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Project Report

Executive Summary

This project aims at the experimentation of 2 important machine learning algorithms – Artificial Neural Networks (ANN) and K-Nearest Neighbours (KNN). Though both the algorithms can be used for Regression and Classification, various control parameters are experimented from a Classification perspective. Some of the control parameters that are studied are: *type of activation functions, No. of hidden layers and no. of nodes in each hidden layer, training size, type of algorithm for KNN, various distance metrics for KNN* etc

Datasets

Dataset 1 – Sgemm_data

- Dataset consists of 241600 observations on 15 variables.
- The description of the variables can be found out by going to the dataset link.
- The dependent variable for the linear regression model is Avgcnt(y): Average GPU run time.
- None of the column contains any missing value, so no missing value imputation is required.

The features – 'Run 1', 'Run 2', and 'Run 3' and 'Run 4 are dropped as the average of these four parameters are calculated and used as target variable

Dataset 2 – Audit data

The second dataset I have chosen is an Audit dataset from Kaggle. The Audit risk dataset consists of data of various firms and their risk factors. They belong to a multitude of sectors ranging from Irrigation, Public Health, Animal Husbandry to Fisheries, Tourism, Science and Technology. This dataset is developed by a 3rd party Audit company that wishes to calculate and assess 'Risk' by analysing the present and historical risk factors thereby facilitating the audit-planning process. The dataset has over 18 columns, with one 'target' variable – 'Risk' (binary).

The primary reason I found this dataset interesting is because I have a strong interest in fraud detection. Initial EDA is performed and columns 'TOTAL', 'Score' and 'LOCATION_ID' are dropped because of redundancy in information and 'Money_Value' feature is imputed with the mean value as it has an unusual number of zeroes. The problem statement is to predict if a firm is under 'Risk' or not.

Tasks – Task 1 – Artificial Neural Networks (ANN)

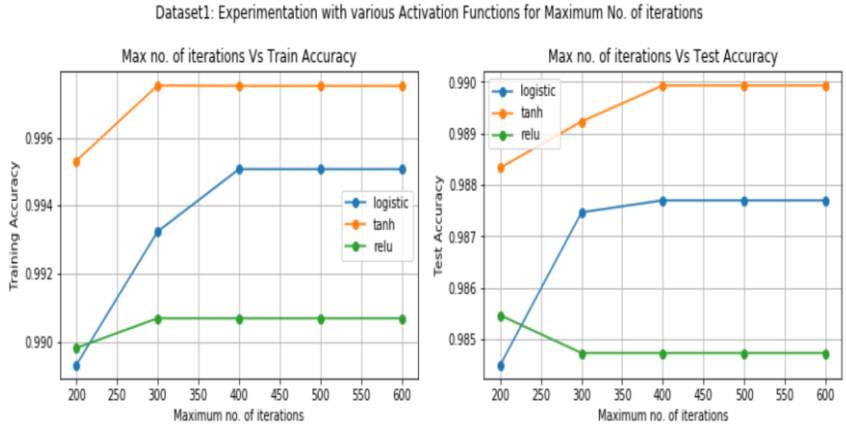
This algorithm is implemented using 'MLPClassifier' package from 'scikit-learn' library. I have performed 3 experiments on ANN. I have considered 3 activation functions – 'tanh','relu' and 'logistic'. Even, the most complicated data distribution can yield good results for the above functions.

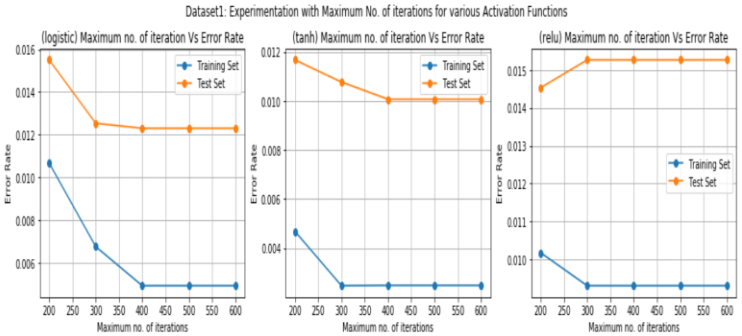
Experiment 1.1 – Experimentation with ' activation functions ' for various values of ' Max iterations '

'Max iterations' parameter determines the maximum number of epochs an ANN model has to run, in order to achieve convergence. The model that has achieved convergence will produce the best results on the test set. Default value of 'max iterations' is 200. I have experimented in the range of 200-600

with 3 activation functions as already mentioned. The best activation function and 'max iterations' value is reported for each dataset at the conclusion of the experiment.

