Supervised Learning

Spring 2021 CS7641 Assignment 1

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# Abstrct

This paper aims to apply different machine learning algorithms, including decision trees, boosting, k-nearest neighbors, support vector machines and neural networks on two different datasets. The prediction performance, optimization steps and efficiency of each algorithms are compared and analyzed in this paper.

# 1 Introduction

Before diving into the results, the information of two selected interesting datasets and the preprocess applied on them will be introduced first. Then the steps of implementation and optimization on all five machine algorithms will be illustrated. Finally, the prediction results and the required time in training and prediction for each algorithm are summarized, comparing which algorithm offers the best performance in terms of speed or accuracy in these two datasets.

## Dataset selection and preprocess

The first dataset I selected is phishing website[1], if the browsing webpage is suspicious or not. There are 11054 instances, 32 features and 2 classes in this dataset. The features include requestURL, redirecting, abnormalURL, popwindows,..etc. The output class is a binary result, 1 means the instance is a phishing website, 0 means not. For each feature, they have only 3 results, 0, +1 or -1. Therefore, this dataset is a typical classification problem and relatively easy to solve by some algorithms. For the second dataset, I tried to find the features which have continuous numbers so that I could tell if the algorithm works well on both discrete and continuous data. Besides, I also looked for the dataset which has more instances but fewer features, so that I could tell if the time complexity for training and prediction depends more on feature or instance size. Since a lot of my family members are suffering from the same disease, I decided to study the diabetes [2]. All the features, including age, times of pregnancy or BMI are continuous numbers, which is different from the first phishing dataset. The output is 0 or 1, showing the patent do/do not have diabetes. The instance size is 15000 and have only 10 features. By analyzing the running time for each algorithm, I expect to tell if the training/testing time depends more on feature/instance size.

For data preprocess, I first dropped all the instance having NA, and meaningless column (e.g., patient ID, index). Each column was normalized, rescale the numbers to be ranging from 0 and 1. Then I splitted 80% dataset into training set and saved 20% for testing. The training set is used for classifier building and validation, and the testing set is only used for verifying the scores obtained by each optimized classifier in the end.

## Algorithm optimization process

For each algorithm, I first used the default arguments for initial tests. Then the gridSearchCV method in sklearn with cross-validation of 5 is used for optimizing multiple parameters simultaneously. The cross-validation is to make sure classifiers do not overfit into specific datasets. After the “nearly-optimized” classifier is built from gridSearchCV method, then the validation curve method is applied for further optimizing on one argument. The f1\_weighted and cv = 5 were selected in validation curve method, the parameters which have the highest score in validation will be chosen as the best classifier.

## Score and execution time comparison between algorithms

After the models with optimized parameters are built, then the prediction accuracy in validation and testing sets is calculated using f1\_score method with weighted average. Compare with the case using recall or precision, f1 score is a better way to determine the model prediction accuracy for even imbalanced datasets [3]. The time for training/testing is also recorded, so that we could finally compare the performance for each algorithm in terms of accuracy and efficiency.

# Implementation and optimization on algorithms

## Decision Trees

For Decision Trees (DT), the pruning action could reduce the size of tree and mitigate the overfitting issue [4]. Therefore, ccp\_alpa, the complexity parameter used for Minimal Cost-Complexity Pruning is the parameter could strongly affect the performance of the classifier [5]. Before fine tune on the cpp\_alpha parameter, the gridSearchCV is applied to find the best other parameters including criterion and splitter for both datasets. I found that for both datasets, gini and entropy (information gain) do not affect too much on the accuracy, so does the splitter method. The returned best estimator showed that gini index with best splitter offers the best scores in both datasets, and the ccp\_alpha plays an important rule in the final f1 scores. While the ccp\_alpha value is 0, no pruning is performed, means the model is too specific for training sets. In the figure 1.a and 1.c, we could clearly see that the accuracy on training is 100% as the ccp\_alpha is 0, however, the performance for the validation is really bad. As the alpha increases, the overfitting is released and the training accuracy becomes lower (red), but the validation scores increase because the model becomes more generalized. As the alpha becomes too high, meaning pruning is too aggressive, then both training and validation score are expected to be lower and lower.

