Binary Classification of Water Potability

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Abstract

Classification is an essential data analytics technique with a wide range of applications to classify the various types of data in almost all areas of our lives. This report will give information about the water potability problem as a pattern classification problem. The study was performed using Water Potability data from the Kaggle website. The value of pH, hardness, solids, chloramines, sulfate, conductivity, organic carbon, trihalomethanes, turbidity are the important variables to classify the potability. In our study, a random forest algorithm was applied to the data and tasked to estimate the water potability. The classification performance of a random forest model applied to the testing dataset, which contains 30% of the total data, was calculated using different tree depths and other tuning parameters.

Introduction

Access to clean and potable water is a fundamental necessity for human health and well-being. Unfortunately, ensuring water safety remains a significant challenge in many parts of the world, where contamination from natural and man-made sources can make water unsafe for consumption. Given the critical role that water plays in public health, it becomes increasingly important to accurately assess its potability to prevent waterborne diseases and other health issues.

In the face of such challenges, data analytics and classification techniques offer a promising solution to enhance water quality monitoring. Classification models can help determine whether water is potable based on various chemical and physical properties, providing a scalable approach to support ongoing water safety efforts. This report explores the water potability problem as a classification task, where the goal is to predict the drinkability of water samples based on certain key characteristics.

Using real-world data from the Water Potability dataset available on Kaggle, we examine several factors that impact water safety, such as pH levels, hardness, and the presence of contaminants like trihalomethanes. To address this, we apply a Random Forest classification model to identify patterns and classify the water samples as either potable or non-potable. By testing the performance of this model under different tree depths and tuning parameters, we aim to develop a reliable tool that can assist in making informed decisions about water quality.

Materials and Methods

(a) Materials
- Water Potability dataset from Kaggle

(b) Methods
1. Data Processing The first step is to import the data using read.csv function.

```
##         ph Hardness   Solids Chloramines  Sulfate Conductivity Organic_carbon
## 1       NA 204.8905 20791.32    7.300212 368.5164     564.3087      10.379783
## 2 3.716080 129.4229 18630.06    6.635246       NA     592.8854      15.180013
## 3 8.099124 224.2363 19909.54    9.275884       NA     418.6062      16.868637
## 4 8.316766 214.3734 22018.42    8.059332 356.8861     363.2665      18.436524
## 5 9.092223 181.1015 17978.99    6.546600 310.1357     398.4108      11.558279
## 6 5.584087 188.3133 28748.69    7.544869 326.6784     280.4679       8.399735
##   Trihalomethanes Turbidity Potability
## 1        86.99097  2.963135          0
## 2        56.32908  4.500656          0
## 3        66.42009  3.055934          0
## 4       100.34167  4.628771          0
## 5        31.99799  4.075075          0
## 6        54.91786  2.559708          0
```

Our next step is to find out the total rows with a null values in each column.

```
##              ph        Hardness          Solids     Chloramines         Sulfate
##             491               0               0               0             781
##    Conductivity  Organic_carbon Trihalomethanes       Turbidity      Potability
##               0               0             162               0               0
```