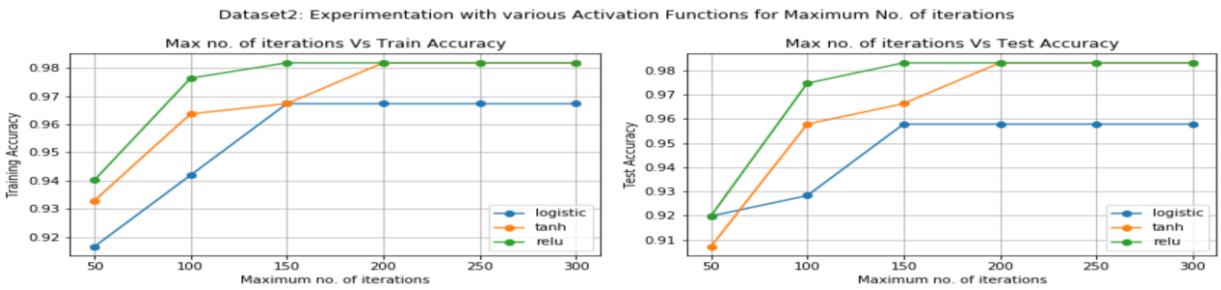
Dataset 1 – From the below plots, it can be inferred that 'tanh' activation function produces the maximum test accuracy for 'maximum no. of iterations' = 600. We can expect the test accuracy to increase with increase in the control parameter, but the test accuracy almost saturates for values above 450. The classification metrics are reported for the best model ('tanh' function, 600 max iterations)

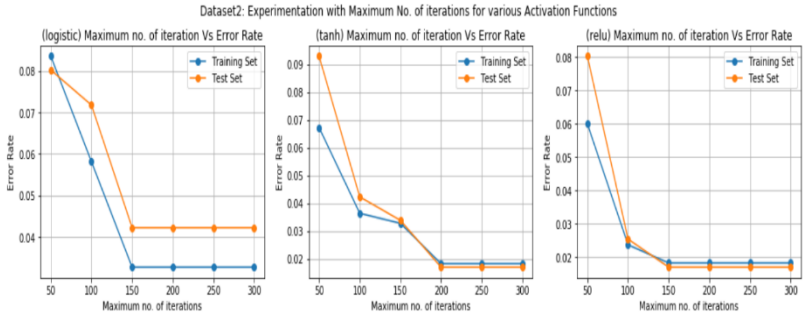




Metrics	Values
Accuracy	0.9899
Recall	0.9928
Precision	0.9929
F1 Score	0.9928

Dataset 2 – The 'relu' function records the best test accuracy of 98.31% for 'max no. of iterations' = 150. 'tanh' function also performs similar to 'relu' at the 150 iterations, but it is inferred that 'relu' is better because it records a higher test accuracy for almost all values of the control parameter when compared with 'tanh'. It can be seen that the model achieves convergence at 150 iterations as both training & test accuracy values are flat for values>150. Hence, we fix 150 as the optimal value for 'max no. of iterations' control parameter. The classification metrics are reported for the best model ('relu', 150 iterations).



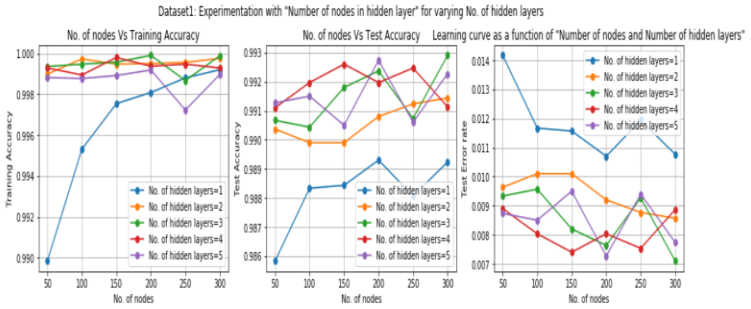


Metrics	Values
Accuracy	0.9831
Recall	0.978
Precision	0.978
F1 Score	0.978

Experiment 1.2 – Experimentation with ' Hidden layer size' and 'Number of nodes ' control parameter

