Assignment 3: Wine Data

CIS 435

Section 56

Summer Quarter

School of Continuing Studies

Northwestern University

Daniel Prusinski

Business Intelligence Data Analyst

Target Corporation

Minneapolis, MN

In Compliance with Master of Science Predictive Analytics

Preliminary Data Analysis:

Before delving into the meat and potatoes of an analysis, it is important to conduct a preliminary exploratory data analysis. This gives an initial foundation that will prove to be the reference point moving forward into more complex analysis. The meta data states there are 14 attributes with 178 instances or rows. In addition, this data is pulled from 3 different cultivars. Cultivar A has the largest sample followed by A, and lastly C. An initial takeaway is that B will have more weight in the analysis simply based on the fact that it represents 40%, A is perfectly represented, and C is underrepresented.

```
                 Class
Attribute                A        B        C
                      (0.33)   (0.4)   (0.27)
==========================================================
Alcohol
  mean               13.7434  12.2782  13.1537
  std. dev.           0.4587   0.5351   0.5252 ← Given the Avg, this distribution of values follows a rather
normal distribution, which leads me to believe it is a veracious attribute. Also, between the different
cultivars the deviation is not far, which shows balance as a variable.
  weight sum              59       71       48 ← This sum validates what is shown in in the green circle above
about B having more weight in the analysis.
  precision           0.0304   0.0304   0.0304
Malic_Acid
  mean                2.0115   1.9329   3.3334
  std. dev.           0.6824   1.0078   1.0749 ← The mean compared to the STDV (Standard Deviation) is
somewhat similar, which points to a rather tumultuous distribution. In conclusion, the distribution might
require a log transformation.
  weight sum              59       71       48
  precision           0.0383   0.0383   0.0383
Ash
  mean                2.4555   2.2451   2.4354
  std. dev.           0.2253   0.3139   0.1817
  weight sum              59       71       48
  precision            0.024    0.024    0.024
Ash_Alcalinity
  mean               17.0506  20.2594  21.4208
  std. dev.           2.5279   3.3209   2.2327
  weight sum              59       71       48
  precision           0.3129   0.3129   0.3129

Magnesium
  mean              106.3338  94.5915  99.2981
  std. dev.            10.4831  16.6495  10.8441 ← This STDV is quite high for such a small mean. I am
concerned about this distribution
  weight sum                59       71       48
  precision             1.7692   1.7692   1.7692

Total_Phenols
  mean                  2.8396   2.2618    1.681
  std. dev.             0.3357   0.5412   0.3553 ← This STDV is quite high for such a small mean. I am
concerned about this distribution
  weight sum                59       71       48
  precision             0.0302   0.0302   0.0302

Flavanoids
  mean                   2.983   2.0793   0.7802
  std. dev.             0.3944   0.7013   0.2896
  weight sum                59       71       48
  precision             0.0362   0.0362   0.0362

Nonflavanoid_Phenols
  mean                  0.2908   0.3646   0.4478
  std. dev.             0.0701   0.1229    0.123 ← The mean compared to the STDV (Standard Deviation) is
somewhat similar, which points to a rather tumultuous distribution. In conclusion, the distribution might
require a log transformation.
  weight sum                59       71       48
  precision             0.0139   0.0139   0.0139

Proanthocyanins
  mean                  1.8982    1.631   1.1518
  std. dev.             0.4095   0.5992   0.4046
  weight sum                59       71       48
  precision             0.0317   0.0317   0.0317

Color_Intensity
  mean                  5.5241   3.0796   7.3996
  std. dev.             1.2265   0.9159   2.2849
  weight sum                59       71       48
  precision             0.0895   0.0895   0.0895

Hue
  mean                  1.0611   1.0559   0.6836
```

std. dev. 0.1151 0.2013 0.1129← The mean compared to the STDV (Standard Deviation) is somewhat similar, which points to a rather tumultuous distribution. In conclusion, the distribution might require a log transformation.

```
 weight sum              59       71       48
 precision            0.016    0.016    0.016
OD280_OD315
 mean                3.1579   2.7843   1.6842
 std. dev.           0.3543   0.4923   0.2688
 weight sum              59       71       48
 precision           0.0226   0.0226   0.0226
Proline
 mean             1115.8573  519.8261   629.683
 std. dev.         220.0034  154.7719  113.0791
 weight sum              59        71        48
 precision          11.6833   11.6833   11.6833
```

Many of the above variables do not have normal distributions, which raises data quality concerns. Additionally, Proline is significantly larger than any other variable, which has the potential to skew results.

