion matrix from the test set#####

#Confusion Matrix of RDA
confusionMatrix(data = predict(RDATune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA

## Prevalence	0
## Detection Rate	0
## Detection Prevalence	0
## Balanced Accuracy	NA

#Confusion matrix of MDA

```
confusionMatrix(data = predict(MDATune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 6 0 0 0 0 0 0

B 1 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.9412

95% CI : (0.7131, 0.9985)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 7.111e-06

##

Kappa : 0.9183

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.8571 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.9167 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.8333 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.9091 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.3529 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.3529 0.3529 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.9286 0.9583 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA

## Prevalence	0
## Detection Rate	0
## Detection Prevalence	0
## Balanced Accuracy	NA

#Confusion matrix of NB

```
confusionMatrix(data = predict(NBTune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 7 0 0 0 0 0 0

B 0 3 0 0 0 0 0

C 0 1 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 1 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8426

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 1.0000 0.6000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 1.0000 0.94118 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 1.0000 NA 1.0000 1.0000 1.0000

Neg Pred Value 1.0000 0.8571 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0.00000 0.05882 0.1176 0.1176

Detection Rate 0.4118 0.1765 0.00000 0.05882 0.1176 0.1176

Detection Prevalence 0.4118 0.1765 0.05882 0.05882 0.1176 0.1176

Balanced Accuracy 1.0000 0.8000 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 0.94118

Pos Pred Value NA

Neg Pred Value NA

```
## Prevalence          0.00000
## Detection Rate      0.00000
## Detection Prevalence 0.05882
## Balanced Accuracy    NA
```

#Confusion matrix of KNN

```
confusionMatrix(data = predict(KNNTune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA

## Prevalence	0
## Detection Rate	0
## Detection Prevalence	0
## Balanced Accuracy	NA

#Confusion matrix of NN

```
confusionMatrix(data = predict(NNTune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA

## Prevalence	0
## Detection Rate	0
## Detection Prevalence	0
## Balanced Accuracy	NA

#Confusion matrix of FDA

```
confusionMatrix(data = predict(FDATune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

Neg Pred Value NA

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

#Confusion matrix of SVM