The primary challenge of implementing an ANN model is to find the best values for 'No. of Hidden layers' and 'No. of nodes in each layer' that reports the best test accuracy. This can be done by using Grid search hyper-parameter optimization, which is not implemented for the entire parameter space, but implemented in a specific range of 1-5 hidden layers and 200 - 600 nodes for each hidden layer considering computational expenses and complexity. The models obtained in Experiment 1.1 are used for further experimentation. (Dataset 1 -'tanh' activation function, Dataset 2 -'relu' activation function)

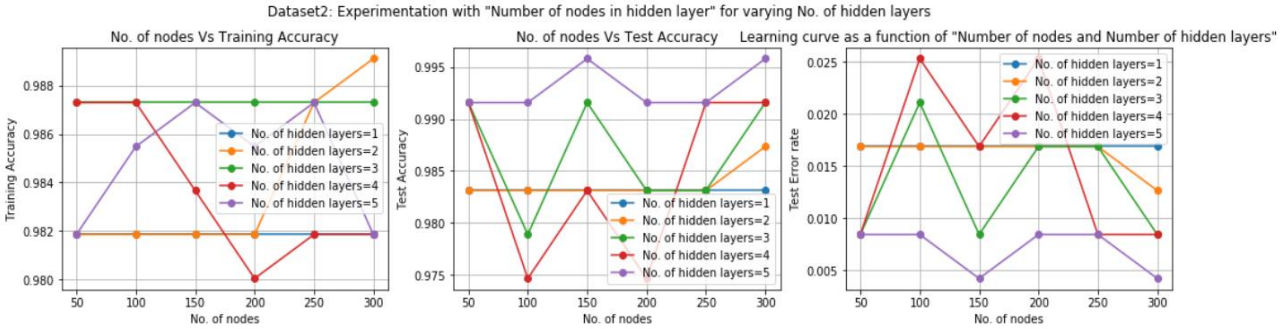
Dataset 1 – The below plots record the test error rates for various 'hidden layer size' and 'no. of nodes' in each hidden layer. The lowest test error rate of 0.7% is recorded for 3 hidden layers and 300 nodes for each hidden layer. This corresponds to a neural net model with 1 input layer, 3 hidden layers with 300 nodes each and 1 output layer. This model is slightly better than the one obtained in Expt 1.1.



Metrics	Values
Accuracy	0.992
Recall	0.9949
Precision	0.9937
F1 Score	0.9943

Dataset 2 – The best test accuracy of 99.58% is recorded for a model with 5 hidden layers and 300 nodes. This corresponds to a neural net model with 1 input layer, 5 hidden layers with 300 nodes each and 1 output layer. The 'precision' metric is 100% which tells us that all the values that were predicted by the model as positive are indeed positive actually. This model is better than the one obtained in experiment 1.1 and has a very high test accuracy equalling almost 100%

Metrics	Values
Accuracy	0.9958
Recall	0.989
Precision	1.0
F1 Score	0.9945

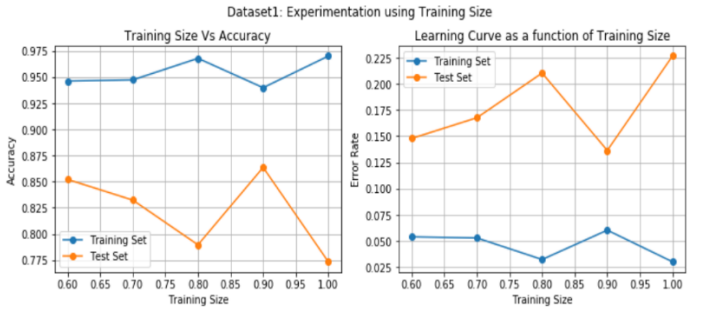


From the above plots, it can be inferred that there is no definite relationship between 'test accuracy' and 'hidden layer size'. As the No. of nodes increase, we don't see any discernible trend in test accuracy curve.