Wine data in Weka using NaiveBayesSimple:

```
Scheme:weka.classifiers.bayes.NaiveBayes
Relation:     Wine
Instances:    178
Attributes:   14
 Test mode:10-fold cross-validation
=== Stratified cross-validation ===
=== Summary ===
Correctly Classified Instances         172             96.6292 %
Incorrectly Classified Instances         6              3.3708 %
Kappa statistic                          0.9489
Mean absolute error                      0.0217
Root mean squared error                  0.1294
Relative absolute error                  4.9371 %
Root relative squared error             27.6176 %
Total Number of Instances              178
=== Detailed Accuracy By Class ===
             TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
               0.949     0         1          0.949    0.974      0.998    A
               0.958     0.028     0.958      0.958    0.958      0.997    B
               1         0.023     0.941      1        0.97       1        C
```

```
Weighted Avg.    0.966     0.017     0.967     0.966     0.966     0.998
=== Confusion Matrix ===
  a  b  c   <-- classified as
 56  3  0 |  a = A
  0 68  3 |  b = B
  0    0 48 |  c = C
```

Initial analysis of NaiveBayesSimple:

NaiveBayesSimple correctly classified 172 of the instances and from a practical perspective has great output. This approach has a better classification than J48.

Wine data in Weka using IBK (kNN algorithm):

```
Scheme:weka.classifiers.lazy.IBk -K 1 -W 0 -A
"weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R
first-last\""
Relation:     Wine
Instances:    178
Attributes:   14
Test mode:10-fold cross-validation

=== Classifier model (full training set) ===

IB1 instance-based classifier
using 1 nearest neighbour(s) for classification


Time taken to build model: 0 seconds

=== Stratified cross-validation ===
=== Summary ===

Correctly Classified Instances         169               94.9438 %
Incorrectly Classified Instances         9                5.0562 %
Kappa statistic                          0.9238
Mean absolute error                      0.0413
Root mean squared error                  0.1821
Relative absolute error                  9.3973 %
Root relative squared error             38.8682 %
Total Number of Instances              178

=== Detailed Accuracy By Class ===

               TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
                 1         0.042      0.922      1         0.959      0.983    A
                 0.873     0          1          0.873     0.932      0.941    B
                 1         0.031      0.923     1         0.96       0.983    C
Weighted Avg.    0.949     0.022      0.953     0.949     0.949      0.966

=== Confusion Matrix ===

  a  b  c   <-- classified as
 59  0  0 |  a = A
  5 62  4 |  b = B
  0   0 48 |  c = C
```

Initial analysis of IBK (kNN algorithm):

IBK does not classify as well as Naïve Bayes, and the Root Mean Squared error is larger. It is better than J48 and the root mean square error is not as high.

Wine data in Weka using jRP:

```
=== Run information ===
Scheme:weka.classifiers.rules.JRip -F 3 -N 2.0 -O 2 -S 1
Relation:     Wine
Instances:    178
Attributes:   14
              Alcohol
              Malic_Acid
              Ash
              Ash_Alcalinity
              Magnesium
              Total_Phenols
              Flavanoids
              Nonflavanoid_Phenols
              Proanthocyanins
              Color_Intensity
              Hue
              OD280_OD315
              Proline
              Type
Test mode:10-fold cross-validation

=== Classifier model (full training set) ===

JRIP rules:
===========

(Flavanoids <= 1.39) and (Color_Intensity >= 4) => Type=C (46.0/0.0)
(OD280_OD315 <= 1.3) => Type=C (2.0/0.0)
(Proline >= 760) => Type=A (61.0/4.0)
 => Type=B (69.0/2.0)
```

```
Number of Rules : 4


Time taken to build model: 0.05 seconds

=== Stratified cross-validation ===
=== Summary ===

Correctly Classified Instances         167               93.8202 %
Incorrectly Classified Instances        11                6.1798 %
Kappa statistic                      0.9059
Mean absolute error                     0.048
Root mean squared error                   0.1991
Relative absolute error                10.9333 %
Root relative squared error              42.4986 %
Total Number of Instances              178

=== Detailed Accuracy By Class ===

               TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
                 0.932     0.034      0.932     0.932     0.932      0.973    A
                 0.944     0.056      0.918     0.944     0.931      0.97     B
                 0.938     0.008      0.978     0.938     0.957      0.97     C
Weighted Avg.    0.938     0.036      0.939     0.938     0.938      0.971

=== Confusion Matrix ===

  a  b  c   <-- classified as
 55  4  0 |  a = A
  3 67  1 |  b = B
  1  2 45 |  c = C
```

