MLND Capstone Project

Predict Wine Class

Definition

Project Overview

Wine tasting is the sensory examination and evaluation of wine. While the practice of wine tasting is as ancient as its production, a more formalized methodology has slowly become established from the 14th century onwards. Modern, professional wine tasters (such as sommeliers or buyers for retailers) use a constantly evolving specialized terminology which is used to describe the range of perceived flavours, aromas and general characteristics of a wine. More informal, recreational tasting may use similar terminology, usually involving a much less analytical process for a more general, personal appreciation. (Source: Wikipedia)

One of the goal of AI/ML algorithms is to reduce dependency on human intelligence and develop scientific methods for decision making. Here we will be exploring various algorithm to develop model to predict wine class scientifically.

In this project we are going to analyse the data, which is the result of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The aim is to develop a model to predict class of wine based on 13 parameters which is result of laboratory test of the wine. As per UCI website the original dataset had 30 attributes but available dataset has 30 attributes.

Problem Statement

It is a typical classification problem where we have to predict class based on the given attributes/features, I will explore various classifiers at predicting a certain wine type from available UCI's wine dataset.

The initial data set had around 30 variables, but on UCI’s website only 13-dimensional version is available. (All attributes are continuous)

1) Alcohol	6) Total phenols	11) Hue
2) Malic acid	7) Flavanoids	12) OD280/OD315 of diluted wines
3) Ash	8) Nonflavanoid phenols	13) Proline
4) Alcalinity of ash	9) Proanthocyanins	
5) Magnesium	10) Colour intensity	

In a classification context, this is a well posed problem with "well behaved" class structures. Number of Instances: class-1(59), class-2(71), class-3(48), Total 178 records in csv format.
https://archive.ics.uci.edu/ml/machine-learning-databases/wine/

Metrics

I will use accuracy and scikit-learn Classification Report as evaluation matrix which reports precision, recall and f1-score.
Accuracy measures how often the classifier makes the correct prediction. It's the ratio of the number of correct predictions to the total number of predictions (the number of test data points).

Precision = [True Positives/(True Positives + False Positives)]
Recall(sensitivity) = [True Positives/(True Positives + False Negatives)]

Precision and Recall can be combined to get the F1 score, which is weighted average(harmonic mean) of the precision and recall scores. This score can range from 0 to 1, with 1 being the best possible F1 score(we take the harmonic mean as we are dealing with ratios).

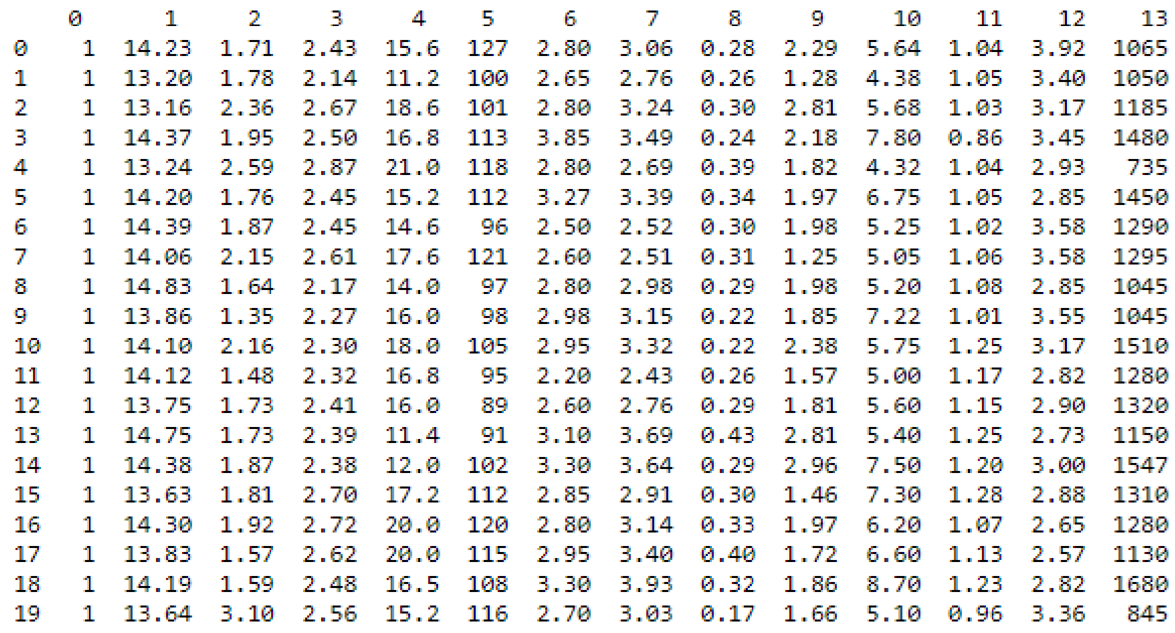
F1 Score = 2*(Recall * Precision) / (Recall + Precision)