Experiment 1.3 – Experimentation using 'Training Size' parameter

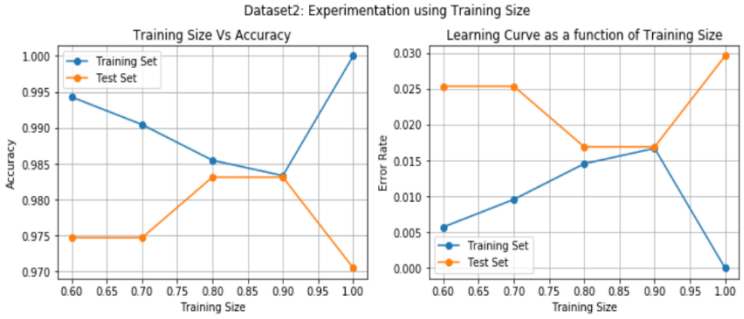
In this experiment, the control parameter is the training size. This experiment is performed to understand the relationship between Training set size and train/test error rates. The best model that is obtained until now is used for further experimentation here

Dataset 1 – From the below plots, it can be inferred that for a training size of 90% of total training set, the best test accuracy of 86.35% is reported. The classification metrics for the best model is reported below. There is a fluctuating trend in test accuracy for varying training set sizes.



Metrics	Values
Accuracy	0.8635
Recall	0.8964
Precision	0.8565
F1 Score	0.876

Dataset 2 – The lowest test error rate of 1.69% is recorded for a training set size of 90% of total training set. Here again, the trend of test error rate is fluctuating and non-linear with respect to training set size.



Metrics	Values
Accuracy	0.9831
Recall	0.978
Precision	0.978
F1 Score	0.978

The key takeaway from this experiment is that training set size and test accuracy have no definite relationship. It is wrong to infer that, with more tranining data, we can produce a better model which would generalize better in the presence of new data. It can be inferred that the distribution of data is of primary importance when a model is trying to learn using a specific machine learning algorithm. Though we don't really have a control over the nature of the data we collect, we can address this aspect by performing K-fold cross validation which will give the best subset of data that produces the best test accuracy. 5-fold cross validation is implemented as a separate experiment for both the algorithms and both the datasets after the experimentation for KNN.

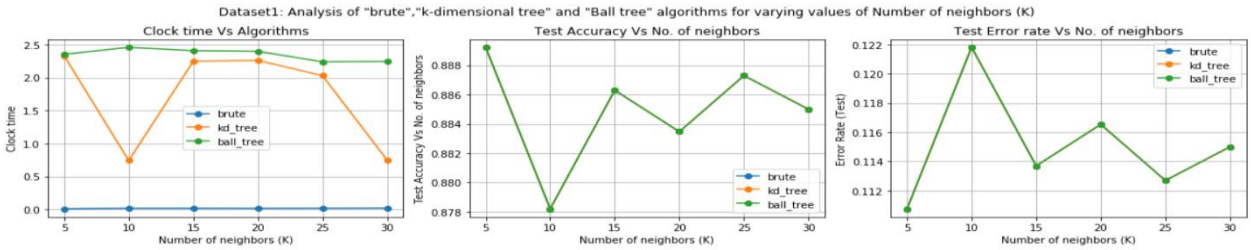
Tasks – Task 2 – K Nearest Neighbours (KNN)

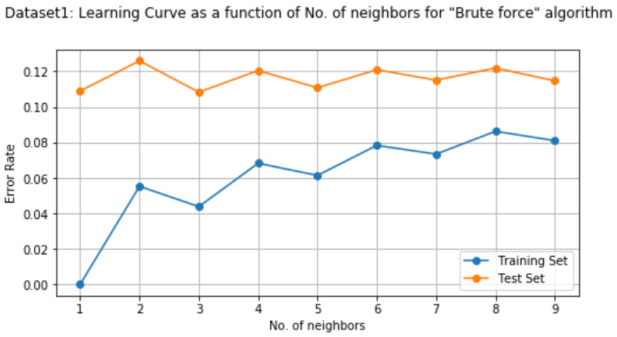
This supervised learning algorithm is implemented using 'KNeighborsClassifier' package from scikit-learn library. I have performed 3 experiments involving control parameters - *algorithm* used to compute nearest neighbors, *distance metric*, *training set size* and *No. of nearest neighbors (k).*

Experiment 2.1 – Experimentation with type of 'algorithm' used as a function of No. of neighbors (k)

The 'No. of neighbors' control parameter denotes the number of neighbors that are to be clustered together as similar. The 'algorithm' that does this function can be 'brute-force', kd_tree' and 'ball_tree'. Brute force involves calculation of distances between 2 points for all the data space. K-d tree involves indexing the data by creating trees which are easier to traverse for finding similarity. Ball-tree is also an indexing algorithm wherein data is visualized as hyperspheres in a binary tree. All the tree algorithms perform similarly with a difference only in time taken. The tree algorithms are faster for higher dimensions. Clock time is also projected to understand the fastest working algorithm for each dataset.