Initial analysis of JRIP):

JRIP and IBK have similar output, but JRIP is the least precise classifier.

Wine data in Weka using J48 classifier:

```
Scheme:weka.classifiers.trees.J48 -C 0.25 -M 2
Relation:     Wine
Instances:    178
Attributes:   14
Test mode:10-fold cross-validation
=== Classifier model (full training set) ===
J48 pruned tree
------------------
```

```
Flavanoids <= 1.57
|   Color_Intensity <= 3.8: B (13.0)
|   Color_Intensity > 3.8: C (49.0/1.0)
Flavanoids > 1.57
|   Proline <= 720: B (54.0/1.0)
|   Proline > 720
|   |   Color_Intensity <= 3.4: B (4.0)
|   |   Color_Intensity > 3.4: A (58.0)
Number of Leaves  :          5
Size of the tree :      9
=== Stratified cross-validation ===
=== Summary ===
Correctly Classified Instances         167               93.8202 %
Incorrectly Classified Instances        11                6.1798 %
Kappa statistic                          0.9058
Mean absolute error                        0.0486
Root mean squared error                      0.2019
Relative absolute error                 11.0723 %
Root relative squared error               43.0865 %
Total Number of Instances                178
=== Detailed Accuracy By Class ===

               TP Rate   FP Rate   Precision   Recall  F-Measure   ROC Area  Class
                 0.983     0.034      0.935     0.983     0.959      0.977    A
                 0.944     0.056      0.918     0.944     0.931      0.937    B
                 0.875     0.008      0.977     0.875     0.923      0.946    C
Weighted Avg.    0.938     0.036      0.94      0.938     0.938      0.953

=== Confusion Matrix ===

  a  b  c   <-- classified as
 58  1  0 |  a = A
  3 67  1 |  b = B
  1  5 42 |  c = C
```

Initial analysis of J48:

J48 correctly classified 167 of the instances and from a practical perspective has great output. This tree is rather small and only has 5 leaves. In accordance with the principle of Parsimony, I feel capable to explain these results to clients. The root mean squared error is often compared as an inverses calculation to the correlation coefficient. This data is from wine, and I am not as concerned with False Negatives as compared with medical diagnostic data. As my analysis furthers, I am curious to analyze the relationship between Proline and color intensity given that they led to such an apt decision tree.

1.A Rank the top three methods according to the rate of correctly classified instances:

1. NaiveBayesSimple: C.C. 172 96.6292 %
2. IBK (kNN algorithm): 169 94.9438 %
3. J48 and JRIP have the same % value: 93.8202 %*
   a. In my opinion, JRIP is better because it has a small root mean square error.

1.B Compare the difference between jRIP and j48. Are the two methods concluding the same classification rules? If not, what are the differences?

The output for the two different methods can be seen above.

The two methods are not concluding the same classification rules.

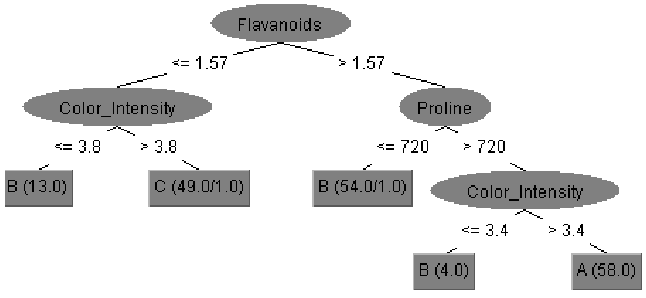
```
jRIP has the following rules → (Flavanoids <= 1.39) and (Color_Intensity >= 4) =>
Type=C (46.0/0.0)
(OD280_OD315 <= 1.3) => Type=C (2.0/0.0)
(Proline >= 760) => Type=A (61.0/4.0)
 => Type=B (69.0/2.0)
```

```
J48 has the following rules→ Flavanoids <= 1.57
|   Color_Intensity <= 3.8: B (13.0)
|   Color_Intensity > 3.8: C (49.0/1.0)
Flavanoids > 1.57
|   Proline <= 720: B (54.0/1.0)
|   Proline > 720
|   |   Color_Intensity <= 3.4: B (4.0)
|   |   Color_Intensity > 3.4: A (58.0)
```

