1. Datasets

I wanted to explore the differences between a medium-sized dataset and a large dataset when implementing the various machine learning algorithms. Both datasets were discovered in the UCI Machine Learning Repository [1].

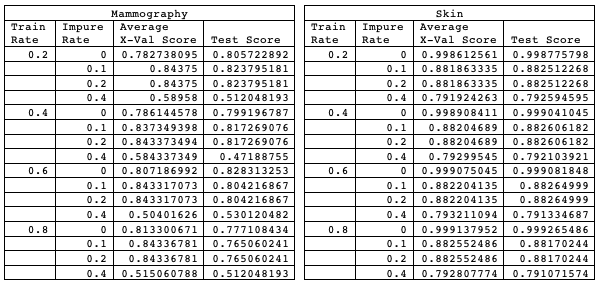
The first one chosen is based off of mammography data that is used to identify whether a tumour is malignant or benign [2]. This dataset had 6 attributes with a binary output and consisted of 961 samples. I chose this dataset because of my interest in healthcare and because I believe the application of machine learning has the potential to play a massive role in improving patient care. The second sample chosen was of identifying whether a particular RGB value corresponds to a human skin colour [3]. This dataset only had 3 attributes and the output was also binary, however the number of samples totalled 245,057. 50,859 were valid skin samples while 194,198 were not. My main reason for choosing this dataset was to contrast its large size to the mammography data. Its binary output also helped maintain consistency between the datasets.

Only the mammography data required pre-processing. It was reduced to 830 total samples due to missing values for some of the attributes. 427 of these were benign while 403 were malignant. Some of the attributes, such as shape, were nominal and needed to be broken into multiple attributes to prevent some algorithms, like neural networks, from weighting one “better” than the other. I broke shape down into 4 mutually exclusive binary attributes: round, oval, lobular, and irregular. This way, “round” won’t be valued as a lower weight than “oval” if its index value was simply less in the mapping. I followed the same procedure for margin and density. Finally, in order to prevent the instances from being far too specific, I transformed the age attribute into a decade attribute. This would place, for example, ages 60-69 into the 60 decade. The total number of attributes came out to 15 after the pre-processing.

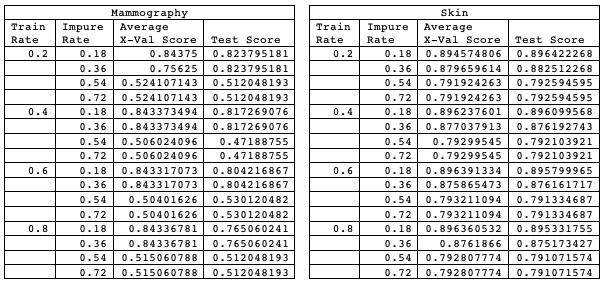
2. Experiments

The data was processed using the Scikit-learn library for Python 3 [4]. In each run, the training set made use of a 4-folded cross-validation procedure and the average was compared with the results of the testing set. Of the data available the training sizes/rates used were 20%, 40%, 60%, and 80% of the total number of instances available.

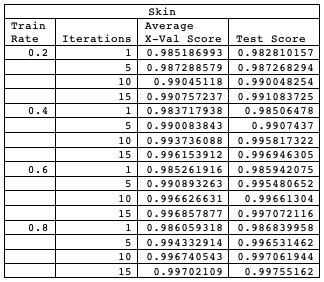
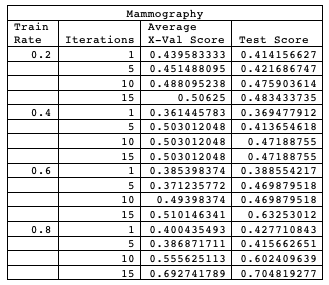
The decision tree algorithm used information gain to split the data because the difference in performance between it and Gini is marginal when the two are compared over a wide range of practical applications [5]. The awaying factor was the abundance of documentation on information gain available. Pruning was applied by preventing further splits if the level of impurity that may result is less than some threshold. The results were as follows.