Analysis

Data Exploration

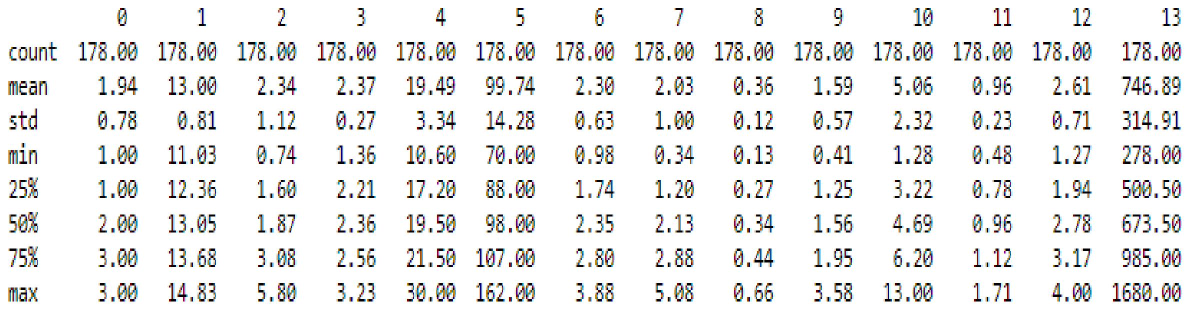
Index	Description	Data Type
0	Wine Class (1, 2, 3)	int64
1	Alcohol	float64
2	Malic acid	float64
3	Ash	float64
4	Alcalinity of ash	float64
5	Magnesium	int64
6	Total phenols	float64
7	Flavanoids	float64
8	Nonflavanoid phenols	float64
9	Proanthocyanins	float64
10	Colour intensity	float64
11	Hue	float64
12	OD280/OD315 of diluted wines	float64
13	Proline	int64

Sample data



```
    0      1     2     3     4    5     6     7     8     9    10    11    12    13
0   1  14.23  1.71  2.43  15.6  127  2.80  3.06  0.28  2.29  5.64  1.04  3.92  1065
1   1  13.20  1.78  2.14  11.2  100  2.65  2.76  0.26  1.28  4.38  1.05  3.40  1050
2   1  13.16  2.36  2.67  18.6  101  2.80  3.24  0.30  2.81  5.68  1.03  3.17  1185
3   1  14.37  1.95  2.50  16.8  113  3.85  3.49  0.24  2.18  7.80  0.86  3.45  1480
4   1  13.24  2.59  2.87  21.0  118  2.80  2.69  0.39  1.82  4.32  1.04  2.93   735
5   1  14.20  1.76  2.45  15.2  112  3.27  3.39  0.34  1.97  6.75  1.05  2.85  1450
6   1  14.39  1.87  2.45  14.6   96  2.50  2.52  0.30  1.98  5.25  1.02  3.58  1290
7   1  14.06  2.15  2.61  17.6  121  2.60  2.51  0.31  1.25  5.05  1.06  3.58  1295
8   1  14.83  1.64  2.17  14.0   97  2.80  2.98  0.29  1.98  5.20  1.08  2.85  1045
9   1  13.86  1.35  2.27  16.0   98  2.98  3.15  0.22  1.85  7.22  1.01  3.55  1045
10  1  14.10  2.16  2.30  18.0  105  2.95  3.32  0.22  2.38  5.75  1.25  3.17  1510
11  1  14.12  1.48  2.32  16.8   95  2.20  2.43  0.26  1.57  5.00  1.17  2.82  1280
12  1  13.75  1.73  2.41  16.0   89  2.60  2.76  0.29  1.81  5.60  1.15  2.90  1320
13  1  14.75  1.73  2.39  11.4   91  3.10  3.69  0.43  2.81  5.40  1.25  2.73  1150
14  1  14.38  1.87  2.38  12.0  102  3.30  3.64  0.29  2.96  7.50  1.20  3.00  1547
15  1  13.63  1.81  2.70  17.2  112  2.85  2.91  0.30  1.46  7.30  1.28  2.88  1310
16  1  14.30  1.92  2.72  20.0  120  2.80  3.14  0.33  1.97  6.20  1.07  2.65  1280
17  1  13.83  1.57  2.62  20.0  115  2.95  3.40  0.40  1.72  6.60  1.13  2.57  1130
18  1  14.19  1.59  2.48  16.5  108  3.30  3.93  0.32  1.86  8.70  1.23  2.82  1680
19  1  13.64  3.10  2.56  15.2  116  2.70  3.03  0.17  1.66  5.10  0.96  3.36   845
```