From this perspective it appears that both methods are the same, but analyzing the number of rules shows a different perspective. JRIP is known as a bottom-up process that analyzes all the examplee. J48 is a top-down approach that separates the example data into subsets (decision tree). In this instance, both have the same end-result but took different approaches (UMN.edu). The values and order of the classification rules are different.

The decision tree demonstrataes the top down approach from J48.

.



Part 2: Changing the data and algorithms:

The next step in this exploratory data analysis (EDA) is to make a few changes to the data as well as the algorithms in an effort to learn how they respond in a different environment.

Changes to the data: In my preliminary analysis of the variables, Proline has the following summary statistics:

Proline

mean	1115.8573	519.8261	629.683
std. dev.	220.0034	154.7719	113.0791
weight sum	59	71	48
precision	11.6833	11.6833	11.6833

The mean is much higher than any other variable by quite a bit, in fact no other mean for a variable is larger than 21. While the standard deviation suggests a normal distribution, I am still going to remove this variable from the overall data.

Changes to Algorithms:

At first I wanted to use the “Use training set” option in Weka, but upon further research I found this approach uses the whole data set provided which is pointless if one cannot test it on other data. Therefore, I will not be using this option to explore algorithmic changes.

I want to know the output of J48, JRIP Naïve Bayes, and IBK if the number of folds are changed from 10 to 5. The folds have the following effect on analyzing the data:

Use 10 fold CV (Rushdi Shams, stackoverflow.com)

- Weka takes 100 labeled data
- it produces 10 equal sized sets. Each set is divided into two groups: 90 labeled data are used for training and 10 labeled data are used for testing.
- it produces a classifier with an algorithm from 90 labeled data and applies that on the 10 testing data for set 1.
- It does the same thing for set 2 to 10 and produces 9 more classifiers
- it averages the performance of the 10 classifiers produced from 10 equal sized (90 training and 10 testing) set

Given that our data is not massive, by lessening the folds it gives the algorithm less opportunity to learn and is based more on the actual initial production of the algorithm. In addition, I want to simulate a “real-life” situation where I would be using one of these algorithms on millions/billions of rows of data and I will utilize a smaller percentage of the data. The default is 66%, and I will be changing that to 33% in an effort to simulate a larger data set than what is actually given in this instance.

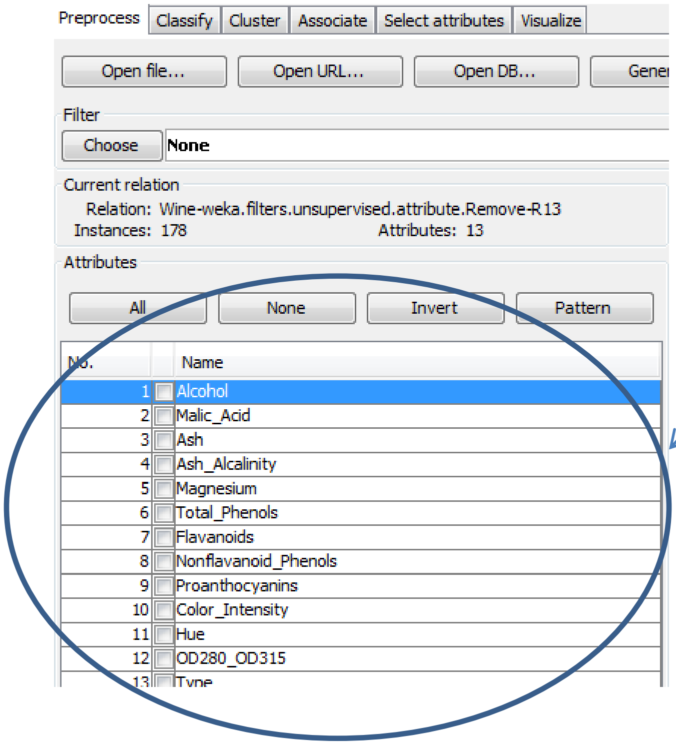
As I work through each algorithm without variable Proline, I will note and analyze the changes to the individual algorithms one at a time.