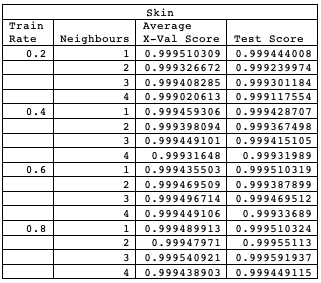
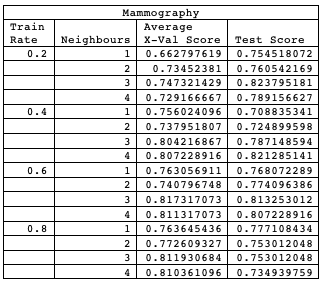
The boosted tree version of this made use of the AdaBoost algorithm to focus in on attributes that have more predictive power. By boosting the weights, I expected to be able to get away with a larger impurity allowance without sacrificing too much accuracy. The results below mostly confirmed my hypothesis.



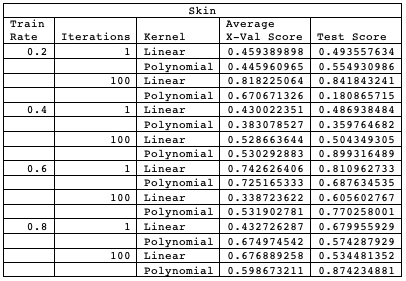
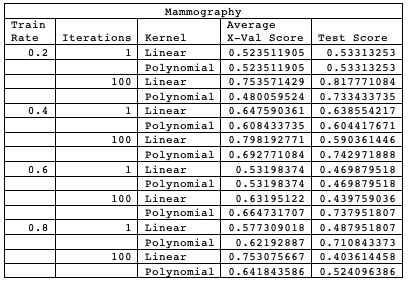
When choosing the implementation for the neural network experiments, I decided to use the logistic sigmoid activation function paired with a stochastic gradient descent solver. ReLU activation was also considered but it was ultimately not chosen because it has the possibility to cause a detriment to learning when paired with this solver in that gradients cannot flow backwards [6]. The results over several different iterations are below.



For the KNN algorithm, I chose a uniform weight distribution because the spread of values was large in both datasets and there was a large potential for overfitting otherwise (especially on the skin data). For example, just because a specific RGB in the brown range isn’t a skin sample shouldn’t mean that a close RGB should be classified as a non-skin sample as well, especially since we know that there are a wide variety of brown tinges that do correspond to common skin colours. The results when varying the number of neighbours are below.



For SVM learning, the kernels chosen were linear and polynomial of degree-2. Since linear is simply a degree-1 polynomial, I wanted to compare it with the next logical progression and analyze the results. For each training rate, the different kernels were applied against a single iteration and 100 iterations to record the effect of repetition on the datasets. The results are as follows.



3. Analysis

To ease readability in the graphs in this section, dashed lines join the average cross-validation scores, while the solid lines join test scores.

The decision trees for the mammography data had the least error on the testing data when the training rate was 60% for impurities 0 and 0.4. This implies that beyond this rate tended to overfit the data for these pruning levels. There is further evidence of this fact by the trend of the error rate decreasing on the testing data as the training portion rises. In contrast, the best testing scores for impurities 0.1 and 0.2 was only 20%. Beyond this point, the error rate on the training data hardly increased. So while the best single run was on impurity level 0 with an error rate of 18.2%, both impurity levels 0.1 and 0.2 only needed a 20% training portion to accomplish a very close error rate of 18.6%. This leads me to believe that very little score is sacrificed by pruning and the gains in performance can far outweigh the deficit. Although, this would not be a worthwhile trade-off for this problem domain due to the repercussions of misclassifying cancer tissue.

As opposed to the mammography output, the error and testing scores were very similar in all test runs for the skin data. The un-pruned tree was the significantly better structure in this case with a <0.1% error rate on both the training data and the testing data as it gets a higher training portion. Impurities 0.1 and 0.2 are tied in scores once again across all training rates. Their lowest error rate is at 11.8% however it’s very close for all training portions. Very little is sacrificed if only 20% of the data is used to train for all impurity levels. This may be attributed to the fact that there are only 3 features and that it’s very easy to tell apart most colours as not being representative of skin pigment. Colours that are green, purple, and red fit such colours and the decision tree algorithm does a fantastic job of identifying this with a small training portion.

