Analysis Report for Assignment 1

OMSCS CS-7641

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Part 0 Problem introduction

After researching and comparing among the potential classification problems, I found two interesting ones. First is the employee turnover problem and second is white wine quality analysis.

My bachelor's background was in Human Resource Management. One of the most intriguing topics during that four years was how to achieve a high employee retention. We covered other topics too, such as performance assessment, salary management and human behavior. However, none of the topics, or lessons really taught me about the fundamental yet critical question: what do employees care the most at work and why they tend to leave? HR is a human related field, it's expected to rely more on human behavioral data analytics. This dataset is a very good example. Besides, this is a binary classification problem and the dataset size is small, which is a good start for testing the classifiers. The data contains couple of categorical features, so data preprocessing is necessary.

The second problem is to predict the quality for white wine. This dataset contains 11 numerical attributes and the target attribute, 'quality', is a continuous score. It's needed to be converted to a classification problem. Here for simplicity and reusability of the code, I also converted this problem to a binary classification. If the score is higher than 5, then the quality is considered "good", otherwise "bad". Also, the attributes of the dataset are not in the same range, so the data needs to be normalized for certain algorithms.

The rest of the report will split into 2 parts for the problems, 5 classifiers will be "implemented" and analyzed with various sets of hyper-parameters. I will compare their performances in terms of accuracy and runtime.

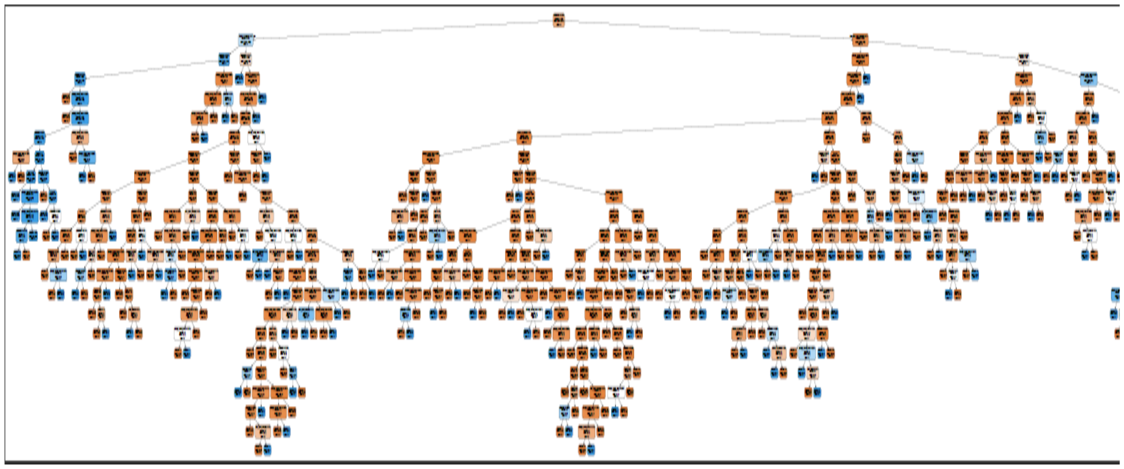
Part I Employee turnover problem

1.1.1 Decision Tree

The following visualization is the first tree generated. This is a basic tree without any pruning and parameter tuning. The performance of the tree is as follows in the table. The technique of cross validation is employed here (cv = 5). The default split criterion is "gini". This is a very huge tree, which cannot be even hosted on one page.

Basic Tree	
SCORE TYPE	SCORE
CV_Score_AVG	0.975421
CV_Score_STD	0.00323
Train_Score	1
Test_Score	0.974545

Precision	0.934156
Recall	0.96105
F1_Score	0.947412
ROC_AUC_SCORE	0.969912
Runtime	0.524626



1.1.2 Pruning

This is not necessarily perfect, I have a feeling that it could do a better if pruned in some way. Pruning is a set of ways to limit the growing of the tree. Here I tried to set an upper limit of the tree's depth and the minimum number of samples required to be at a leaf node. The latter one guarantees that the model does not further split a node when the samples are exhausting.

To achieve the best tree, the GridSearchCV technique was implemented. Here, I need to specify a set of parameters: tree depth and minimum number of samples to split the leaf nodes. This technique helps to discover the best parameter combination in the list given.

Here are the potential parameters list. I tend to make it cover as many possibilities as possible.