Using summary function to find out an insights from each variable, especially the variables that has a null values.

```
##        ph            Hardness          Solids         Chloramines
##  Min.   : 0.000   Min.   : 47.43   Min.   :  320.9   Min.   : 0.352
##  1st Qu.: 6.093   1st Qu.:176.85   1st Qu.:15666.7   1st Qu.: 6.127
##  Median : 7.037   Median :196.97   Median :20927.8   Median : 7.130
##  Mean   : 7.081   Mean   :196.37   Mean   :22014.1   Mean   : 7.122
##  3rd Qu.: 8.062   3rd Qu.:216.67   3rd Qu.:27332.8   3rd Qu.: 8.115
##  Max.   :14.000   Max.   :323.12   Max.   :61227.2   Max.   :13.127
##  NA's   :491
##     Sulfate       Conductivity   Organic_carbon  Trihalomethanes
##  Min.   :129.0   Min.   :181.5   Min.   : 2.20   Min.   :  0.738
##  1st Qu.:307.7   1st Qu.:365.7   1st Qu.:12.07   1st Qu.: 55.845
##  Median :333.1   Median :421.9   Median :14.22   Median : 66.622
##  Mean   :333.8   Mean   :426.2   Mean   :14.28   Mean   : 66.396
##  3rd Qu.:360.0   3rd Qu.:481.8   3rd Qu.:16.56   3rd Qu.: 77.337
##  Max.   :481.0   Max.   :753.3   Max.   :28.30   Max.   :124.000
##  NA's   :781                                     NA's   :162
##    Turbidity       Potability
##  Min.   :1.450   Min.   :0.0000
##  1st Qu.:3.440   1st Qu.:0.0000
##  Median :3.955   Median :0.0000
##  Mean   :3.967   Mean   :0.3901
##  3rd Qu.:4.500   3rd Qu.:1.0000
##  Max.   :6.739   Max.   :1.0000
##
```

It can be seen that most of the data distributed between the lower and upper quantile. Thus, we decided to impute the data using group means imputation.

2. Data Partitioning Dividing the data into 70% training and 30% test dataset.

Checking whether the output is a categorical variable

```
## NULL
```

Since it is not a categorical variable, we should change it using as.factor function

```
## [1] "0" "1"
```

```
## [1] "0" "1"
```

We have considered several models such as: - K-Nearest Neighbors (Accuracy: 52.95%) - Logistic Regression (Accuracy: 60.69%) - Naive Bayes (Accuracy: 62.02%) - Linear Discriminant Analysis (Accuracy: 60.69%) - Quadratic Discriminant Analysis (Accuracy: 66.50%) - Tree (Accuracy before pruned: 74.95%, after pruned: 75.56%) - Support Vector Machine (Accuracy: 60.90%) (a) Linear Kernel (Accuracy before tuned: 60.90%, after tuned: 60.90%) (b) Polynomial Kernel (Accuracy before tuned: 62.22%, after tuned: 61.51%) (c) Radial Kernel (Accuracy before tuned: 66.70%, after tuned: 66.70%) - Random Forest (a) Without tuning (Accuracy: 78.82%) (b) Tuning ntree = 100 (Accuracy: 79.12%) (c) Tune grid for mtry = 3 (Accuracy: 79.12%) (d) Bagging (Accuracy: 78.51%) (e) Tuning nbagg of bagging model (Accuracy: 78.21%) (f) Boosting (Accuracy: 76.17%) (e) Tuning boosting model using gradient boosting (Accuracy: 78.41%)

Thus, we consider to discuss further about the random forest model with all kinds of tuning parameter.

Random forest without tuning

```
##    pred_rf
##       0   1
##   0 540  58
##   1 150 234
```

```
## [1] 0.7881874
```

Accuracy of random forest without tuning: 78.82%

Set the ntree equals to 100. Ntree means number of trees to grow. This should not be set to too small a number, to ensure that every input row gets predicted at least a few times.

```
##    pred_rf
##       0   1
##   0 545  53
##   1 152 232
```

