## Predicting the Oligomerization of Fluorescent Protein

## Rnewbie

February 22, 2558 BE

```
library(RCurl)
## Loading required package: bitops
library(prospectr)
## Loading required package: RcppArmadillo
library(caret)
## Loading required package: lattice
## Loading required package: ggplot2
library(RWeka)
set.seed(3)
x <- getURL("https://raw.githubusercontent.com/Rnewbie/OliFP/master/OliFP.csv")
OliFP <- read.csv(text=x, header = TRUE)</pre>
data <- OliFP
PCP <- data[, 2:532]
DPC <- data[, 533:932]</pre>
AAC <- data[, 933:952]
AAC_DPC <- cbind(AAC, DPC)
AAC_PCP <- cbind(AAC, PCP)
DPC_PCP <- cbind(DPC, PCP)</pre>
ALL <- data[, 5:952]
Oligomerization <- data $Oligomerization
set.seed(1)
x \leftarrow list(AAC = AAC,
          DPC = DPC,
          PCP = PCP,
          AAC_DPC = AAC_DPC,
          AAC_PCP = AAC_PCP,
          DPC PCP = DPC PCP,
          ALL = ALL)
J48 <- lapply(x, function(x){
  data <- cbind(Oligomerization, x)</pre>
  Monomer <- subset(data, Oligomerization == "Monomer")</pre>
  Oligomer <- subset(data, Oligomerization == "Oligomer")</pre>
  sel <- kenStone(Monomer[-1], k = 150, metric = "mahal", pc=2)</pre>
  train_Monomer <- Monomer[sel$model, ]</pre>
  test_Monomer <- Monomer[sel$test, ]</pre>
  sel <- kenStone(Oligomer[-1], k = 149, metric = "mahal", pc=2)</pre>
  train_Oligomer <- Oligomer[sel$model, ]</pre>
  test Oligomer <- Oligomer[sel$test, ]</pre>
  Train <- rbind(train_Monomer, train_Oligomer)</pre>
```

```
Test <- rbind(test_Monomer, test_Oligomer)</pre>
  x <- J48(Oligomerization~., data = Train)
  cv <- evaluate_Weka_classifier(x,</pre>
                                          numFolds=10.
                                          complexity = FALSE,
                                          seed=1,
                                          class=TRUE)
  external <- evaluate Weka classifier(x,
                                        newdata = Test,
                                        numFolds=10,
                                        complexity = FALSE,
                                        seed=1,
                                        class=TRUE)
 Model <- summary(x)</pre>
 results <- list(Training = Model, Cross_Validation_10_Fold = cv, Testing = external)
 return(results)
})
J48
## $AAC
## $AAC$Training
## === Summary ===
##
## Correctly Classified Instances
                                           269
                                                             89.9666 %
## Incorrectly Classified Instances
                                            30
                                                             10.0334 %
## Kappa statistic
                                             0.7993
## Mean absolute error
                                             0.1599
## Root mean squared error
                                            0.2828
## Relative absolute error
                                            31.9819 %
## Root relative squared error
                                            56.5525 %
## Coverage of cases (0.95 level)
                                            98.6622 %
## Mean rel. region size (0.95 level)
                                           73.2441 %
## Total Number of Instances
                                           299
## === Confusion Matrix ===
##
##
     a b <-- classified as
## 133 17 |
              a = Monomer
   13 136 | b = Oligomer
##
## $AAC$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
##
## === Summary ===
##
## Correctly Classified Instances
                                           234
                                                             78.2609 %
## Incorrectly Classified Instances
                                                             21.7391 %
## Kappa statistic
                                             0.5651
## Mean absolute error
                                             0.2321
                                            0.4343
## Root mean squared error
## Relative absolute error
                                            46.4215 %
                                            86.8685 %
## Root relative squared error
```

```
## Coverage of cases (0.95 level)
                                            88.6288 %
## Mean rel. region size (0.95 level)
                                            68.7291 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area
                                                                                                    Class
                             0.255
##
                    0.820
                                      0.764
                                                  0.820
                                                           0.791
                                                                       0.567
                                                                                0.814
                                                                                          0.787
                                                                                                    Monom
##
                    0.745
                             0.180
                                       0.804
                                                  0.745
                                                           0.774
                                                                       0.567
                                                                                0.814
                                                                                          0.751
                                                                                                    Oligo
## Weighted Avg.
                    0.783
                             0.218
                                       0.784
                                                  0.783
                                                           0.782
                                                                       0.567
                                                                                0.814
                                                                                          0.769
## === Confusion Matrix ===
##
              <-- classified as
##
        b
##
   123 27 |
              a = Monomer
##
     38 111 |
                b = Oligomer
##
## $AAC$Testing
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                                             81.5789 %
                                            62
## Incorrectly Classified Instances
                                                             18.4211 %
                                            14
## Kappa statistic
                                             0.6316
## Mean absolute error
                                             0.1819
## Root mean squared error
                                             0.4055
## Relative absolute error
                                            36.3454 %
## Root relative squared error
                                            81.0351 %
## Coverage of cases (0.95 level)
                                            86.8421 %
## Mean rel. region size (0.95 level)
                                            55.2632 %
## Total Number of Instances
                                            76
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area Class
##
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                       0.632
                                                                                0.853
                                                                                          0.809
                                                                                                    Monom
##
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                       0.632
                                                                                0.853
                                                                                          0.809
                                                                                                    Oligo
## Weighted Avg.
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                       0.632
                                                                                0.853
                                                                                          0.809