After using gridSearchCV and finely searchgin alpha, the optimized parameters for Decision Trees classification for both datasets are shown in below table, and the learning curves for training/validation sets are plotted in Figure 1.b and 1.d.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Diabetes | | | | Phishing | | | |
| criterion | splitter | ccp\_alpha | F1 score | criterion | splitter | ccp\_alpha | F1 score |
| gini | best | 0.0003 | 0.92 | gini | best | 0.0001 | 0.963 |

Chart

Description automatically generated

1. The accuracy under variant ccp\_alpha value for (a) diabetes and (c) phishing datasets. The calculated accuracy using the optimized parameters for Decision Trees classifier are shown in (b) and (d) for diabetes and phishing, respectively.

## Boosting

The idea of boosting is an ensemble technique in creating a strong classifier from a mount of weak classifiers [6]. In this assignment, AdaBoost was implemented [6]. By following the same procedure mentioned in decision tree, gridSearchCV was first applied to find the best parameters for weak classifier. The best parameters of the decision trees are with splitter of best and max\_depth of 1, act as the stumps instead of huge trees. One of the important parameters for AdaBoost classifier is the n\_estimator, which means the numers of models to iteratively train. In Figure 2.a and 2.d, the validation scores are really low for both datasets as the n\_estimators are lower than 10, means the number of estimators is insufficient for making right decision from voting. As n\_estimators get higher, the accuracy increases and then get saturated, demonstrates the fact that after a specific point of n\_estimator, accuracy will be converged. Another important parameter is learning rate, which shrinks the contribution of each classifier [6]. The performance from default (=1) works pretty well, and the performance will decrease a lot while learning rate is larger than 2, where the model got trained too fast for worse accuracy. The final performances of the optimized AdaBoost classifier are shown in Figure 2.c and 2.f. As we could see, from the learning curve, the scores increase dramatically as the size is larger, means that the adaBoost classifier needs sufficient data size for making good training. The final scores of validation sets for both datasets are high with low biases and perform better than a single Decision Tree shown before. This observation is expected because we know that the AdaBoost is not prone to overfit compared with DT in theory [7], therefore, better scores in “testing” could be expected as well which will be discussed in section 3.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Diabetes | | | | Phishing | | | |
| criterion | n\_estimator | Learning rate | F1 score | criterion | n\_estimator | Learning rate | F1 score |
| entropy | 225 | 1.1 | 0.96 | gini | 75 | 1.0 | 0.971 |

Graphical user interface

Description automatically generated

***Figure 2*** - The accuracy under variant n\_estimator for (a) diabetes and (d) phishing datasets. The accuracy under variant learning\_rate for (b) diabetes and (e) phishing datasets. The accuracy using the optimized parameters AdaBoost classifier are shown in (c) and (f) for diabetes and phishing, respectively.

## k-Nearest Neighbors

For k-Nearest Neighbors (KNN), the most important parameter is for sure the number of neighbors. Besides, I also have interest on the weight function used in prediction, either uniform, meaning all points in each neighborhood are weighted equally, or distance, while the weight points by the inverse of their distance. In figure 3.a and 3.d, the plots show the influence of neighbor numbers using uniform weight. For diabetes, the training score is high and validation score is low as the k = 1, showing the fact that the model has high variance due to overfitting issue. As the k increases, the scores from training and validation start converging, means the variance is getting reduced, however the bias becomes higher. For the case of phishing the validation scores the highest for k – 1, indicating that this dataset might have a lot of repeated instance making the weights strongly biased. As the k increases, the same trend seen in diabetes occurs, the variance decreases while the bias increases.