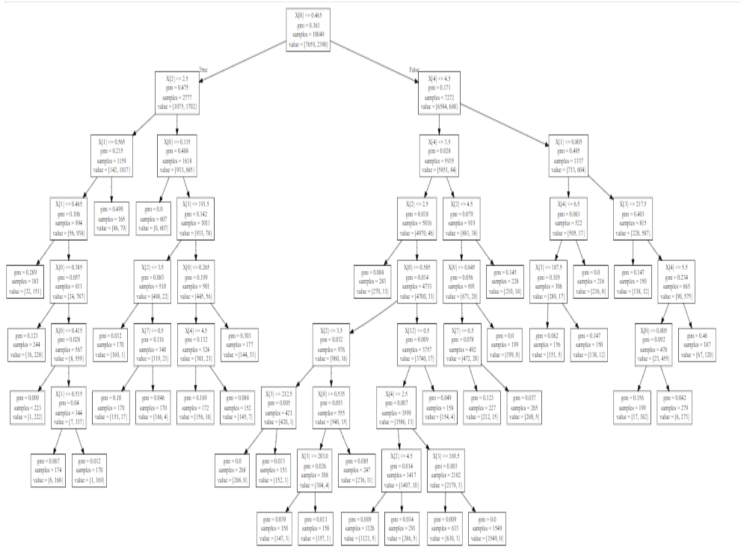
{'max_depth': [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20], 'min_samples_leaf': [50, 100, 150, 20
0, 250, 300, 350, 400, 450]}

After the grid search (I set cv = 5 for consistency). Here return the best parameters:

{'max_depth': 8, 'min_samples_leaf': 150}

Use above best parameters to fit the tree again and the new tree is much more simple without sacrificing significant performance. In fact, the runtime after pruning dropped dramatically by 50%.

SCORE TYPE	SCORE
CV_Score_AVG	0.968256
CV_Score_STD	0.003137
Train_Score	0.970246
Test_Score	0.964646
Precision	0.948307
Recall	0.900931
F1_Score	0.924012
ROC_AUC_SCORE	0.942771
Runtime	0.26997



1.1.3 Feature Selection

From the fitted decision tree, the importance of the attributes can be found. Due to the nature of decision tree, each feature provides different information gain as shown in the list below. I then dropped the features with an importance less than 0.05 and built the tree again (with pruning, otherwise it still would be a huge tree). This time, with the best parameters (5, 50), the accuracy stays the same, but the runtime drastically dropped.

Features	Importance
satisfaction	0.58045
time_spend_company	0.149701
evaluation	0.123546
number_of_projects	0.094283
average_montly_hours	0.051456
salary	0.000516
management	0.000048
work_accident	0
promotion	0
IT	0
RandD	0
accounting	0
hr	0
marketing	0
product_mng	0
sales	0
support	0

Lean/Pruned Tree	
SCORE TYPE	SCORE
CV_Score_AVG	0.968256
CV_Score_STD	0.003137
Train_Score	0.970246
Test_Score	0.964646
Precision	0.948307
Recall	0.900931
F1_Score	0.924012
ROC_AUC_SCORE	0.942771
Runtime	0.103695

1.2.1 K-NN

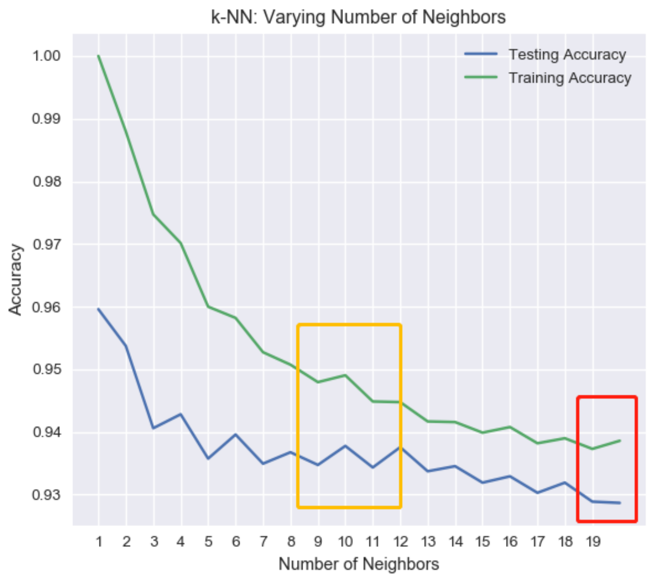
Unlike decision tree, the data need to be scaled for K-NN, for better performance. Still, 5-fold cross-validation is embedded in the model. Here is the training result with 5 neighbors. We can tell that the runtime increased significantly than the Decision Tree. It demonstrates the 'laziness' of the K-NN algorithm.