##
## === Confusion Matrix ===
##
           <-- classified as
##
    a b
   31 7 | a = Monomer
    7 31 | b = Oligomer
##
##
## $DPC
## $DPC$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           284
                                                             94.9833 %
## Incorrectly Classified Instances
                                            15
                                                              5.0167 %
```

```
## Kappa statistic
                                             0.8997
## Mean absolute error
                                            0.0877
## Root mean squared error
                                            0.2094
## Relative absolute error
                                           17.5344 %
## Root relative squared error
                                           41.8741 %
## Coverage of cases (0.95 level)
                                           98.9967 %
## Mean rel. region size (0.95 level)
                                           69.5652 %
## Total Number of Instances
                                           299
## === Confusion Matrix ===
##
            <-- classified as
##
        b
##
   144
          6 I
              a = Monomer
      9 140 |
                b = Oligomer
##
##
## $DPC$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
##
## === Summary ===
##
## Correctly Classified Instances
                                           256
                                                             85.6187 %
## Incorrectly Classified Instances
                                                             14.3813 %
                                            43
## Kappa statistic
                                            0.7123
## Mean absolute error
                                            0.1612
                                            0.3688
## Root mean squared error
## Relative absolute error
                                           32.242 %
## Root relative squared error
                                           73.7594 %
## Coverage of cases (0.95 level)
                                           89.2977 %
## Mean rel. region size (0.95 level)
                                           59.5318 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
                                                                                                    Class
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                               ROC Area PRC Area
##
                    0.887
                             0.174
                                      0.836
                                                  0.887
                                                           0.861
                                                                      0.714
                                                                               0.878
                                                                                          0.841
                                                                                                    Monom
##
                    0.826
                             0.113
                                      0.879
                                                  0.826
                                                           0.851
                                                                      0.714
                                                                               0.878
                                                                                          0.854
                                                                                                    Oligo
## Weighted Avg.
                    0.856
                             0.144
                                      0.857
                                                  0.856
                                                           0.856
                                                                      0.714
                                                                               0.878
                                                                                          0.848
##
## === Confusion Matrix ===
##
##
        b <-- classified as
##
   133 17 |
              a = Monomer
     26 123 |
                b = Oligomer
##
##
## $DPC$Testing
## === 10 Fold Cross Validation ===
##
## === Summary ===
                                                             81.5789 %
## Correctly Classified Instances
                                            62
## Incorrectly Classified Instances
                                                             18.4211 %
                                            14
## Kappa statistic
                                            0.6316
## Mean absolute error
                                            0.1946
## Root mean squared error
                                            0.4175
```

```
## Relative absolute error
                                            38.8854 %
## Root relative squared error
                                            83.4403 %
## Coverage of cases (0.95 level)
                                            85.5263 %
## Mean rel. region size (0.95 level)
                                            55.2632 %
## Total Number of Instances
##
## === Detailed Accuracy By Class ===
##
                                                           F-Measure MCC
##
                    TP Rate FP Rate Precision Recall
##
                                                  0.789
                    0.789
                             0.158
                                       0.833
                                                           0.811
                                                                       0.632
##
                    0.842
                             0.211
                                       0.800
                                                  0.842
                                                           0.821
                                                                       0.632
## Weighted Avg.
                    0.816
                             0.184
                                       0.817
                                                  0.816
                                                           0.816
                                                                       0.632
##
## === Confusion Matrix ===
##
##
    a b
           <-- classified as
##
   30 8 | a = Monomer
    6 32 \mid b = Oligomer
##
##
## $PCP
## $PCP$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           296
                                                              98.9967 %
## Incorrectly Classified Instances
                                                               1.0033 %
                                             3
## Kappa statistic
                                             0.9799
## Mean absolute error
                                             0.0156
## Root mean squared error
                                             0.0883
## Relative absolute error
                                             3.1216 %
## Root relative squared error
                                            17.6679 %
## Coverage of cases (0.95 level)
                                           100
                                            53.1773 %
## Mean rel. region size (0.95 level)
## Total Number of Instances
                                           299
##
## === Confusion Matrix ===
##
##
          b <-- classified as
              a = Monomer
##
   149
          1 |
      2 147 |
               b = Oligomer
##
## $PCP$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                                             81.2709 %
                                           243
## Incorrectly Classified Instances
                                            56
                                                              18.7291 %
## Kappa statistic
                                             0.6254
## Mean absolute error
                                             0.1928
## Root mean squared error
                                             0.4285
## Relative absolute error
                                            38.5587 %
## Root relative squared error
                                            85.7063 %
```