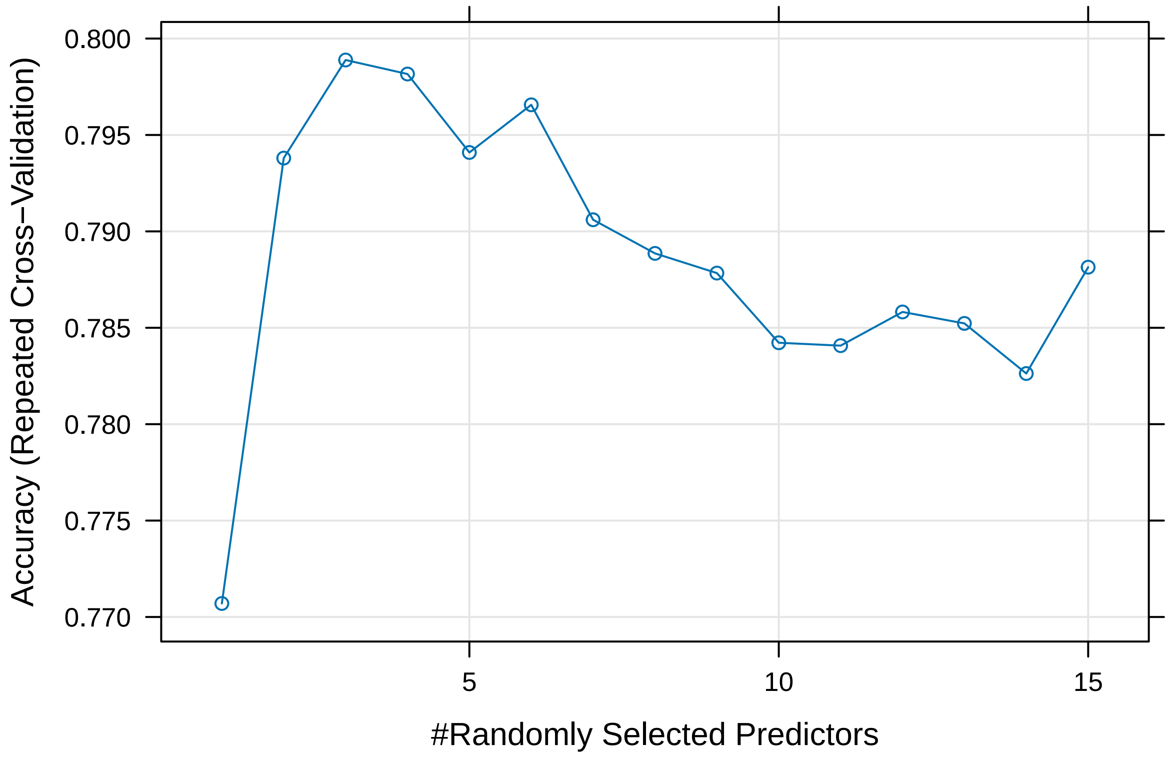
```
## [1] 0.7912424
```

Using ntree equals to 100, it improve our model to an accuracy of 79.12%

Next, we would like to tune the mtry parameter. Mtry is a number of variables randomly sampled as a candidates at each split. to ensure that every input rows get predicted at least a few times.

First of all, we will try using the grid search of the number of mtry. Each axis of the grid is an algorithm parameter, and points in the grid are specific combinations of parameters. Because we are only tuning one parameter, the grid search is a linear search through a vector of candidate values.

```
## Random Forest
##
## 2294 samples
##    9 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 2064, 2065, 2065, 2064, 2065, 2064, ...
## Resampling results across tuning parameters:
##
##   mtry  Accuracy   Kappa
##    1    0.7707006  0.4893730
##    2    0.7938004  0.5478491
##    3    0.7988880  0.5612796
##    4    0.7981602  0.5611924
##    5    0.7940915  0.5529922
##    6    0.7965641  0.5581623
##    7    0.7906012  0.5466602
##    8    0.7888583  0.5424857
##    9    0.7878362  0.5399807
##   10    0.7842225  0.5335831
##   11    0.7840738  0.5318851
##   12    0.7858199  0.5353187
##   13    0.7852269  0.5351170
##   14    0.7826270  0.5289025
##   15    0.7881425  0.5409338
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 3.
```



We can see that the most accurate value for mtry is 3 with an accuracy of 79.88% of the training accuracy. Then, we will apply mtry equals to 3 to our model. Let's see if there is any significant difference to the model.