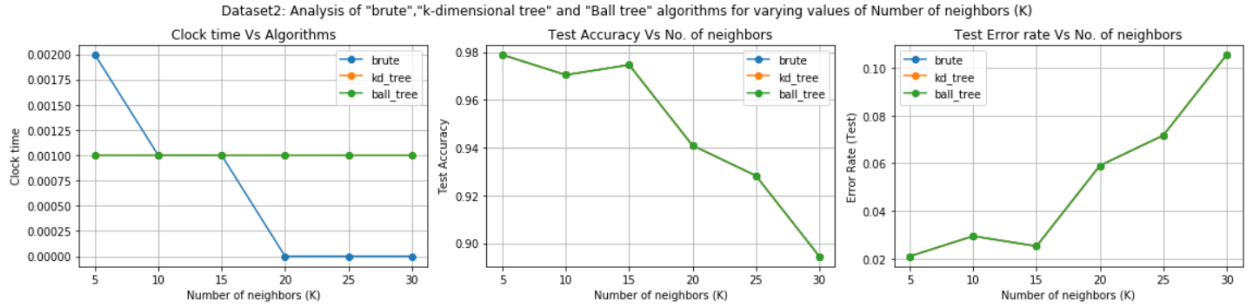
Dataset 1 – It can be inferred from below plots that 'Brute-force' is the fastest algorithm outperforming others by taking very little time. As expected, all the algorithms record the same test accuracy for varying 'No. of neighbors' (k). The best model is the one with k=3 recording a test accuracy of 89.17%.

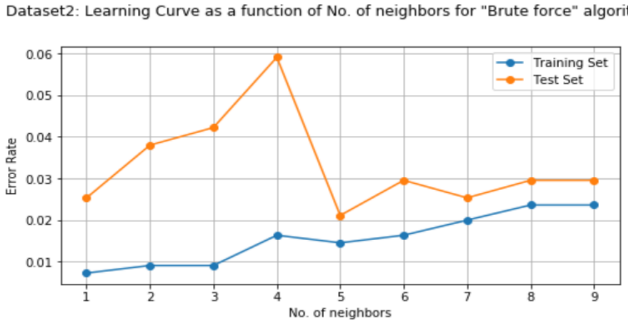




Metrics	Values
Accuracy	0.8917
Recall	0.9326
Precision	0.9151
F1 Score	0.9238

Dataset 2 – It is interesting to note that brute is faster compared to other tree algorithms in this dataset as well. This is primarily dependent on the 'No. of features'. The best model is in the range of k=5. The lowest error rate of 2.11% is reported for a value of k=5 as evidenced by the plots below.



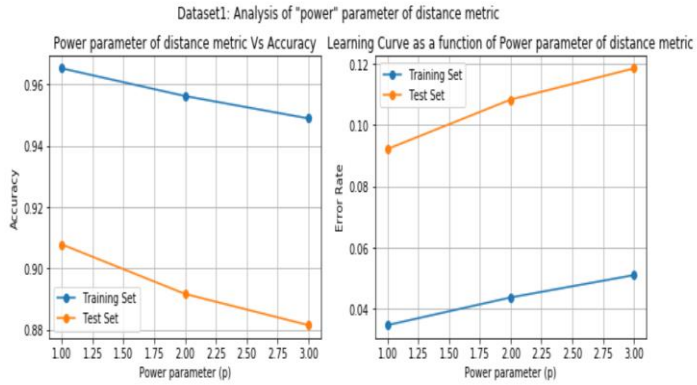


Metrics	Values
Accuracy	0.9789
Recall	0.989
Precision	0.9574
F1 Score	0.9729

Experiment 2.2 – Experimentation using distance metrics (Euclidean, Manhattan)

In this experiment, the control parameter is the distance metric. The power of the minkowski metric is varied in the range of 1 to 3 to correspond to various distance metrics such as Manhattan (power=1) and Euclidean (power=2). We try to find the best distance metric through this experiment for each dataset.