Question 2:

a. Will j48 Decision Tree change? What do you think?

The j48 Decision Tree will change because the Proline variable has been removed. Given that I am only using 5 folds, I think that will negatively affect the process as well.

Documented Changes:



Filter

Choose None

Current relation

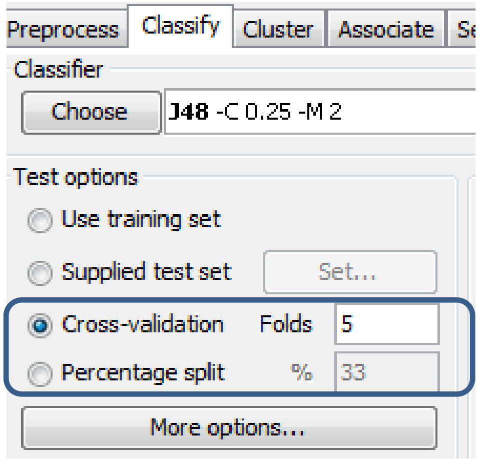
Relation: Wine-weka.filters.unsupervised.attribute.Remove-R13

Instances: 178 Attributes: 13

Attributes

No.		Name
1	□	Alcohol
2	□	Malic_Acid
3	□	Ash
4	□	Ash_Alcalinity
5	□	Magnesium
6	□	Total_Phenols
7	□	Flavanoids
8	□	Nonflavanoid_Phenols
9	□	Proanthocyanins
10	□	Color_Intensity
11	□	Hue
12	□	OD280_OD315
13	□	Type

Proline has been removed from the list of attributes being analyzed.



Classifier

Choose J48 -C 0.25 -M 2

Test options

○ Use training set

○ Supplied test set

● Cross-validation Folds 5

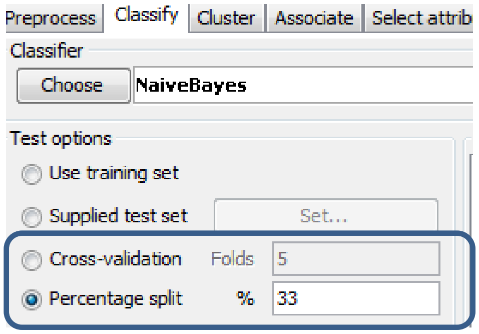
○ Percentage split % 33

Note the changes made to the J48 test options with cross-validation being 5 folds and the percentage split is now 33%.

After change analysis:

```
Scheme:weka.classifiers.trees.J48 -C 0.25 -M 2
Relation:     Wine-weka.filters.unsupervised.attribute.Remove-R13
Instances:    178
Attributes:   13
Test mode:5-fold cross-validation
Number of Leaves  :          7
Size of the tree :       13
Flavanoids <= 1.57
|   Color_Intensity <= 3.8: B (13.0)
|   Color_Intensity > 3.8: C (49.0/1.0)
Flavanoids > 1.57
|   Alcohol <= 12.77: B (49.0)
|   Alcohol > 12.77
|   |   Magnesium <= 88: B (6.0)
|   |   Magnesium > 88
|   |   |   Color_Intensity <= 3.8
|   |   |   |   Hue <= 1.2: A (4.0)
|   |   |   |   Hue > 1.2: B (2.0)
|   |   |   Color_Intensity > 3.8: A (55.0)
Correctly Classified Instances         159               89.3258 %
Incorrectly Classified Instances        19               10.6742 %
Root mean squared error                  0.2576
```

Despite less folds as well as a smaller percentage of data to work with, J48 correctly classified 89% of the data correctly and in addition has a root mean squared error of .25. In my opinion, removing Proline has the greatest effect on J48 based on how the algorithm is a top down approach and since Proline was used in node that was not the bottom leaf I automatically assumed it would take an accuracy hit.