5-NN	
SCORE TYPE	SCORE
CV_Score_AVG	0.941586
CV_Score_STD	0.005206
Train_Score	0.959996
Test_Score	0.935758
Precision	0.84603
Recall	0.893311
F1_Score	0.869028
ROC_AUC_SCORE	0.921184
Runtime	6.465076

1.2.2 Play with k, the number of neighbors

The following chart shows the trends of training accuracy and testing accuracy when k varies. For this problem, I tried k values from 1 to 20, the accuracy (both training and testing) decreases as k value increases. However, if k is too small, the model overfits. According to the chart, an "ideal" k value is 19, since when it's 20, training and testing accuracies diverse. A good k value should keep the difference between training and testing accuracy as small as possible and keep itself small too. More k means more runtime. In this situation it seems k = 10 is a good fit (k = 11 sacrifices the accuracies). The right-handed table shows the performance of the knn when k = 10.

As expected, the accuracies decrease compared to k = 5, but the difference between Train_Score and Test_Score decrease by 53.49%!

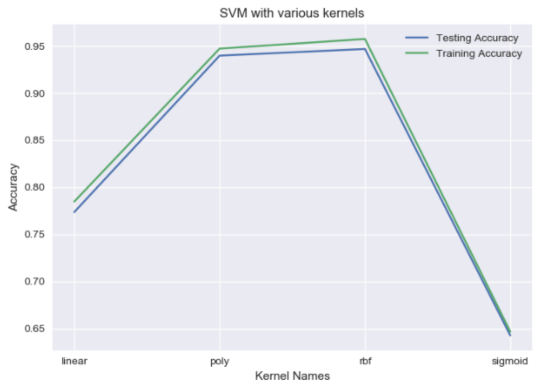


10-NN	
SCORE TYPE	SCORE
CV_Score_AVG	0.938103
CV_Score_STD	0.006772
Train_Score	0.94905
Test_Score	0.937778
Precision	0.865884
Recall	0.874682
F1_Score	0.870261
ROC_AUC_SCORE	0.916115
Runtime	6.827148

1.3.1 Support Vector Machine, kernels

The SVM exploration concentrates more on the kernel functions. Below on the left is the performance of a basic SVM – with gamma = 'auto', C = 1.00 and kernel function as Gaussian Kernel. The right-sided chart shows the training and testing accuracy with different kernels.

SVM with Gaussian kernel	
SCORE TYPE	SCORE
CV_Score_AVG	0.951338
CV_Score_STD	0.004641
Train_Score	0.957508
Test_Score	0.946869
ROC_AUC_SCORE	0.926737
Runtime	6.093823

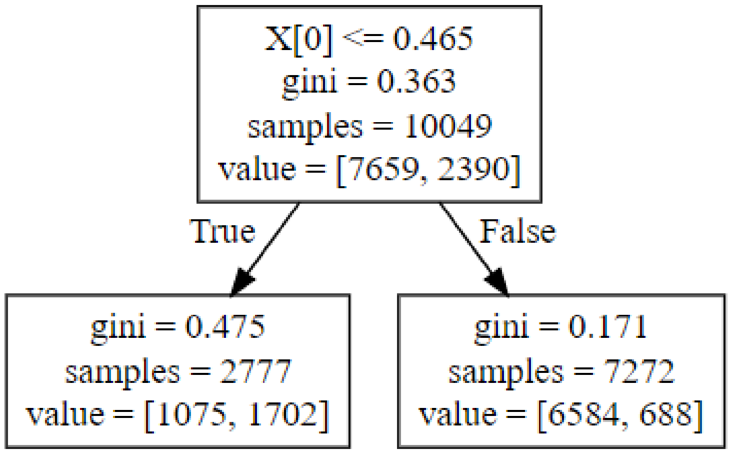


"rtf", in the third position on the x-axis, stands for "Radial Basis Function kernel" also known as Gaussian kernel. Based on the performance of the 4 kernels, the linear kernel doesn't do a good job, so maybe this is not a linear separable problem so either a polynomial or Gaussian kernel significantly increases the model's performance.