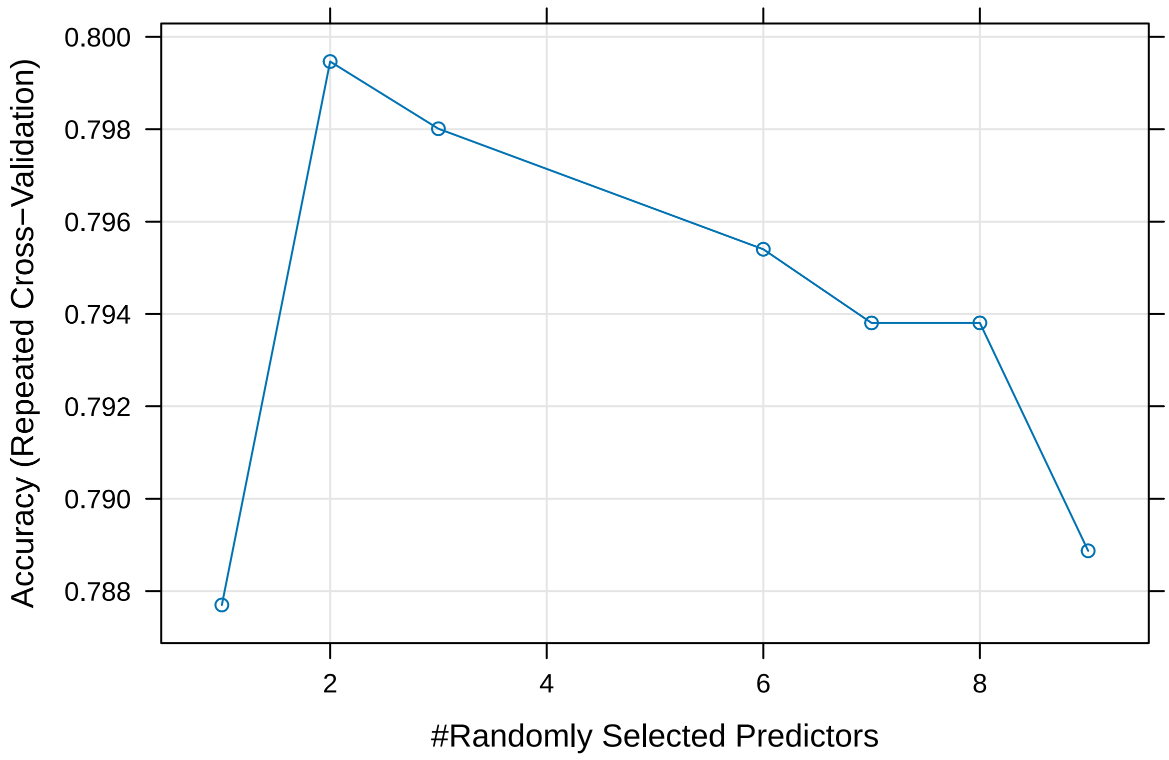
```
##    pred_rf
##       0   1
##   0 545  53
##   1 152 232
```

```
## [1] 0.7912424
```

It can be seen that the accuracy is 79.12%, which means it didn't improve our model. Let's tree to tune the mtry value using other method which is random search.

```
## Random Forest
##
## 2294 samples
##    9 predictor
##    2 classes: '0', '1'
##
```

```
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 2064, 2065, 2065, 2064, 2065, 2064, ...
## Resampling results across tuning parameters:
##
##   mtry  Accuracy   Kappa
##   1     0.7876989  0.5269460
##   2     0.7994659  0.5592872
##   3     0.7980103  0.5587034
##   6     0.7954009  0.5557769
##   7     0.7938055  0.5535527
##   8     0.7938067  0.5531342
##   9     0.7888716  0.5423211
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 2.
```



We can see that the most accurate value for mtry is 3 with an accuracy of 79.67% of the training accuracy. Then, we will apply mtry equals to 3 to our model. This means that tuning using grid search and random search will give the same mtry value whcih is 3. Aside from tuning the ntree and mtry, we will try to model our data using bagging and boosting model.

Bagging Bagging is an ensemble algorithm that fits multiple models on different subsets of a training dataset, then combines the predictions from all models.