Classifier: NaiveBayes

Test options

○ Use training set

○ Supplied test set

○ Cross-validation Folds 5

● Percentage split % 33

Note the changes made to the Naïve Bayes test options with cross-validation being 5 folds and the percentage split is now 33%.

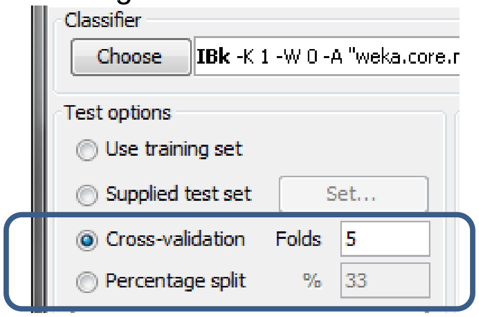
After change analysis:

```
Scheme:weka.classifiers.bayes.NaiveBayes
Relation:     Wine-weka.filters.unsupervised.attribute.Remove-R13
Instances:    178
Attributes:   13
Test mode:5-fold cross-validation
```

```
Correctly Classified Instances        170               95.5056 %
Incorrectly Classified Instances        8                4.4944 %
Total Number of Instances             178
Root mean squared error                 0.1555
```

Despite less folds as well as a smaller percentage of data to work with, Naïve Bayes correctly classified 95% of the data correctly and in addition has a root mean squared error of .1555. There are quite a few variables in this data set that have a strong correlation coefficient, which is one reason that the Naïve Bayes is doing so well at classification.

Preliminary thought process before changes on IBk: I think the changes will not affect this algorith based on the fact that it is in the class of lazy classifiers.



Classifier

Choose | IBk -K 1 -W 0 -A "weka.core.r

Test options

○ Use training set

○ Supplied test set | Set...

● Cross-validation | Folds | 5

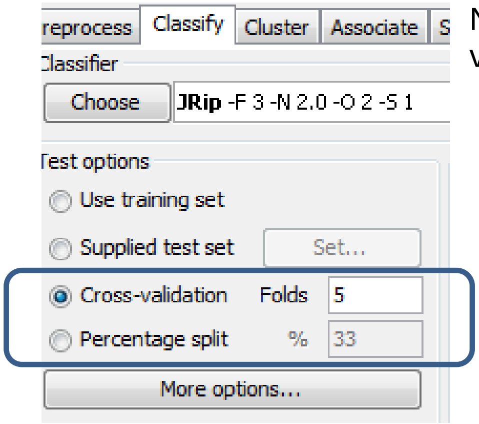
○ Percentage split | % | 33

Note the changes made to the IBk test options with cross-validation being 5 folds and the percentage split is now 33%.

<u>After change analysis:</u>

```
Scheme:weka.classifiers.lazy.IBk -K 1 -W 0 -A
"weka.core.neighboursearch.LinearNNSearch -A \"weka.core.EuclideanDistance -R
first-last\""
Relation:     Wine-weka.filters.unsupervised.attribute.Remove-R13
Test mode:5-fold cross-validation
Correctly Classified Instances        167               93.8202 %
Incorrectly Classified Instances       11                6.1798 %
Root mean squared error                 0.2011
```

Despite less folds as well as a smaller percentage of data to work with, IBk correctly classified 93% of the data correctly and in addition has a root mean squared error of .20. My personal preference is to go with an unsupervised learning method because the data is driving the decision making without initial third party intervention.



JRip -F 3 -N 2.0 -O 2 -S 1

○ Use training set

○ Supplied test set

● Cross-validation Folds 5

○ Percentage split % 33

Note the changes made to the JRIP test options with cross-validation being 5 folds and the percentage split is now 33%.

After change analysis:

```
Scheme:weka.classifiers.rules.JRip -F 3 -N 2.0 -O 2 -S 1
Relation:     Wine-weka.filters.unsupervised.attribute.Remove-R13
Test mode:5-fold cross-validation
(OD280_OD315 <= 2.11) and (Hue <= 0.81) => Type=C (39.0/0.0)
(Flavanoids <= 0.92) => Type=C (10.0/1.0)
(Alcohol >= 12.85) => Type=A (68.0/9.0)
 => Type=B (61.0/0.0)
Number of Rules : 4
Correctly Classified Instances         159               89.3258 %
Incorrectly Classified Instances        19               10.6742 %
Root mean squared error                  0.26
```

Given the changes, JRIP and J48 have very similar output.