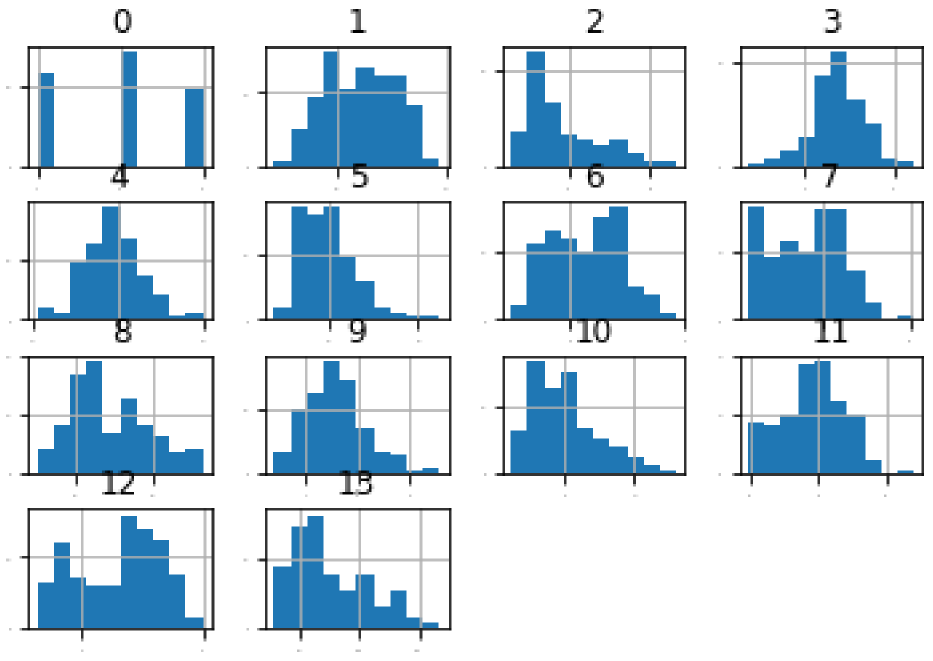
Data Description



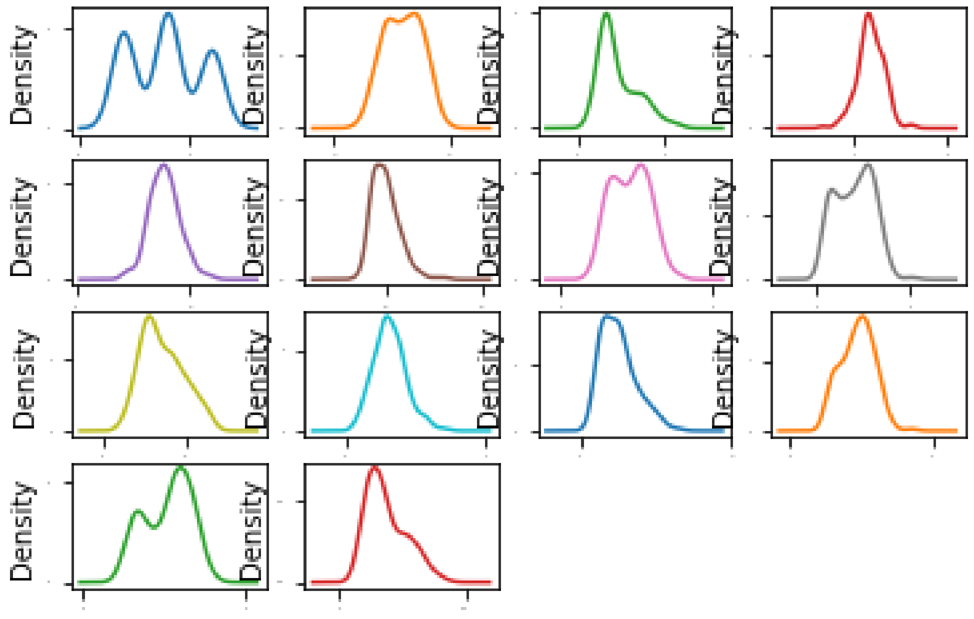
```
            0       1       2       3       4       5       6       7       8       9      10      11      12       13
count  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00  178.00   178.00
mean     1.94   13.00    2.34    2.37   19.49   99.74    2.30    2.03    0.36    1.59    5.06    0.96    2.61   746.89
std      0.78    0.81    1.12    0.27    3.34   14.28    0.63    1.00    0.12    0.57    2.32    0.23    0.71   314.91
min      1.00   11.03    0.74    1.36   10.60   70.00    0.98    0.34    0.13    0.41    1.28    0.48    1.27   278.00
25%      1.00   12.36    1.60    2.21   17.20   88.00    1.74    1.20    0.27    1.25    3.22    0.78    1.94   500.50
50%      2.00   13.05    1.87    2.36   19.50   98.00    2.35    2.13    0.34    1.56    4.69    0.96    2.78   673.50
75%      3.00   13.68    3.08    2.56   21.50  107.00    2.80    2.88    0.44    1.95    6.20    1.12    3.17   985.00
max      3.00   14.83    5.80    3.23   30.00  162.00    3.88    5.08    0.66    3.58   13.00    1.71    4.00  1680.00
```