ROC Area PRC Area

0.868

0.814

0.841

0.868

0.868

0.868

Class

Monom

Oligo

```
## Coverage of cases (0.95 level)
                                            82.6087 %
## Mean rel. region size (0.95 level)
                                            52.1739 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area
                                                                                                    Class
##
                    0.813
                             0.188
                                      0.813
                                                  0.813
                                                           0.813
                                                                      0.625
                                                                                0.813
                                                                                          0.765
                                                                                                    Monom
##
                    0.812
                             0.187
                                       0.812
                                                  0.812
                                                           0.812
                                                                      0.625
                                                                                0.813
                                                                                          0.768
                                                                                                    Oligo
                                      0.813
                                                  0.813
## Weighted Avg.
                    0.813
                             0.187
                                                           0.813
                                                                      0.625
                                                                                0.813
                                                                                          0.767
## === Confusion Matrix ===
##
              <-- classified as
##
        b
##
   122 28 |
              a = Monomer
##
     28 121 |
                b = Oligomer
##
## $PCP$Testing
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                                             85.5263 %
                                            65
## Incorrectly Classified Instances
                                                             14.4737 %
                                            11
## Kappa statistic
                                            0.7105
## Mean absolute error
                                            0.1478
## Root mean squared error
                                            0.3767
## Relative absolute error
                                            29.5314 %
## Root relative squared error
                                            75.2755 %
## Coverage of cases (0.95 level)
                                            85.5263 %
## Mean rel. region size (0.95 level)
                                            50
                                                    %
## Total Number of Instances
                                            76
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area Class
##
                    0.868
                             0.158
                                       0.846
                                                  0.868
                                                           0.857
                                                                      0.711
                                                                                0.880
                                                                                          0.824
                                                                                                    Monom
##
                    0.842
                             0.132
                                       0.865
                                                  0.842
                                                           0.853
                                                                      0.711
                                                                                0.880
                                                                                          0.862
                                                                                                    Oligo
## Weighted Avg.
                    0.855
                             0.145
                                       0.856
                                                  0.855
                                                           0.855
                                                                      0.711
                                                                                0.880
                                                                                          0.843
##
## === Confusion Matrix ===
##
           <-- classified as
##
    a b
  33 5 | a = Monomer
    6 32 | b = Oligomer
##
##
## $AAC_DPC
## $AAC_DPC$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           292
                                                             97.6589 %
## Incorrectly Classified Instances
                                                              2.3411 %
```

```
## Kappa statistic
                                             0.9532
## Mean absolute error
                                             0.0381
## Root mean squared error
                                             0.138
## Relative absolute error
                                             7.6186 %
## Root relative squared error
                                            27.6017 %
## Coverage of cases (0.95 level)
                                           100
                                                    %
## Mean rel. region size (0.95 level)
                                            60.3679 %
## Total Number of Instances
                                           299
## === Confusion Matrix ===
##
             <-- classified as
##
        b
##
   144
          6 I
              a = Monomer
      1 148 |
                b = Oligomer
##
##
## $AAC_DPC$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
##
## === Summary ===
##
## Correctly Classified Instances
                                           251
                                                             83.9465 %
## Incorrectly Classified Instances
                                                              16.0535 %