1.4.1 'Adaboosted' version of decision tree

In the first part exploration of the decision tree classifiers, pruning was implemented by limiting the tree depth and minimum samples for each leaf. In this section, one form of ensemble learning, boosting technique is implemented. Here a more 'aggressive' pruning will be used for each tree estimator (weak learners). The most intriguing hyperparameters are the number of the estimators, or iterations and the learning rate. As an example, the following is a fitted tree with depth = 1 and criterion = 'gini'.

Weak Learner	
SCORE NAME	SCORE
CV_Score_AVG	0.82456
CV_Score_STD	0.008389
Train_Score	0.82456
Test_Score	0.812323
Precision	0.589616
Recall	0.701948
F1_Score	0.640897
ROC_AUC_SCORE	0.774428
Runtime	0.050991



Apparently, this tree has relatively poor performance (weak learner). What about an adaboost classifier built on top of the learner? Here is the performance of the adaboosted version of the decision tree with the same pruning (depth = 1 and minimum samples of a leaf = 10). Iterations of 5000 and learning rate of 0.05 are the parameter values here.

Adaboosted tree with 5000 iterations and learning rate of 0.05	
SCORE TYPE	SCORE
CV_Score_AVG	0.960593
CV_Score_STD	0.003753
Train_Score	0.962484
Test_Score	0.960404
Precision	0.923474
Recall	0.909399
F1_Score	0.916382
ROC_AUC_SCORE	0.942893
Runtime	148.1826

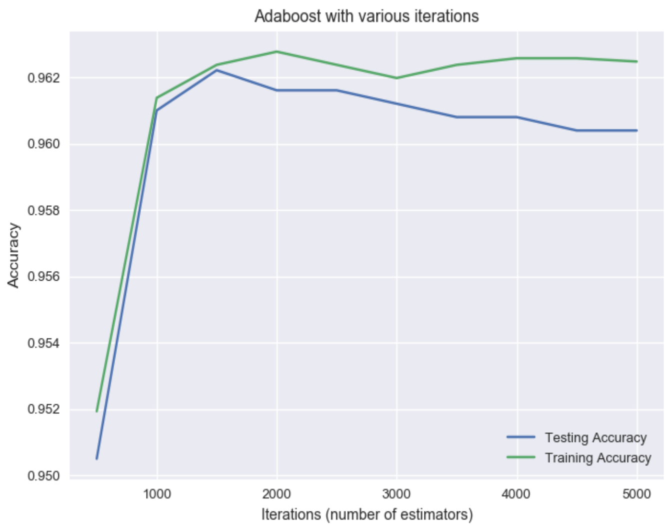
The accuracy substantially increases, and overfitting is largely improved. Compared to the previous pruned tree in 1.1.2, the test score is lower by 0.44% while the train and test accuracy difference dropped by 62.86%!

1.4.2 Explore the number of iterations

The number of iterations also states how many weak estimators are used in the adaboost classifier. From 1 estimator to many, the accuracy goes up. I would be intuitive if an iteration – accuracy learning curve is displayed.

Here is the result. It's obvious that when number of iterations = 1500, the model performs best because of 1. least overfitting; 2. Relatively high accuracy. The curve almost doesn't fluctuate, which means the learning rate is fine with the value of 0.05. But overfitting seems to emerge with more and more iterations.

The performance of the adaboosted tree with iteration of 1500 is shown in the right-handed table. The difference between train and test accuracy decreases by 92% (compared to iteration = 5000)!



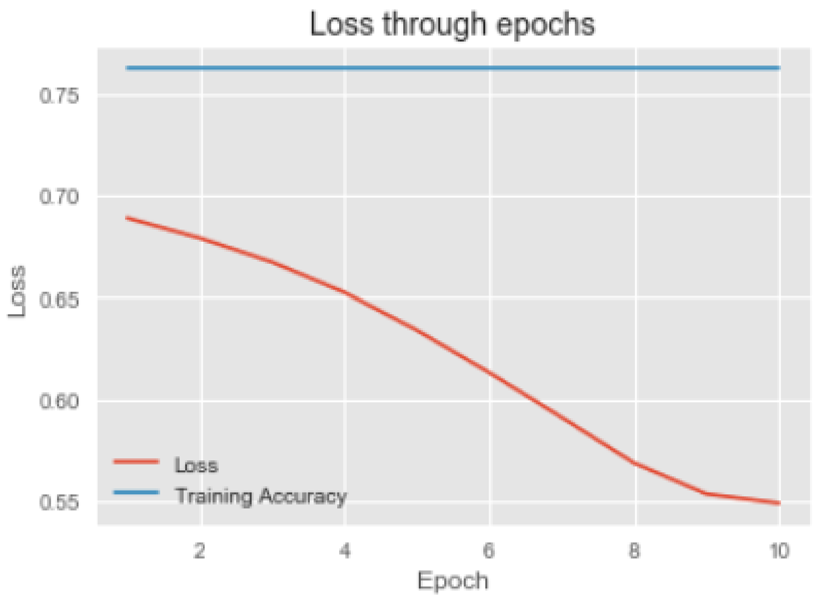
Adaboosted tree with 1500 iterations and learning rate of 0.05	
SCORE TYPE	SCORE
CV_Score_AVG	0.960892
CV_Score_STD	0.005193
Train_Score	0.962384
Test_Score	0.962222
Precision	0.931424
Recall	0.908552
F1_Score	0.919846
ROC_AUC_SCORE	0.943796
Runtime	44.423687