Algorithms and Techniques

Histogram



Density



Benchmark

I will use following result on Kaggle as benchmark:
https://www.kaggle.com/brynja/testing-classifiers-for-wine-variety-prediction

Accuracy: 0.98592

Sensitivity: 0.95455

Specificity: 1.00000

Precision: 1.00000

I will try tune my algorithms and try few ensembles to improve accuracy and get better result than above mention model. However if I talk in term of independent project I would keep LogisticRegression as benchmark model and would compare other model with it for benchmarking the result.

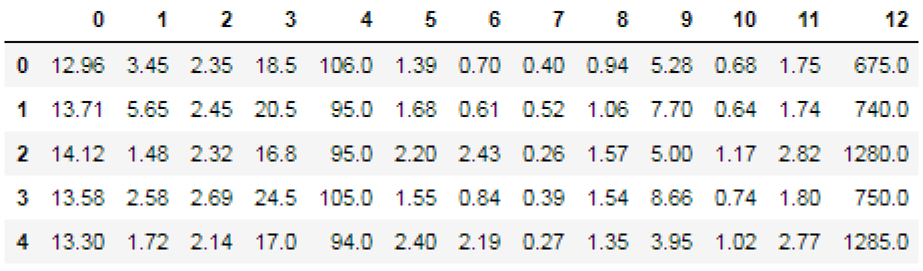
Methodology

Data Pre-processing

The given data is well processed data having no anomalies, none of the attributed had null or garbage values. And we have good number of samples from each class. The only preprocessing I did on data is doing StandardScaler transform.

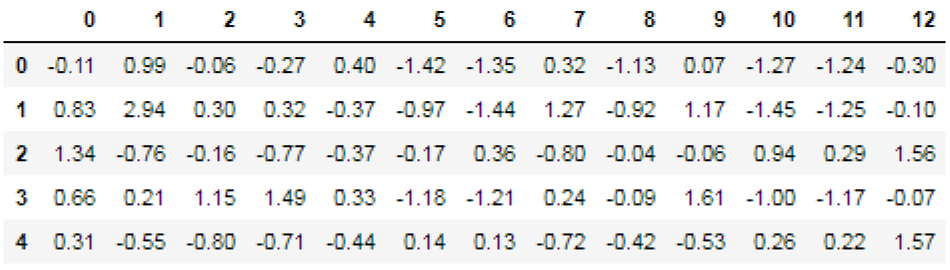
Standardization is a useful technique to transform attributes with a Gaussian distribution and differing means and standard deviations to a standard Gaussian distribution with a mean of 0 and a standard deviation of 1. It is most suitable for techniques that assume a Gaussian distribution in the input variables and work better with rescaled data.

Data



	0	1	2	3	4	5	6	7	8	9	10	11	12
0	12.96	3.45	2.35	18.5	106.0	1.39	0.70	0.40	0.94	5.28	0.68	1.75	675.0
1	13.71	5.65	2.45	20.5	95.0	1.68	0.61	0.52	1.06	7.70	0.64	1.74	740.0
2	14.12	1.48	2.32	16.8	95.0	2.20	2.43	0.26	1.57	5.00	1.17	2.82	1280.0
3	13.58	2.58	2.69	24.5	105.0	1.55	0.84	0.39	1.54	8.66	0.74	1.80	750.0
4	13.30	1.72	2.14	17.0	94.0	2.40	2.19	0.27	1.35	3.95	1.02	2.77	1285.0