## Kappa statistic
                                             0.6789
## Mean absolute error
                                             0.1738
## Root mean squared error
                                             0.3848
## Relative absolute error
                                            34.7643 %
## Root relative squared error
                                            76.95
## Coverage of cases (0.95 level)
                                            88.9632 %
## Mean rel. region size (0.95 level)
                                            61.0368 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
                                                                                                     Class
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area
##
                    0.833
                             0.154
                                       0.845
                                                  0.833
                                                           0.839
                                                                       0.679
                                                                                0.870
                                                                                          0.840
                                                                                                     Monom
##
                    0.846
                             0.167
                                       0.834
                                                  0.846
                                                           0.840
                                                                       0.679
                                                                                0.870
                                                                                          0.840
                                                                                                     Oligo
## Weighted Avg.
                    0.839
                             0.160
                                       0.840
                                                  0.839
                                                           0.839
                                                                       0.679
                                                                                0.870
                                                                                          0.840
##
## === Confusion Matrix ===
##
##
              <-- classified as
        b
                a = Monomer
##
   125 25 l
     23 126 |
                b = Oligomer
##
##
## $AAC_DPC$Testing
## === 10 Fold Cross Validation ===
##
## === Summary ===
                                                             85.5263 %
## Correctly Classified Instances
                                            65
## Incorrectly Classified Instances
                                                              14.4737 %
                                            11
## Kappa statistic
                                             0.7105
## Mean absolute error
                                             0.1485
## Root mean squared error
                                             0.3562
```

```
## Relative absolute error
                                            29.6792 %
## Root relative squared error
                                            71.1894 %
## Coverage of cases (0.95 level)
                                            90.7895 %
## Mean rel. region size (0.95 level)
                                            61.8421 %
## Total Number of Instances
##
## === Detailed Accuracy By Class ===
##
                                                           F-Measure MCC
##
                    TP Rate FP Rate Precision Recall
##
                                                  0.789
                    0.789
                             0.079
                                       0.909
                                                           0.845
                                                                       0.717
                    0.921
                             0.211
                                       0.814
                                                  0.921
                                                           0.864
                                                                       0.717
## Weighted Avg.
                    0.855
                             0.145
                                       0.862
                                                  0.855
                                                           0.855
                                                                       0.717
##
## === Confusion Matrix ===
##
##
    a b
            <-- classified as
##
   30 8 | a = Monomer
    3 35 \mid b = Oligomer
##
##
## $AAC_PCP
## $AAC_PCP$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           296
                                                              98.9967 %
## Incorrectly Classified Instances
                                                               1.0033 %
                                             3
## Kappa statistic
                                             0.9799
## Mean absolute error
                                             0.0156
## Root mean squared error
                                             0.0883
## Relative absolute error
                                             3.1216 %
## Root relative squared error
                                            17.6679 %
## Coverage of cases (0.95 level)
                                           100
                                            53.1773 %
## Mean rel. region size (0.95 level)
## Total Number of Instances
                                           299
##
## === Confusion Matrix ===
##
##
          b <-- classified as
              a = Monomer
##
   149
          1 |
               b = Oligomer
      2 147 |
##
## $AAC_PCP$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                           238
                                                             79.5987 %
## Incorrectly Classified Instances
                                            61
                                                              20.4013 %
## Kappa statistic
                                             0.592
## Mean absolute error
                                             0.2085
## Root mean squared error
                                             0.4482
## Relative absolute error
                                            41.7058 %
## Root relative squared error
                                            89.6348 %
```