1.5.1 Neural Network

I used Keras to build sequential models with different layers, number of nodes, and activation functions. I tried 4 hidden layers with 5 nodes for each and 3 hidden layers with 12, 8 and 8 for each. Also, I tried both 'tanh' and 'sigmoid' as the activation functions for the output layer. Batch processing is implemented here (mini batches with 300 samples). The optimization algorithm I chose is Adam, it's an alternative optimization algorithm for classic gradient decent or stochastic gradient decent.

However, my training accuracy does not improve in any cases, even after the less relevant attributes are dropped. The training accuracy is stuck at 76.22% and it seems all predicted results are "0", which means the model predicts everyone to stay under all circumstances.

I'm still confused why the model does not work. More investigations should involve for this issue. Here is the learning curve for the network (4 layer, 'relu' as activation for the hidden layers and tanh for output layer; Adam as the optimization algorithm).



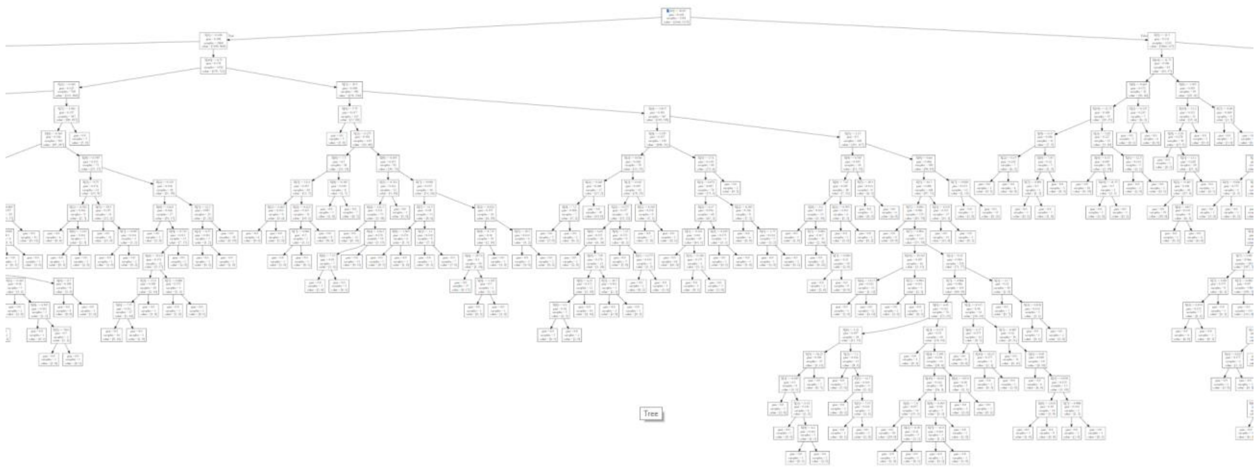
Part II White Wine Quality

2.1.1 Decision Tree

When looking at the basic tree (without specifying any hyperparameters), I found the tree built for wine quality does not perform as well as the one for employee turnover. I assume it's caused by the data scales. To confirm the reason, I trained two trees, one with original data and the other with scaled data.