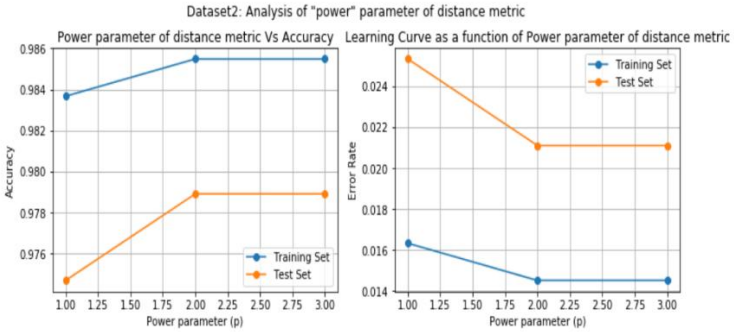
Dataset 1 – It can be inferred that though there isn't a significant difference in test accuracy for various metrics, the Manhattan distance(p=1) records the best test accuracy of 90.78%. It can be seen that accuracy decreases as the power of the distance metric (minkowski metric) increases.



Metrics	Values
Accuracy	0.9078
Recall	0.9463
Precision	0.9245
F1 Score	0.9353

Dataset 2 – For this dataset, it can be interpreted from the below plots that monkowski metric with power=2 and power=3 perform better than the Manhattan distance. We choose the Euclidean metric as the best distance metric with the lowest error rate of 2.11%. In this scenario, as power increases the accuracy decreases and becomes flat.

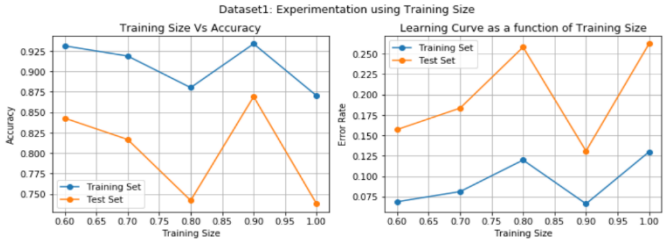
Metrics	Values
Accuracy	0.9789
Recall	0.989
Precision	0.9574
F1 Score	0.9729



Experiment 2.3 – Experimenting with Training Size

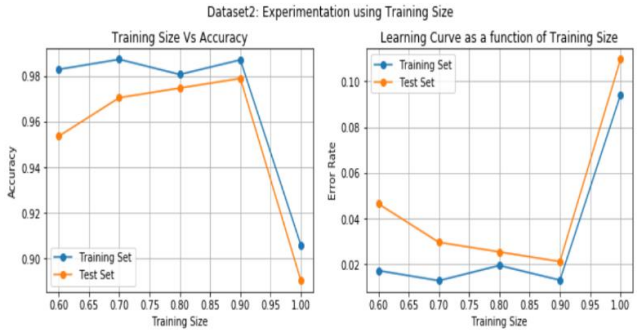
In this experiment, the control parameter is the training size. This experiment is performed to understand the relationship between Training set size and train/test error rates. The best model that is obtained until now is used for further experimentation here.

Dataset 1 - The best model is the one with a training size of 90% of the entire train set. Looking at the confusin matrix, the test accuracy is 86.91% with a Recall rate of 90.48%.



Metrics	Values
Accuracy	0.8691
Recall	0.9048
Precision	0.8592
F1 Score	0.8814

Dataset 2 – Here also, the best model is the one with traning size of 90% of original training set, the Test accuracy is peaking at 97.89%. As already interpreted, the distribution of data is the key point to consider. Based on the distribution of the data, the learnings can be different, and the model can perform differently on the test set.



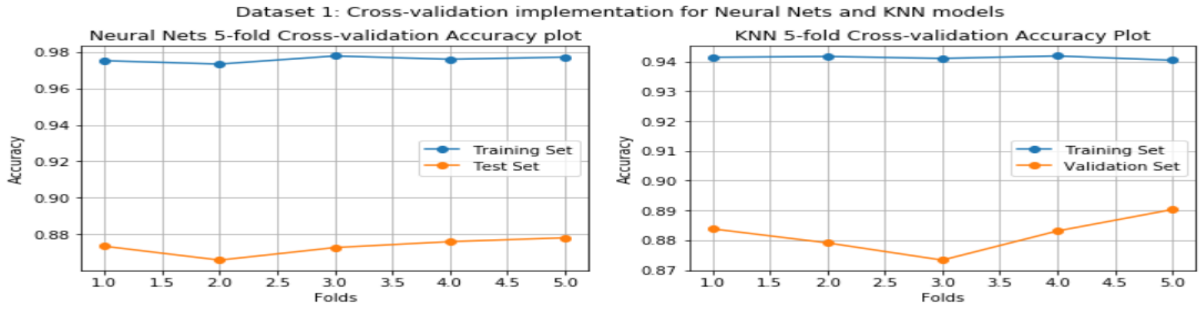
Metrics	Values
Accuracy	0.9789
Recall	0.989
Precision	0.9574
F1 Score	0.9729