ROC Area PRC Area

0.882

0.882

0.882

0.833

0.858

0.846

Class

Monom

Oligo

```
## Coverage of cases (0.95 level)
                                            80.2676 %
## Mean rel. region size (0.95 level)
                                            51.1706 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                               ROC Area PRC Area
                                                                                                    Class
                             0.201
##
                    0.793
                                      0.799
                                                  0.793
                                                           0.796
                                                                      0.592
                                                                               0.796
                                                                                          0.743
                                                                                                    Monom
##
                    0.799
                             0.207
                                       0.793
                                                  0.799
                                                           0.796
                                                                      0.592
                                                                               0.796
                                                                                          0.752
                                                                                                    Oligo
                                                           0.796
## Weighted Avg.
                    0.796
                             0.204
                                       0.796
                                                  0.796
                                                                      0.592
                                                                               0.796
                                                                                          0.747
## === Confusion Matrix ===
##
             <-- classified as
##
        b
##
   119 31 |
              a = Monomer
##
     30 119 |
                b = Oligomer
##
## $AAC PCP$Testing
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                                             81.5789 %
                                            62
## Incorrectly Classified Instances
                                                             18.4211 %
                                            14
## Kappa statistic
                                            0.6316
## Mean absolute error
                                            0.1869
## Root mean squared error
                                            0.4258
## Relative absolute error
                                            37.3452 %
## Root relative squared error
                                            85.1027 %
## Coverage of cases (0.95 level)
                                            81.5789 %
## Mean rel. region size (0.95 level)
                                            50
                                                    %
## Total Number of Instances
                                            76
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                               ROC Area PRC Area Class
##
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                      0.632
                                                                               0.832
                                                                                          0.779
                                                                                                    Monom
##
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                      0.632
                                                                               0.832
                                                                                          0.791
                                                                                                    Oligo
## Weighted Avg.
                    0.816
                             0.184
                                       0.816
                                                  0.816
                                                           0.816
                                                                      0.632
                                                                               0.832
                                                                                          0.785
##
## === Confusion Matrix ===
##
           <-- classified as
##
    a b
  31 7 | a = Monomer
    7 31 | b = Oligomer
##
##
## $DPC_PCP
## $DPC_PCP$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           291
                                                             97.3244 %
## Incorrectly Classified Instances
                                                              2.6756 %
```

```
## Kappa statistic
                                             0.9465
## Mean absolute error
                                             0.0506
## Root mean squared error
                                             0.1591
## Relative absolute error
                                            10.126 %
## Root relative squared error
                                            31.8213 %
## Coverage of cases (0.95 level)
                                           100
## Mean rel. region size (0.95 level)
                                            74.9164 %
## Total Number of Instances
                                           299
## === Confusion Matrix ===
##
        b <-- classified as
##
##
   149
         1 |
              a = Monomer
                b = Oligomer
##
      7 142 |
##
## $DPC_PCP$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
##
## === Summary ===
##
## Correctly Classified Instances
                                           243
                                                             81.2709 %
## Incorrectly Classified Instances
                                                             18.7291 %
## Kappa statistic
                                             0.6254
## Mean absolute error
                                             0.1927
## Root mean squared error
                                            0.4213
## Relative absolute error
                                            38.5419 %