As taking the *distance* was used in weights shown in Figure 3.b and 3.e, the training sets are almost independent of neighbor numbers, both datasets shows similar results, that the models are overfitted because the centered points has more power on making decision than its neighbors, making the model exhibiting high variance, which could be observed from the difference between training and validation. The learning curves using the optimized parameters for KNN are plotted in Figure 3.c and 3.f for both datasets, and we could find that comparing with other classifier, KNN tends to have larger bias and larger variance. The details of comparison will be demonstrated in following sections.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Diabetes | | | | Phishing | | | |
| weights | leaf\_size | neighbors | F1 score | weights | leaf\_size | neighbors | F1 score |
| uniform | 30 | 5 | 0.877 | uniform | 30 | 1 | 0.951 |
| distance | 30 | 10 | 0.878 | distance | 30 | 10 | 0.954 |

Graphical user interface, chart, line chart

Description automatically generated

***Figure 3*** - The scores under different number of neighbors using *uniform* for (a) diabetes and (d) phishing datasets. The scores under different number of neighbors using *distance* for (b) diabetes and (e) phishing datasets are also shown. The learning curve of KNN classifier with optimized parameters are shown in (c) and (f) for diabetes and phishing.

## Support Vector Machines

SVM creates virtual planes to separate classes using different Kernel functions [8], therefore, the most interest parameter will be the Kernel selected in algorithm. Linear, polynomial (poly), Radia Basis Fuction(rbf) and sigmoid are the Kernel tested. Besides, the regularization parameter (C) and Kernel coefficient (gamma) control the regulation also affect strongly on the performance of the classifier. I used the same strategy for narrowing down the searching range using gridSearchCV first, found rbf and poly Kernal works the best in my datasets. Then optimize C and gamma for rbf and poly Kernel respectively, also searched for the best degree. In Figure 4.a and 4.d, the performance using rbf Kernel with optimized C and gamma performed pretty well in both datasets. As the size increases, both variance and bias decreases. For poly Kernel, the degree of polynomial was optimized in Figure 4.b and 4.e for both datasets. In both cases, the biases are high and variances are low at low degree. And as the degree increases, scores of training set keep increasing, but the validation goes down after the minimum degree, means the model becomes overfitting to training set due to resulting in high variance.

Compared with the results obtained from poly and rbf Kernel, we could see in both cases, rbf Kernel works better than the poly Kernels especially for diabetes cases. It implies that the polynomial Kernel might work well for discrete data type, but not the continuous numbers like BMI, age features included in the diabetes dataset. The learning curves are plotted in Figure 4.c and 4.f with the optimized degree, Kernel, gamma and C in SVM classifier. The accuracy is not that different compared to the results analyzed in previous section, but the required time for optimizing the parameters do take longer than the algorithm listed before. The details about the required time for training/query will be discussed in details in later section.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Diabetes | | | | Phishing | | | |
| Kernel | C | gamma | F1 score | Kernel | C | gamma | F1 score |
| rbf | 17.5 | 1.875 | 0.901 | rbf | 10 | 0.3333 | 0.965 |
| Poly – 4 degree | 4 | 1.875 | 0.865 | Poly – 5 degree | 1 | 0.3333 | 0.962 |

Chart, line chart

Description automatically generated

***Figure 4*** - The accuracy using the optimized *rbf* Kernel for (a) diabetes and (d) phishing datasets. The accuracy under variant degree of *poly* Kernel for (b) diabetes and (e) phishing datasets are also shown. The accuracy using the optimized parameters of SVM classifier are shown in (c) and (f) for diabetes and phishing, respectively.