Cross Validation Implementation

Cross validation is performed to mainly understand if we can obtain a subset of the training data that can generalize better than the entire training set taken into account. Such a subset can be used for future experimentation to yield better results compared to the conventional models built using the entire training set. In this experiment, 5-fold cross-validation is implemented for both datasets for both the algorithms – ANN and KNN to understand if cross-validation can help boost the test accuracy by giving us the best subset of data that generalizes the best on the test set.

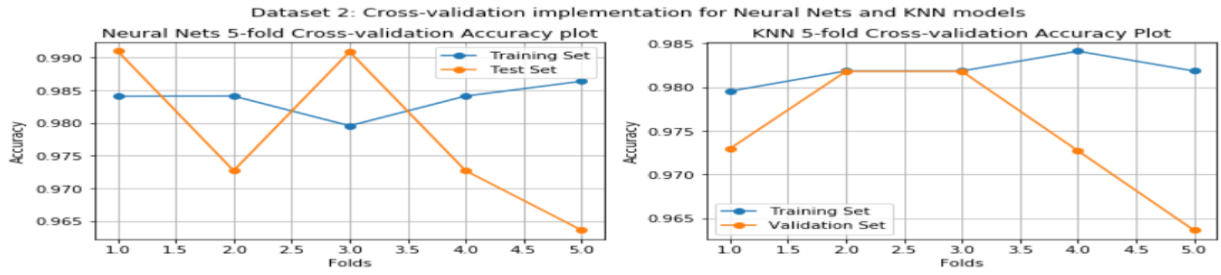
Dataset 1

- The model with entire training set records a test accuracy of 98% for ANN & 89% for KNN.
- In Cross-validation, for ANN, 5th fold records accuracy of 88% which is less than the base accuracy .
- For KNN, there isn't a significant improvisation in the test accuracy (flat at ~88%).



Dataset 2

- The model with entire training set records a test accuracy of 98.31% for ANN & 97.89% for KNN.
- In Cross-validation, for ANN, the 1st fold records a test accuracy of 99% which is considerably more than the base model's accuracy. The 3rd fold also records similar accuracy but yieds a poorer training accuracy. The 1st fold subset of data is a good candidate for future experimentation.
- For KNN, it is to be noted that the 2nd and 3rd folds record an accuracy of 98% which is a little more than the base accuracy, making them eligible for further experimentation for better models(results).



Conclusion / Discussion

Dataset 1 sgemm data

Rank	Algorithm	accuracy
1	ANN	98.99%
2	Boosted model decision tree	98.84%
3	Decision Tree	98.79%
4	SVM	96.91%
5	KNN	89.17%

Dataset 2: audit data

Rank	Algorithm	accuracy
1	**ANN**	**99.58%**
2	**SVM**	**99.16%**
3	**DecissionTree**	**98.31%**
4	**Boosted model decision tree**	**97.89%**
4	**KNN**	**97.89%**

The key takeaways are summarised below:

- Dataset 1 – Best model – Artificial Neural Network– 98.99% test accuracy

Based on the analysis of various algorithms for dataset 1, it can be concluded that Artificial Neural Network is the best algorithm within the scope of performed experimentation. Followed by boosted decision tree and decision tree model

- Dataset 2 – Best model – Artificial Neural Networks – 99.58% test accuracy

  For dataset 2, the experimentation with various algorithms has yielded that ANN is the best model with a stunning accuracy of almost 99.58%.
- Also, there is no "best" algorithm on a universal basis. It solely depends on the dataset, its size, distribution, variance etc. From my perspective, the "best" algorithm would have optimal training accuracy and the best testing accuracy. The "best" model never occurs by chance, it must be worked upon incessantly. Extensive pre-processing, visualization and proper tuning using hyperparameters of the built model is mandatory for to get the "best model".
- Overall, ANN performed better than KNN for both data set.