## Root relative squared error
                                            84.2602 %
## Coverage of cases (0.95 level)
                                            84.6154 %
## Mean rel. region size (0.95 level)
                                            54.3478 %
## Total Number of Instances
                                           299
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area
                                                                                                    Class
##
                    0.800
                             0.174
                                       0.822
                                                  0.800
                                                           0.811
                                                                      0.626
                                                                                0.826
                                                                                          0.795
                                                                                                    Monom
##
                    0.826
                             0.200
                                       0.804
                                                  0.826
                                                           0.815
                                                                      0.626
                                                                                0.826
                                                                                          0.777
                                                                                                    Oligo
## Weighted Avg.
                    0.813
                             0.187
                                       0.813
                                                  0.813
                                                           0.813
                                                                      0.626
                                                                                0.826
                                                                                          0.786
##
## === Confusion Matrix ===
##
##
              <-- classified as
        b
                a = Monomer
##
   120 30 |
     26 123 |
                b = Oligomer
##
##
## $DPC_PCP$Testing
## === 10 Fold Cross Validation ===
##
## === Summary ===
## Correctly Classified Instances
                                            67
                                                             88.1579 %
## Incorrectly Classified Instances
                                                             11.8421 %
                                             9
## Kappa statistic
                                             0.7632
## Mean absolute error
                                            0.1278
## Root mean squared error
                                             0.3424
```

```
## Relative absolute error
                                            25.5345 %
## Root relative squared error
                                            68.4233 %
## Coverage of cases (0.95 level)
                                            88.1579 %
## Mean rel. region size (0.95 level)
                                                    %
                                            50
## Total Number of Instances
                                            76
##
## === Detailed Accuracy By Class ===
##
                                                           F-Measure MCC
##
                    TP Rate FP Rate Precision Recall
##
                                      0.892
                                                  0.868
                    0.868
                             0.105
                                                           0.880
                                                                      0.763
                    0.895
                             0.132
                                       0.872
                                                  0.895
                                                           0.883
                                                                      0.763
## Weighted Avg.
                    0.882
                             0.118
                                       0.882
                                                  0.882
                                                           0.882
                                                                      0.763
##
## === Confusion Matrix ===
##
##
    a b
            <-- classified as
##
   33 5 | a = Monomer
    4 34 | b = Oligomer
##
##
## $ALL
## $ALL$Training
##
## === Summary ===
##
## Correctly Classified Instances
                                           291
                                                             97.3244 %
## Incorrectly Classified Instances
                                                              2.6756 %
                                             8
## Kappa statistic
                                             0.9465
## Mean absolute error
                                             0.0506
## Root mean squared error
                                             0.1591
                                            10.126 %
## Relative absolute error
## Root relative squared error
                                            31.8213 %
## Coverage of cases (0.95 level)
                                           100
## Mean rel. region size (0.95 level)
                                            74.9164 %
## Total Number of Instances
                                           299
##
## === Confusion Matrix ===
##
##
          b <-- classified as
              a = Monomer
##
   149
          1 |
      7 142 |
               b = Oligomer
##
## $ALL$Cross_Validation_10_Fold
## === 10 Fold Cross Validation ===
## === Summary ===
##
## Correctly Classified Instances
                                                             81.6054 %
                                           244
## Incorrectly Classified Instances
                                            55
                                                             18.3946 %
## Kappa statistic
                                             0.6321
## Mean absolute error
                                             0.1894
## Root mean squared error
                                             0.4173
## Relative absolute error
                                            37.873 %
## Root relative squared error
                                            83.4626 %
```