```
confusionMatrix(data = predict(SVMTune, test.FattyAcids), reference = test.OilType)
```

Confusion Matrix and Statistics

##

Reference

Prediction A B C D E F G

A 5 0 0 0 0 0 0

B 2 5 0 0 0 0 0

C 0 0 0 0 0 0 0

D 0 0 0 1 0 0 0

E 0 0 0 0 2 0 0

F 0 0 0 0 0 2 0

G 0 0 0 0 0 0 0

##

Overall Statistics

##

Accuracy : 0.8824

95% CI : (0.6356, 0.9854)

No Information Rate : 0.4118

P-Value [Acc > NIR] : 8.516e-05

##

Kappa : 0.8381

##

McNemar's Test P-Value : NA

##

Statistics by Class:

##

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

Sensitivity 0.7143 1.0000 NA 1.0000 1.0000 1.0000

Specificity 1.0000 0.8333 1 1.0000 1.0000 1.0000

Pos Pred Value 1.0000 0.7143 NA 1.0000 1.0000 1.0000

Neg Pred Value 0.8333 1.0000 NA 1.0000 1.0000 1.0000

Prevalence 0.4118 0.2941 0 0.05882 0.1176 0.1176

Detection Rate 0.2941 0.2941 0 0.05882 0.1176 0.1176

Detection Prevalence 0.2941 0.4118 0 0.05882 0.1176 0.1176

Balanced Accuracy 0.8571 0.9167 NA 1.0000 1.0000 1.0000

Class: G

Sensitivity NA

Specificity 1

Pos Pred Value NA

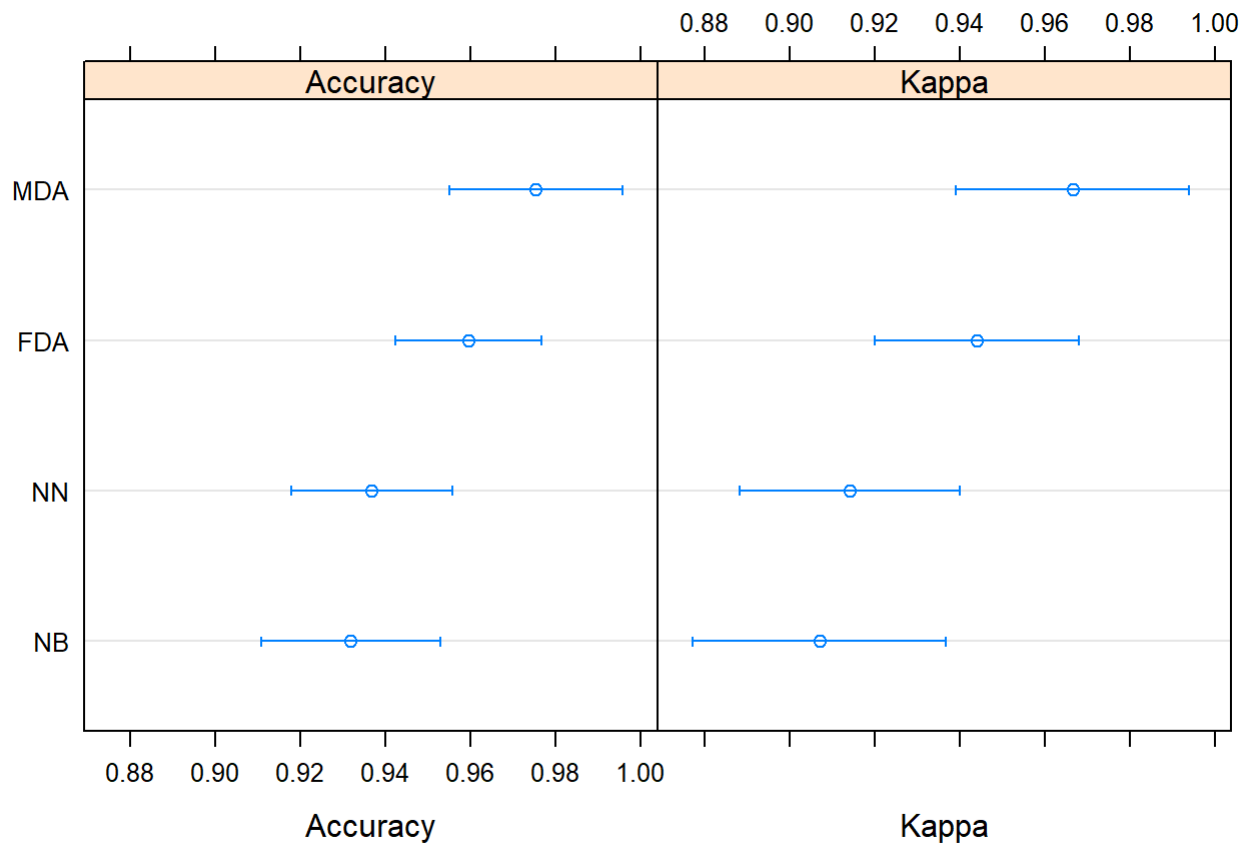
Neg Pred Value NA

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

#Resamples of Training data

Combining the models from Question 13