Rescaled Data



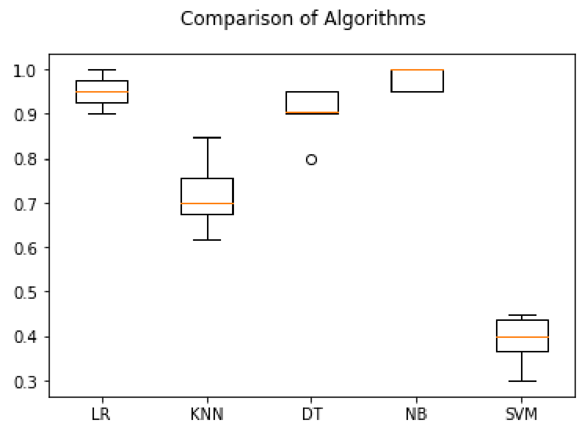
	0	1	2	3	4	5	6	7	8	9	10	11	12
0	-0.11	0.99	-0.06	-0.27	0.40	-1.42	-1.35	0.32	-1.13	0.07	-1.27	-1.24	-0.30
1	0.83	2.94	0.30	0.32	-0.37	-0.97	-1.44	1.27	-0.92	1.17	-1.45	-1.25	-0.10
2	1.34	-0.76	-0.16	-0.77	-0.37	-0.17	0.36	-0.80	-0.04	-0.06	0.94	0.29	1.56
3	0.66	0.21	1.15	1.49	0.33	-1.18	-1.21	0.24	-0.09	1.61	-1.00	-1.17	-0.07
4	0.31	-0.55	-0.80	-0.71	-0.44	0.14	0.13	-0.72	-0.42	-0.53	0.26	0.22	1.57

Implementation

Firstly, I tried few algorithms to check which one is performing better with default parameters. I tried Linear Classification model (Logistics Regression) and non-Linear classification models (KNN, SVM, Decision Tree, Naïve Bayes. Here is the result (Mean accuracy and standard deviation):

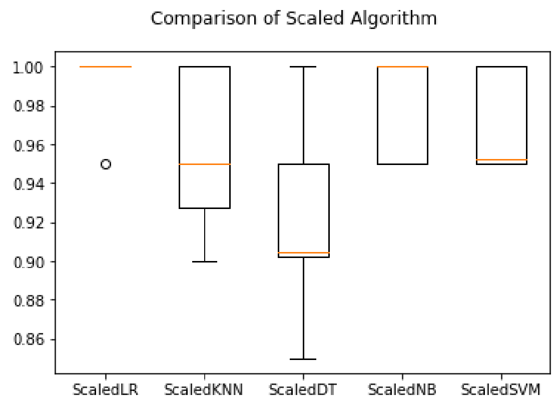
```
Logistic Regression: 0.950680 (0.037812)
KNN: 0.718707 (0.071149)
Decision Tree: 0.908163 (0.049713)
Naïve Bayes: 0.978571 (0.024744)
SVM: 0.394218 (0.051332)
```

As per the result Naive Bayes is performing best out of all the 5 algorithms. Logistic Regression and Decision Tree are also very close to NB.



I tried all these algorithms again with transformed data and here is the result:

```
ScaledLR: 0.992857 (0.017496)
ScaledKNN: 0.957823 (0.040740)
ScaledDT: 0.922789 (0.044577)
ScaledNB: 0.978571 (0.024744)
ScaledSVM: 0.971769 (0.024461)
```



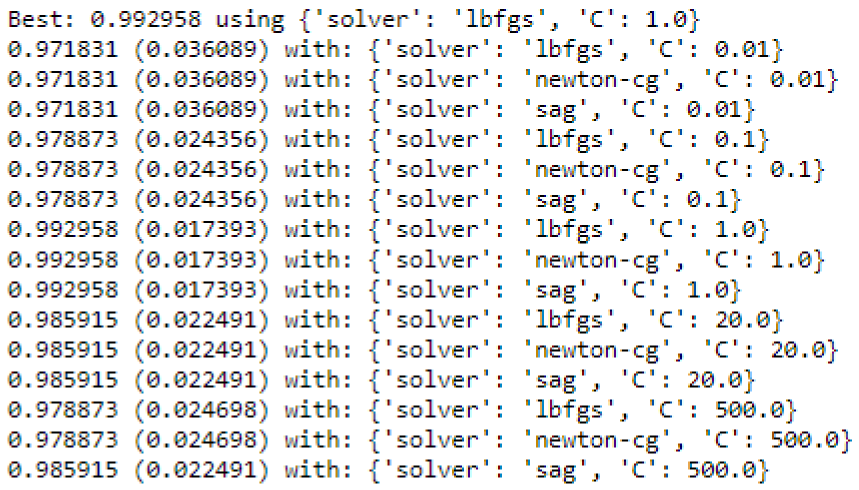
Clearly Logistic Regression is the winner.

Refinement

I tuned parameters of Logistic Regression and SVM using grid search to get the best result out of it.

