

First Machine Learning model to predict cancer proteins with Weka.

Fundamentals in Bioinformatics.

Pedro Sánchez García

MASTER IN BIOINFORMATICS FOR HEALTH SCIENCES TEACHER: DR. CRISTIAN ROBERT MUNTEANU

PRACTICE 0: CLASSIFICATIONS

You have a dataset with protein descriptors for proteins involved in two types of cancers: HCC and HBC. Using Practise/CancerDataSet.csv database and Weka, find the best classification model that can predict if a protein is related with HCC or HBC. You should use 10-fold cross validation, at least one method from *BayesNet*, *Decision Table*, and *Random Forest*. Order the performance of the models using TP Rate.

Random Forest

```
=== Detailed Accuracy By Class ===
                 TP Rate
                          FP Rate
                                                                  MCC
                                                                            ROC Area
                                                                                      PRC Area
                                   Precision
                                              Recall
                                                       F-Measure
                                                                                                Class
                                                                  0,996
                 0,998
                          0,002
                                   0,998
                                              0,998
                                                       0,998
                                                                            1,000
                                                                                      1,000
                                                                                                HBC
                                              0,998
                                   0,998
                                                                            1,000
                                                                                                HCC
                 0,998
                          0,002
                                                       0,998
                                                                  0,996
                                                                                      1,000
Weighted Avg.
                 0,998
                          0,002
                                   0,998
                                              0,998
                                                       0,998
                                                                  0,996
                                                                            1,000
                                                                                      1,000
=== Confusion Matrix ===
         b
             <-- classified as
 1046
      2 |
               a = HBC
    2 1052 |
                b = HCC
```

Decision Table

```
=== Detailed Accuracy By Class ===
                 TP Rate
                          FP Rate Precision
                                              Recall
                                                        F-Measure
                                                                  MCC
                                                                            ROC Area
                                                                                      PRC Area
                                                                                                Class
                 0,948
                          0,491
                                   0,657
                                              0,948
                                                        0,777
                                                                   0,509
                                                                            0,789
                                                                                      0,764
                                                                                                HBC
                                                                   0,509
                                                                                                HCC
                 0,509
                          0,052
                                   0,908
                                              0,509
                                                        0,652
                                                                            0,789
                                                                                      0,827
Weighted Avg.
                 0,728
                          0,271
                                   0,783
                                              0,728
                                                        0,714
                                                                   0,509
                                                                            0,789
                                                                                      0,796
=== Confusion Matrix ===
      b
           <-- classified as
 994 54 |
            a = HBC
 518 536 |
             b = HCC
```

Naive Bayes

```
=== Detailed Accuracy By Class ===
                          FP Rate
                 TP Rate
                                   Precision
                                               Recall
                                                        F-Measure
                                                                   MCC
                                                                             ROC Area
                                                                                       PRC Area
                                                                                                 Class
                 0,169
                          0,078
                                    0,683
                                               0,169
                                                        0,271
                                                                   0,139
                                                                             0,573
                                                                                       0,595
                                                                                                 HBC
                                                                                                 HCC
                 0,922
                          0,831
                                    0,527
                                               0,922
                                                        0,671
                                                                   0,139
                                                                             0,573
                                                                                       0,529
Weighted Avg.
                          0,456
                                               0,547
                                                                                       0,562
                 0,547
                                    0,605
                                                        0,472
                                                                    0,139
                                                                             0,573
=== Confusion Matrix ===
       b
           <-- classified as
 177 871 | a = HBC
  82 972 |
             b = HCC
```

DISCUSSION

Based on the results obtained, Random Forest is the best method, since if we look at it, the TP rate is very close to 1, which indicates a good prediction of the model for both the type of HCC and HBC cancer. In addition, unlike the Decision Table and Naive Bayes methods, the weighted average in Random Forest is high, in such a way that confirms that this is the best model for this problem treated in practice. This highlights its robustness, one of the characteristics for which it is widely applied in gene expression classification, mass spectrometry data analysis, prediction of interactions between proteins ...