Basic Tree before Scale	
SCORE TYPE	SCORE
CV_Score_AVG	0.760745
CV_Score_STD	0.008799
Train_Score	1
Test_Score	0.766852
Precision	0.633094
Recall	0.670476
F1_Score	0.651249
ROC_AUC_SCORE	0.741832
Runtime	0.104009

Basic Tree After Scale	
SCORE TYPE	SCORE
CV_Score_AVG	0.759831
CV_Score_STD	0.008449
Train_Score	1
Test_Score	0.765615
Precision	0.630824
Recall	0.670476
F1_Score	0.650046
ROC_AUC_SCORE	0.740916
Runtime	0.104674

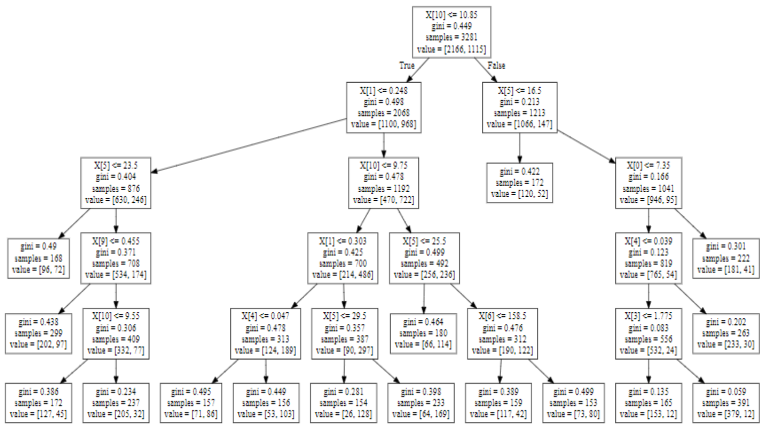


Scaling does not help. Does it mean Decision Tree does not care about training data scale?

2.1.2 Pruning

This tree before pruning is obviously overfitting the data. Here I used grid search to find the 'best parameters'. The parameters to be used are {'max_depth': 5, 'min_samples_leaf': 150}. Here is the result after pruning the tree using these parameters.

After Pruning	
SCORE TYPE	SCORE
CV_Score_AVG	0.745815
CV_Score_STD	0.014814
Train_Score	0.759829
Test_Score	0.742733
Precision	0.607495
Recall	0.586667
F1_Score	0.596899
ROC_AUC_SCORE	0.702216
Runtime	0.039439

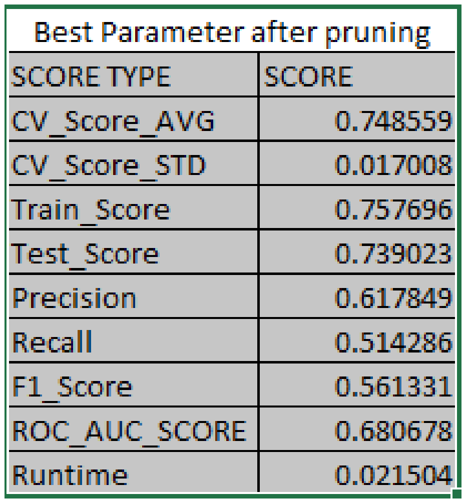

X[10] <= 10.85 gini = 0.449 samples = 3281 value = [2166, 1115]
True
False
X[1] <= 0.248 gini = 0.498 samples = 2068 value = [1100, 968]
X[5] <= 16.5 gini = 0.213 samples = 1213 value = [1066, 147]
X[5] <= 23.5 gini = 0.404 samples = 876 value = [630, 246]
X[10] <= 9.75 gini = 0.478 samples = 1192 value = [470, 722]
gini = 0.422 samples = 172 value = [120, 52]
X[0] <= 7.35 gini = 0.166 samples = 1041 value = [946, 95]
gini = 0.49 samples = 168 value = [96, 72]
X[9] <= 0.455 gini = 0.371 samples = 708 value = [534, 174]
X[1] <= 0.303 gini = 0.425 samples = 700 value = [214, 486]
X[5] <= 25.5 gini = 0.499 samples = 492 value = [256, 236]
X[4] <= 0.039 gini = 0.123 samples = 819 value = [765, 54]
gini = 0.301 samples = 222 value = [181, 41]
gini = 0.438 samples = 299 value = [202, 97]
X[10] <= 9.55 gini = 0.306 samples = 409 value = [332, 77]
X[4] <= 0.047 gini = 0.478 samples = 313 value = [124, 189]
X[5] <= 29.5 gini = 0.357 samples = 387 value = [90, 297]
gini = 0.464 samples = 180 value = [66, 114]
X[6] <= 158.5 gini = 0.476 samples = 312 value = [190, 122]
X[3] <= 1.775 gini = 0.083 samples = 556 value = [532, 24]
gini = 0.202 samples = 263 value = [233, 30]
gini = 0.386 samples = 172 value = [127, 45]
gini = 0.234 samples = 237 value = [205, 32]
gini = 0.495 samples = 157 value = [71, 86]
gini = 0.449 samples = 156 value = [53, 103]
gini = 0.281 samples = 154 value = [26, 128]
gini = 0.398 samples = 233 value = [64, 169]
gini = 0.389 samples = 159 value = [117, 42]
gini = 0.499 samples = 153 value = [73, 80]
gini = 0.135 samples = 165 value = [153, 12]
gini = 0.059 samples = 391 value = [379, 12]

Pruning decreases the variance issue of the model but does not improve the accuracy.