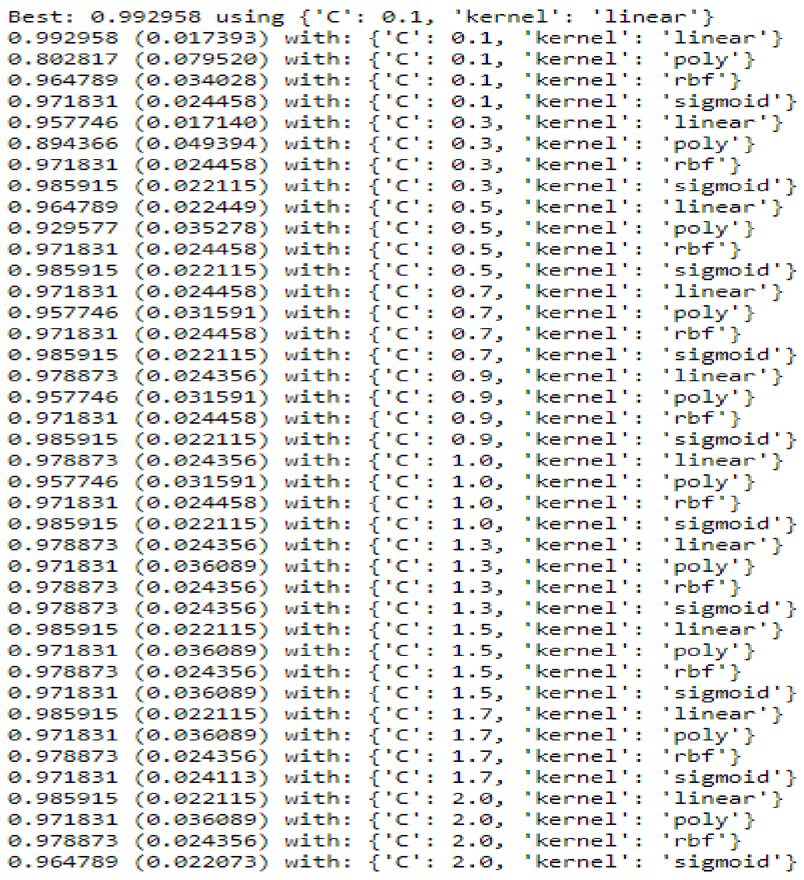
Here is the result of tuning:

```
Logistic Regression: 0.992958 using {'solver': 'lbfgs', 'C': 1.0}
```



```
Best: 0.992958 using {'solver': 'lbfgs', 'C': 1.0}
0.971831 (0.036089) with: {'solver': 'lbfgs', 'C': 0.01}
0.971831 (0.036089) with: {'solver': 'newton-cg', 'C': 0.01}
0.971831 (0.036089) with: {'solver': 'sag', 'C': 0.01}
0.978873 (0.024356) with: {'solver': 'lbfgs', 'C': 0.1}
0.978873 (0.024356) with: {'solver': 'newton-cg', 'C': 0.1}
0.978873 (0.024356) with: {'solver': 'sag', 'C': 0.1}
0.992958 (0.017393) with: {'solver': 'lbfgs', 'C': 1.0}
0.992958 (0.017393) with: {'solver': 'newton-cg', 'C': 1.0}
0.992958 (0.017393) with: {'solver': 'sag', 'C': 1.0}
0.985915 (0.022491) with: {'solver': 'lbfgs', 'C': 20.0}
0.985915 (0.022491) with: {'solver': 'newton-cg', 'C': 20.0}
0.985915 (0.022491) with: {'solver': 'sag', 'C': 20.0}
0.978873 (0.024698) with: {'solver': 'lbfgs', 'C': 500.0}
0.978873 (0.024698) with: {'solver': 'newton-cg', 'C': 500.0}
0.985915 (0.022491) with: {'solver': 'sag', 'C': 500.0}
```

```
SVM : 0.992958 using {'C': 0.1, 'kernel': 'linear'}
```