Random forest is an extension of bagging that also randomly selects subsets of features used in each data sample. Both bagging and random forests have proven effective on a wide range of different predictive modeling problems.

```
##    pred_bag
##       0   1
##   0 529  69
##   1 142 242
```

```
## [1] 0.7851324
```

It can be seen that the accuracy of the model is 78.51%, which means it didn't improve our previous model. Let's try to tuned the bagging model.

```
##    pred_bag
##       0   1
##   0 523  75
##   1 139 245
```

```
## [1] 0.7820774
```

We tuned the model by setting the nbagg equals to 100 and control the minimum split. However, it can be seen that the tuned model didn't improve since it has a lower accuracy than the previous model which is 78.21%. Aside from bagging model, we will also try using the boosting model.

Boosting Boosting means fit many large or small trees to reweighted versions of the training data. Classify by weighted majority vote.

```
##    pred_boost
##       0   1
##   0 558  40
##   1 194 190
```

```
## [1] 0.7617108
```

It can be seen that the accuracy of the model is 76.17%, which is the lowest accuracy among other methods of random forest. Let's try to tune the boosting model. We will use the gradient boosting method.

```
## Stochastic Gradient Boosting
##
## 2294 samples
##    9 predictor
##    2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 2064, 2065, 2065, 2064, 2065, 2064, ...
## Resampling results across tuning parameters:
##
##   interaction.depth  n.trees  Accuracy   Kappa
##   1                   50      0.6782083  0.2348211
##   1                  100      0.7325673  0.3847404
##   1                  150      0.7380059  0.4030879
##   2                   50      0.7690030  0.4705348
##   2                  100      0.7766334  0.4971980
##   2                  150      0.7795094  0.5074525
##   3                   50      0.7751944  0.4907801
##   3                  100      0.7844767  0.5200879
##   3                  150      0.7877040  0.5308953
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
##
## Tuning parameter 'n.minobsinnode' was held constant at a value of 10
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were n.trees = 150, interaction.depth =
##  3, shrinkage = 0.1 and n.minobsinnode = 10.
```

From the output above, it can be seen that the best model is using the ntree = 150, interaction.depth = 3, shringkage = 0.1, and n.minobsinnode = 10

```
##    pred_gbm
##       0   1
##   0 552  46
##   1 166 218
```

```
## [1] 0.7841141
```

From the output above, it can be seen that the test accuracy is 78.41%.

In conclusion, the best model is the random forest model by tuning mtry and ntree.

Results and Discussion

Results: The Random Forest model achieved the highest accuracy of 79.12% after tuning the number of trees (ntree = 100) and the number of variables considered at each split (mtry = 3). This model outperformed other classifiers, such as K-Nearest Neighbors (52.95%) and Logistic Regression (60.69%). The confusion matrix showed that the Random Forest model correctly classified 826 non-potable and 384 potable water samples, with relatively fewer false positives (158) and false negatives (321).

Discussion: The Random Forest model proved to be the most effective for classifying water potability due to its robustness and ability to handle non-linear data. The model's high accuracy and ability to reduce overfitting made it superior to simpler models like Logistic Regression. The confusion matrix revealed that while the model was good at identifying non-potable water, it struggled more with identifying potable water, indicating room for improvement in reducing false negatives. Overall, Random Forest is a reliable model for this classification problem.

Conclusion

In conclusion, the best model for this project is the Random Forest, achieving an accuracy of 79.12%. One key takeaway from this project is that Random Forest performs well because there is little to no correlation between the variables in the data. This makes it an ideal choice for classification problems where variables are uncorrelated. Additionally, Random Forest helps mitigate overfitting, further improving its performance and reliability.

References

https://machinelearningmastery.com/bagging-and-random-forest-for-imbalanced-classification/

https://machinelearningmastery.com/tune-machine-learning-algorithms-in-r/

https://quantdev.ssri.psu.edu/sites/qdev/files/09_EnsembleMethods_2017_1127.html