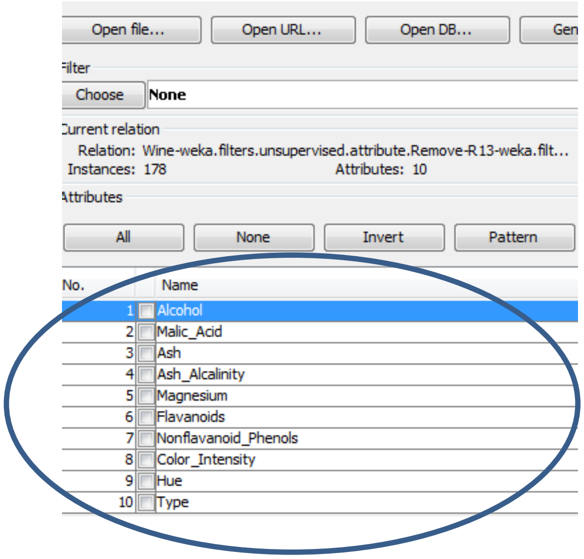
2.b. Have the rules generated from jRP changed? If so, are they compatible?

The rules have changed because Proline is no longer in the analysis, but the rules are compatible just as J48 gathered the next best result from the top-down. This approach does a very similar approach except looking from the bottom up from the data.

2.c. Removing some correlated variables, do the two Naive Bayes results differ? Why or why not?

Initial Variable Removal:

In order to assess how the correlated variables affect the analysis, I removed the most correlated variables from the list. The variables removed include: Proline, Total Phenols, Proanthocyanins, OD280_OD315.

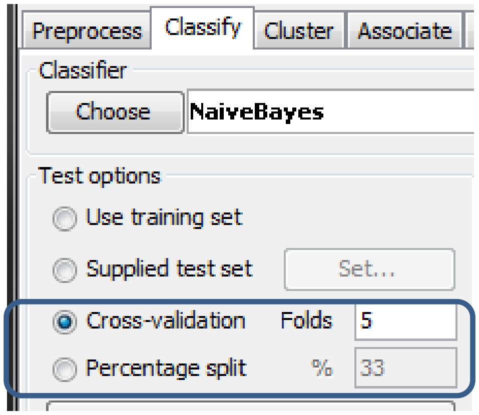


Filter: None

Relation: Wine-weka.filters.unsupervised.attribute.Remove-R13-weka.filt...
Instances: 178
Attributes: 10

No.	Name
1	Alcohol
2	Malic_Acid
3	Ash
4	Ash_Alcalinity
5	Magnesium
6	Flavanoids
7	Nonflavanoid_Phenols
8	Color_Intensity
9	Hue
10	Type

After removing the variables the remainging variables are listed to the right.



Classifier: NaiveBayes

Test options
○ Use training set
○ Supplied test set
● Cross-validation Folds 5
○ Percentage split % 33

Note the changes made to the JRIP test options with cross-validation being 5 folds and the percentage split is now 33%.

After change analysis:
Scheme:weka.classifiers.bayes.NaiveBayes
Relation: Wine-weka.filters.unsupervised.attribute.Remove-R13-weka.filters.unsupervised.attribute.Remove-R6,9,12
Test mode: 5-fold cross-validation

```
Correctly Classified Instances         171               96.0674 %
Incorrectly Classified Instances         7                3.9326 %
Root mean squared error                  0.1423
```

Surprisingly, removing the correlated variables boosted the correctly classified percentage and shrunk the root mean squared error. Initially, I thought the correlation was helping the Naïve Bayes classifier, but now I wonder if the data suffers from a high value of multicollinearity given the removing the correlated variables had a positive effect on the overall classification output.

Concluding Thoughts:

Through this exercise, I have learned how to use 4 different classification algorithms on a relatively small data set. The next step would be to apply this to a rather large data set in an effort to analyze what happens as more data is brought into the decision making process. On a personal note, all four examples had a rather high percentage of correct classification. If I was tasked with picking one, I would resort to an algorithm that correctly classifies above 93% and best adheres to the principle of parsimony.