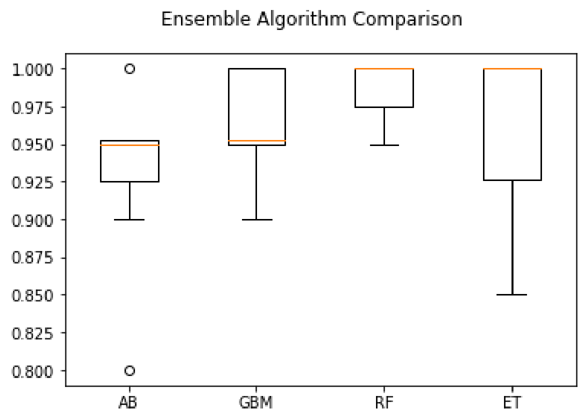


```
Best: 0.992958 using {'C': 0.1, 'kernel': 'linear'}
0.992958 (0.017393) with: {'C': 0.1, 'kernel': 'linear'}
0.802817 (0.079520) with: {'C': 0.1, 'kernel': 'poly'}
0.964789 (0.034028) with: {'C': 0.1, 'kernel': 'rbf'}
0.971831 (0.024458) with: {'C': 0.1, 'kernel': 'sigmoid'}
0.957746 (0.017140) with: {'C': 0.3, 'kernel': 'linear'}
0.894366 (0.049394) with: {'C': 0.3, 'kernel': 'poly'}
0.971831 (0.024458) with: {'C': 0.3, 'kernel': 'rbf'}
0.985915 (0.022115) with: {'C': 0.3, 'kernel': 'sigmoid'}
0.964789 (0.022449) with: {'C': 0.5, 'kernel': 'linear'}
0.929577 (0.035278) with: {'C': 0.5, 'kernel': 'poly'}
0.971831 (0.024458) with: {'C': 0.5, 'kernel': 'rbf'}
0.985915 (0.022115) with: {'C': 0.5, 'kernel': 'sigmoid'}
0.971831 (0.024458) with: {'C': 0.7, 'kernel': 'linear'}
0.957746 (0.031591) with: {'C': 0.7, 'kernel': 'poly'}
0.971831 (0.024458) with: {'C': 0.7, 'kernel': 'rbf'}
0.985915 (0.022115) with: {'C': 0.7, 'kernel': 'sigmoid'}
0.978873 (0.024356) with: {'C': 0.9, 'kernel': 'linear'}
0.957746 (0.031591) with: {'C': 0.9, 'kernel': 'poly'}
0.971831 (0.024458) with: {'C': 0.9, 'kernel': 'rbf'}
0.985915 (0.022115) with: {'C': 0.9, 'kernel': 'sigmoid'}
0.978873 (0.024356) with: {'C': 1.0, 'kernel': 'linear'}
0.957746 (0.031591) with: {'C': 1.0, 'kernel': 'poly'}
0.971831 (0.024458) with: {'C': 1.0, 'kernel': 'rbf'}
0.985915 (0.022115) with: {'C': 1.0, 'kernel': 'sigmoid'}
0.978873 (0.024356) with: {'C': 1.3, 'kernel': 'linear'}
0.971831 (0.036089) with: {'C': 1.3, 'kernel': 'poly'}
0.978873 (0.024356) with: {'C': 1.3, 'kernel': 'rbf'}
0.978873 (0.024356) with: {'C': 1.3, 'kernel': 'sigmoid'}
0.985915 (0.022115) with: {'C': 1.5, 'kernel': 'linear'}
0.971831 (0.036089) with: {'C': 1.5, 'kernel': 'poly'}
0.978873 (0.024356) with: {'C': 1.5, 'kernel': 'rbf'}
0.971831 (0.036089) with: {'C': 1.5, 'kernel': 'sigmoid'}
0.985915 (0.022115) with: {'C': 1.7, 'kernel': 'linear'}
0.971831 (0.036089) with: {'C': 1.7, 'kernel': 'poly'}
0.978873 (0.024356) with: {'C': 1.7, 'kernel': 'rbf'}
0.971831 (0.024113) with: {'C': 1.7, 'kernel': 'sigmoid'}
0.985915 (0.022115) with: {'C': 2.0, 'kernel': 'linear'}
0.971831 (0.036089) with: {'C': 2.0, 'kernel': 'poly'}
0.978873 (0.024356) with: {'C': 2.0, 'kernel': 'rbf'}
0.964789 (0.022073) with: {'C': 2.0, 'kernel': 'sigmoid'}
```

I tried ensembles to see if I can get better accuracy as compared to LR or SVM. I tried (Gradient Boosting, Random Forest, Ada Boost, Extra Trees) with default parameters to check which one is performing best for our case.

Here is the result:

```
AdaBoost: 0.929252 (0.059158)
GradientBoosting: 0.964626 (0.034864)
RandomForest: 0.985714 (0.022588)
ExtraTrees: 0.957483 (0.056206)
```



I tried to tune both GradientBoosting and RandomForest and got best result from GradientBoosting.

```
Best: 1.000000 using {'n_estimators': 10, 'min_samples_split': 6, 'max_
features': 3, 'min_samples_leaf': 1, 'max_depth': 3}
```

Results

Model Evaluation and Validation

Here is the result. The model seems to give ideal result as 1 for accuracy, precision, recall and f1-score. This could be because we have small validation set but we can consider this as fairly accurate model.

```
1.0
[[ 7  0  0]
 [ 0 17  0]
 [ 0  0 12]]
             precision    recall  f1-score   support

        1.0       1.00      1.00      1.00         7
        2.0       1.00      1.00      1.00        17
        3.0       1.00      1.00      1.00        12

avg / total       1.00      1.00      1.00        36
```

Justification

In comparison to the benchmark model on Kaggle this model had given much better result with 100% accuracy. As I mentioned in previous heading that this perfect accuracy can be because we have small data set to validate the model. I am sure even with bigger dataset it would give satisfactory result.