## Neural Networks

Neural Networks performs backpropagation method for optimizing the weight of neuron and the bias [9]. The most interesting parameters to be tuned in Neural Network are the hidden layer size, representing the number of neurons in ith layer, the penalty parameter alpha, activation function and learning rate for weight updats. Again there are too many parameters to be optimized, therefore, the gridSearchCV again used first for narrowing down the range of each parameters. The activation function as relu and the learning\_rate as constant are found to be the best in both cases. Also, the hidden layer size of (250, 500). During the gridSearchCV scan, I found that the larger the neuron size in hidden layer, more time is required for training for each weight. And a larger size of (300, 600) was not selected, demonstrating the fact that more hidden layer size will cause overfitting and increase the bias in validation sets.

The finer scan of penalty parameter alpha is shown in Figure 5.a and 5.c. The small number of alpha could help lowering both bias and variance for validation sets, however, it increase the bias for both training and validation sets dramatically. So the number of alpha has to be carefully tuned. The final results using the optimized Neural Network classifier are shown in Figure 5.b and 5.d, showing low bias for both datasets. And we could clearly see the validation scores is highly depends on the percentage of instance used, more data helps achieving better performance in learning curve

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Diabetes | | | | Phishing | | | |
| Hidden layer | Activation function | Alpha | F1 score | Hidden layer | Activation function | Alpha | F1 score |
| (250, 500) | relu | 0.5 | 0.93 | (250, 500) | relu | 0.005 | 0.963 |

Chart, line chart

Description automatically generated

***Figure 5*** - The accuracy under variant alpah for (a) diabetes and (c) phishing datasets. The accuracy using the optimized parameters Neural Network classifier are shown in (c) and (f) for diabetes and phishing, respectively.

# Comparison

## 3.1 Accuracy

Figure 7 show the calculated accuracy from training set and testing sets for each algorithm in both data sets. From Figure 7.a, most of classifiers work well for diabetes datasets besides KNN, the only one which has lower accuracy in both training and testing sets. However, in phishing datasets, KNN works pretty well and comparable with other algorithms. The main difference between two datasets is the type of features, which is continuous for diabetes and discrete for phishing. While the feature type is continuous, KNN may perform worse than other algorithms. For all algorithm in both datasets, the difference of scores between training and testing are close, this low variance means the built models are generalized. And the prediction accuracy on testing sets are mostly above 90%, demonstrates the fact that the bias for the models are low. Among all algorithms, AdaBoost works the best in both continuous and discrete datasets, and KNN is the one with the worst accuracy. DT also works well for phishing dataset but not diabetes, demonstrating the fact that continuous feature type might degrade the performance from DT. NN is stable, and SVM is highly depends on the Kernel select

Chart, bar chart

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***Figure 6*** - The scores calculated from training (blue) and testing sets (orange) for (a) diabetes and (b) phishing datasets.

## 3.2 Time

The required time for training and testing for each classifier are summarized in Figure 7.a (diabetes) and 7.b (phishing). KNN is the only algorithm which needs longer testing time than training time, because there’s barely needs for training in KNN model, and the testing time is highly depends on the selected neighbors, more neighbor means better accuracy, but sacrifice the time. The most time-consuming model to train from my tests is the Neural Networks, and I think the reason is that (250, 500) hidden layers were chosen for better accuracy. If the number of layers could be reduced, for sure the time could be reduced a lot, but the calculated biases and weights might not be that accurate if the “neurons” are not enough. Good news for Neural Networks is, testing time is way faster than training time and also faster compared with other algorithms. Decision trees is the algorithm works really efficient in both training and testing, because there’s only one tree got built and just one pass for each test set. The accuracy is still above average from the previous accuracy tests, but the performance of decision tree might not be that good for more complexity datasets. The required time of training and testing for AdaBoost algorithm are highly depends on the n\_estimator settings. I found that the time required for training takes really long while the n\_estimator parameter was set too high. Therefore, same optimization work for AdaBoost is to find a balance between accuracy and efficiency.

Chart, bar chart

Description automatically generated***Figure 7*** - The time required for performing training (blue) and testing (orange) for (a) diabetes and (b) phishing datasets, the time in y axis is shown in log scale.

# References

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