2.1.3 Feature Selection

The decision tree ranks the importance of the features as listed below. The features with importance weights less than 0.03 are eliminated and the tree was built again. As the results shown below.

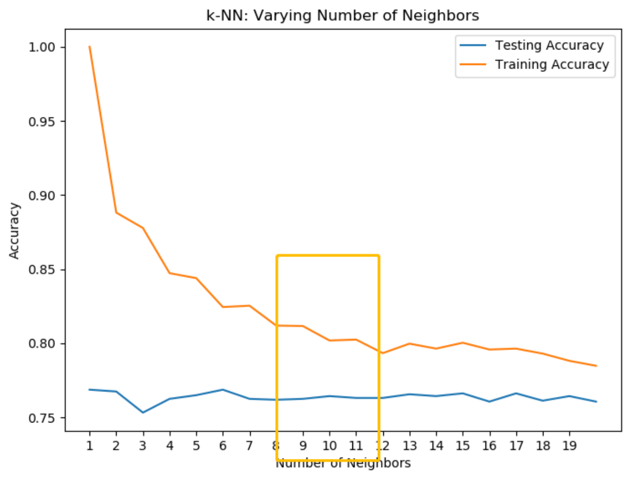
Feature	Importance
alcohol	0.543606
volatile acidity	0.294541
free sulfur dioxide	0.095869
total sulfur dioxide	0.026539
sulphates	0.016281
fixed acidity	0.012524
chlorides	0.009598
residual sugar	0.001043
citric acid	0
density 0	0
pH 0	0



Best Parameter after pruning	
SCORE TYPE	SCORE
CV_Score_AVG	0.748559
CV_Score_STD	0.017008
Train_Score	0.757696
Test_Score	0.739023
Precision	0.617849
Recall	0.514286
F1_Score	0.561331
ROC_AUC_SCORE	0.680678
Runtime	0.021504

2.2.1 K-NN

As 1.2.1 and 1.2.2 implies, finding best k value for K-NN algorithm is critical so here is the correlation of the accuracy and values of k. It shows that when k = 10, the bias and variance are balanced. The 10-NN model performs better than decision tree, both on training and testing accuracies.

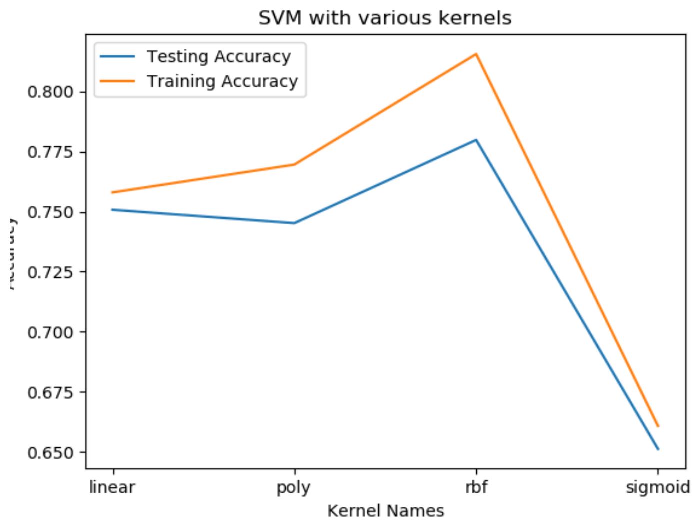


10-NN	
SCORE TYPE	SCORE
CV_Score_AVG	0.769279
CV_Score_STD	0.011408
Train_Score	0.80189
Test_Score	0.764378
Precision	0.68
Recall	0.518095
F1_Score	0.588108
ROC_AUC_SCORE	0.70044
Runtime	0.62492