Conclusion

Free-Form Visualization

Here are the highlights of the model:

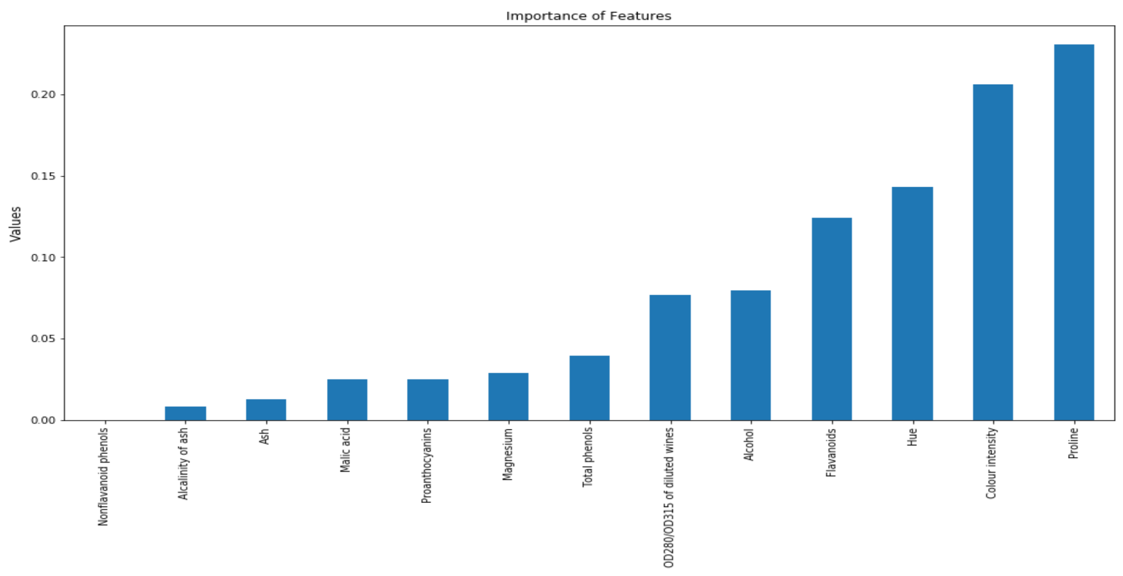
Top 3 and bottom 3 feature as per Importance:

```
Most imp feature = Proline
Least imp feature = Nonflavanoid phenols

3 most imp features of the model:
Proline
Colour intensity
Hue

3 least imp features of the model:
Nonflavanoid phenols
Alcalinity of ash
Ash
```

Plot for importance of features:



I was assuming that first feature (Alcohol) would be the most important feature but it turned out that Feature[12] Proline is the most important feature. And model mostly depend on top 6 features as they carry most of the importance.

Reflection

My solution mainly focussed on optimizing the models by tuning the parameters and in this solution I tried lots of models like Linear model(Logistic Regression), non-Linear classification model (KNN, SVM, Decision Tree, Naïve Bayes) and ensembles (Gradient Boosting, Random Forest, Ada Boost, Extra Trees) to get the best result.

My biggest time consuming tasks in this project was to choose which dataset to choose and approach to adopt. For choosing dataset I decided to go for multiclass classification model as it looked more challenging than linear regression or binary classification problem. I wanted to choose a dataset where I have to do data wrangling and play with data to make to eligible for modelling but could not find suitable data source. My most favourite spot for choosing data for ML is UCI website and I tried various dataset like Sonar Dataset (binary classification), breast cancer data (binary classification), poker hand data (ANN model) and Wine Classification data. Finally I decided to go ahead with data and Kaggle already had a solution for 98% accuracy so getting better accuracy was the challenging task and that's what made me to choose this data set.

For deciding which algorithm to choose I decide to follow the strategy of choosing top 2 algorithms by doing spot check and then tuning the parameter to get best result. I also tried ensemble to better the result.

Improvement

I would definitely like to try this solution with the complete original features (30) and bigger data set. I could also try to include only the important or top 6 features to build the model for more generalize solution.