```
res13 = resamples(list(MDA=MDATune,NB=NBTune,NN=NNtune,FDA=FDATune))
dotplot(res13)
```



Confidence Level: 0.95

Q 13.2 b

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

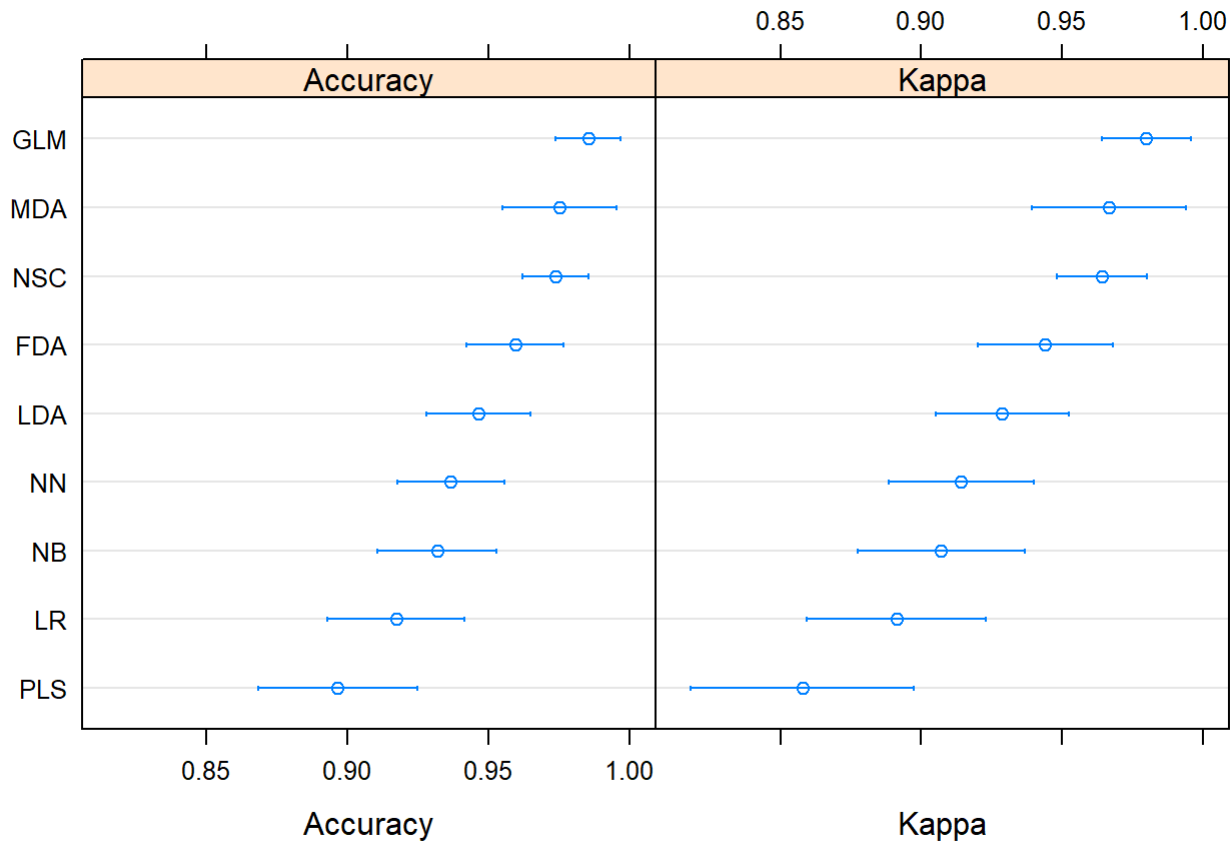
Answer (13.2 b)

Based on the output of the `resamples` function on the training data and using the classification statistic “**Accuracy**”, and also matching with the Confusion Matrix data for test data, we can say that **MDA (Mixed Discriminant Analysis)** is the best model as far as accuracy of prediction is concerned.

And from the data, we can also see that **NB (Naive Bayes)** is the model with the least accurately prediction.

(Overall)

```
# Combining the models from Question 12 & Question 13
res1213 = resamples(list(MDA=MDATune,NB=NBTune,NN=NN Tune,FDA=FDATune,LR=lr.FattyAcids,LDA=lda.FattyAcids,PLS=pls.FattyAcids,
GLM=glm.Tuned.LR.FattyAcids,NSC=nsc.Tuned.FattyAcids))
dotplot(res1213)
```



Confidence Level: 0.95

If we combine the outputs of Question 12 and Question 13, based on the output of the resamples function on the training data and using the classification statistic “**Accuracy**”, and also matching with the Confusion Matrix data for test data, we can say that **GLM (Penalized Model for Logistic Regression)** is the best model as far as accuracy of prediction is concerned.

Again if we combine the outputs of Question 12 and Question 13, from the data, we see that **PLS (Partial Least Squares Discriminant Analysis)** is the model with the least accurate prediction.