ROC Area PRC Area

0.862

0.862

0.862

0.844

0.792

0.818

Class

Monom

Oligo

```
## Coverage of cases (0.95 level)
                                            84.9498 %
## Mean rel. region size (0.95 level)
                                            54.3478 %
## Total Number of Instances
                                           299
##
##
  === Detailed Accuracy By Class ===
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area
##
                                                                                                     Class
##
                    0.800
                             0.168
                                       0.828
                                                  0.800
                                                            0.814
                                                                       0.632
                                                                                0.831
                                                                                           0.803
                                                                                                     Monom
                                                           0.818
##
                    0.832
                             0.200
                                       0.805
                                                  0.832
                                                                       0.632
                                                                                0.831
                                                                                           0.780
                                                                                                     Oligo
                                       0.816
                                                  0.816
## Weighted Avg.
                    0.816
                             0.184
                                                           0.816
                                                                       0.632
                                                                                0.831
                                                                                           0.792
## === Confusion Matrix ===
##
              <-- classified as
##
          b
##
    120 30 |
                a = Monomer
##
     25 124 |
                b = Oligomer
##
## $ALL$Testing
## === 10 Fold Cross Validation ===
##
## === Summary ===
##
## Correctly Classified Instances
                                                              88.1579 %
                                            67
## Incorrectly Classified Instances
                                                              11.8421 %
## Kappa statistic
                                             0.7632
## Mean absolute error
                                             0.1278
## Root mean squared error
                                             0.3424
## Relative absolute error
                                            25.5345 %
## Root relative squared error
                                            68.4233 %
                                            88.1579 %
## Coverage of cases (0.95 level)
## Mean rel. region size (0.95 level)
                                            50
                                                    %
## Total Number of Instances
                                            76
##
## === Detailed Accuracy By Class ===
##
##
                    TP Rate FP Rate Precision Recall
                                                           F-Measure MCC
                                                                                ROC Area PRC Area Class
##
                    0.868
                             0.105
                                       0.892
                                                  0.868
                                                            0.880
                                                                       0.763
                                                                                0.862
                                                                                           0.844
                                                                                                     Monom
##
                    0.895
                             0.132
                                       0.872
                                                  0.895
                                                            0.883
                                                                       0.763
                                                                                0.862
                                                                                           0.792
                                                                                                     Oligo
## Weighted Avg.
                    0.882
                             0.118
                                       0.882
                                                  0.882
                                                            0.882
                                                                       0.763
                                                                                0.862
                                                                                          0.818
##
## === Confusion Matrix ===
##
            <-- classified as
##
    a b
    33 5 | a = Monomer
##
     4 34 | b = Oligomer
```

Performance table of J48 for training, 10-fold cross validation and external validation.

```
library(knitr)
x <- getURL("https://raw.githubusercontent.com/Rnewbie/OliFP/master/OliFPJ48.csv")
OliFPJ48 <- read.csv(text=x, header = TRUE)
kable(OliFPJ48, align = 'c', format = "markdown")</pre>
```

Des	Acc.tr	Sen.tr	$\operatorname{Spe.tr}$	$\mathrm{MCC.tr}$	Acc.cv	Sen.cv	Spe.cv	MCC.cv	Acc.tes	Sen.tes	Spe.tes	MCC
AAC	89.97	91.28	88.67	0.80	78.26	74.50	82.00	0.57	81.58	81.58	81.58	0.0
DPC	94.98	93.96	96.00	0.90	85.62	82.55	88.67	0.71	81.58	84.21	78.95	0.0
PCP	99.00	98.66	99.33	0.98	81.27	81.21	81.33	0.63	85.51	84.21	86.84	0.
AAC+DPC	97.99	99.33	96.64	0.96	83.95	84.56	83.33	0.68	85.53	92.11	78.95	0.
AAC+PCP	99.00	98.66	99.33	0.98	79.60	79.87	79.33	0.59	81.58	81.58	81.58	0.0
DPC+PCP	97.32	95.30	99.33	0.95	81.27	82.55	80.00	0.63	88.16	89.47	86.84	0.
$\operatorname{ALL}$	97.32	95.30	99.33	0.95	81.61	83.22	80.00	0.63	88.16	89.47	86.84	0.