2.3.1 Support Vector Machine, kernels

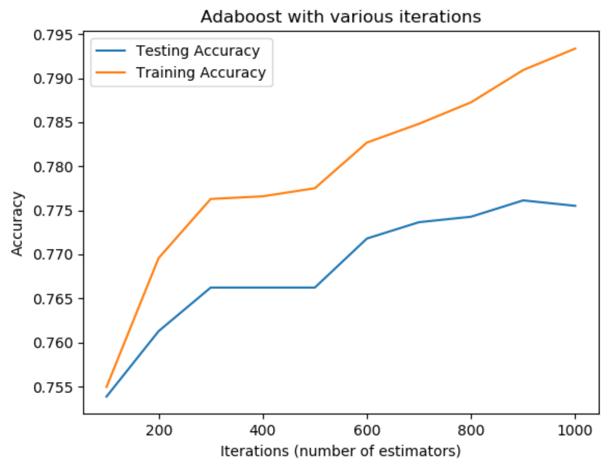
The left chart suggests that Gaussian kernel fits the best. The svm model with Gaussian kernel is by far the strongest predictive model for wine data.

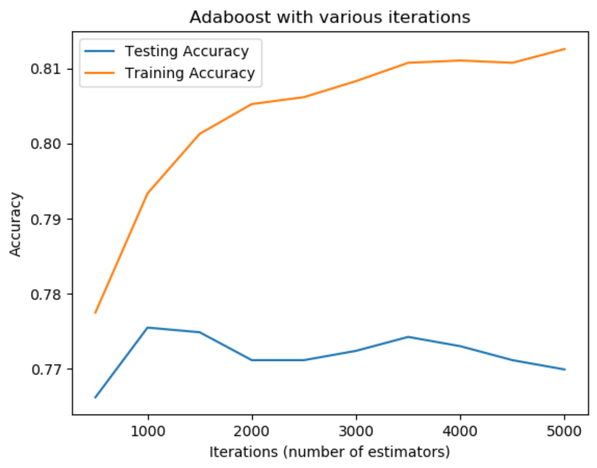
SVM with Gaussian kernel	
SCORE TYPE	SCORE
CV_Score_AVG	0.783605
CV_Score_STD	0.007524
Train_Score	0.815605
Test_Score	0.779839
Precision	0.683297
Recall	0.6
F1_Score	0.638945
ROC_AUC_SCORE	0.73315
Runtime	1.660538



2.4.1 Boosting (Adaboost) version of the decision tree

First, find the best number of iterations. From the charts, 900 seems to be a fair iteration. The result of adaboosted tree with iteration = 900 and learning rate = 0.05 is shown in the table. The ensembled model does not outperform svm with Gaussian kernel. Still, it shows that overfitting comes with excessive iterations.

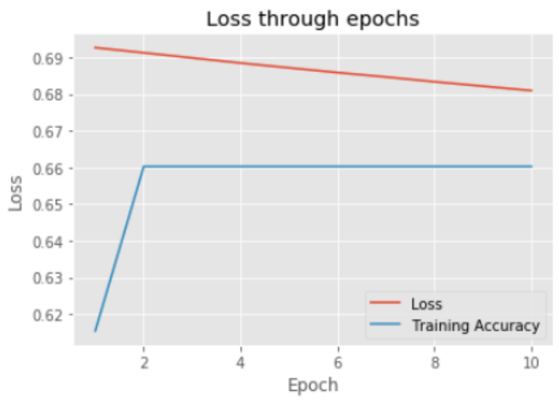




Adaboosted tree with 900 iterations and learning rate of 0.05	
SCORE TYPE	SCORE
CV_Score_AVG	0.765324
CV_Score_STD	0.024624
Train_Score	0.790917
Test_Score	0.776129
Precision	0.670146
Recall	0.611429
F1_Score	0.639442
ROC_AUC_SCORE	0.73337
Runtime	16.246744

2.5.1 Neural Network

Similar with HR turnover problem, the result of the neural network is the same here, although the value of loss and accuracy are not exactly the same, but they follow the similar pattern: decreasing loss does not improve the model accuracy.



Part 3 Conclusion

5 models, each for 2 datasets, were implemented in this assignment. Here are my conclusions:

1. Data size is critical for machine learning;
2. Use Cross Validation as possible as I can;
3. Adaboost is a great version of ensemble learning;
4. Data does not have to be scaled for KNN;
5. KNN is computation consuming;
6. Gaussian kernel is robust for these two problems;
7. Decision Tree is very expressive, readable and intuitive;
8. Decision Tree helps on feature selection;
9. Data preprocessing is important;
10. Neural networks are worth exploring more