The most noteworthy change in the results when using AdaBoost on the mammography data was that even with a high impurity level like 0.36, the algorithm was able to have an error rate of 18.6% on the testing set at a 20% training rate. This is the same as the error rates at impurity levels 0.1 and 0.2 before. The boosting seemed to have allowed additional impurities to creep in to the splits without forgoing any accuracy at all in this case. However, as the boosting is stressed even more with impurity levels 0.54 and 0.72, the excessive pruning hugely detriments score, even dipping below 50% at its worst.

Boosting on the skin data was ineffective and, in the case of no pruning, yielded much worse results if anything. This may be due to the fact there’s no one important attribute out of red, green, or blue, and so there would be nothing to gain out of weighting these. Weighting them would be counter-intuitive in this regard, which would result in inaccurate labels.

The neural network results on the mammography dataset are unsurprising in that the error rate on the testing set decreases as more iterations are added, with the exception of 5 iterations near the end. What did surprise me was how poorly it did in general. The lowest error rate was 29.5% over both training error and testing error. There was also a sharp rise in training error for 5 iterations between 40% and 60% training rate. Since the testing error dropped in this interval at 5 iterations, there may have been some misrepresenting of the data occurring because that would explain the underfit.

In contrast, the neural network scored extremely well on the skin dataset. The error rates were as low as 0.3% on the training data and 0.2% on the testing data. There was also no indication of overfitting, the scores simply improved as more training was provided and as more iterations were added.

KNN on mammography data was the most successful with 20% of the samples used for training with K = 3. The largest drop in error rate was 9.2% for K = 1 between the 20% and 40% training portion. This was a training error drop and leads to the conclusion that the extra 20% training was much more important earlier on. Especially when considering that training error dropped noticeably for K = 3 and K = 4 in the same interval.

KNN on the skin data was, simply put, the most successful of all the experiments. The error rate in the worst case was <0.1% and while the best score was for the K = 3 test data, the difference was marginal. The success of this experiment could be attributed to the size and spread of the dataset such that there was always a close neighbour nearby.

The SVM approach yielded a great deal of variability in the results on the mammography dataset. The polynomial kernel at 100 iterations was the most consistent, hovering at around a 25% testing error rate until overfitting began after increasing the training portion past 60%. However, the lowest error rates were for the linear kernel at 100 iterations, even though overfitting had a massive effect on the testing error rate as the training portion increased.

This approach on the skin data had even more variability, the most seen in all the experiments. The most immediately noticeable item of interest is the testing error dropping close to 70% when increasing the training portion from 20% to 40% for the 100 iteration polynomial run of the algorithm. This experiment demonstrated very well how important the training portion can be and how quickly scores can vary based off of this parameter. At its worst, the testing error exceeded 80%, that’s impressively inept considering that random chance at labelling correctly is 50%.

4. Discussion

The overall best performer for both datasets was the KNN algorithm. This is easier to see in the case of the skin data because the spread of scores was incredibly low while always remaining closer to perfect scores than any other algorithm tested. While KNN did not hold the highest score for the mammography data, it was close, and the lowest score was well above that of the decision tree (19.1% higher).

The worst performer on the mammography data was the neural network. The variability in scores was 34.4% but the real issue was that most of the runs scored less than 50% on a binary label. It would be interesting to see how greatly increasing the iteration count would affect the scores because they did have some positive impact. Unfortunately, this was not done because increasing it on the skin data was far too slow to be feasible and consistency between the input parameters for both datasets was a key component to the experiments.

While the SVM algorithm had some low error rates, it also had some of the highest for the skin data, including one run that was 81.9%. The huge range was the primary reason for it being the worst performer for this dataset. I attempted higher order polynomials but the execution could not complete. However, it may not have actually helped in this case due to the sporadic scoring seen. At some training sizes, the linear kernel actually performed better.

In general, the graphs showed more consistent scoring between training and testing sets for the skin data. One reason to explain this is that certain colours, such as purple, can be very easily determined as non-skin. In contrast, the determination of malignant breast tissue can be very challenging. For example, while it may be true that breast cancer is more common as age increases, it’s certainly not the case that younger individuals cannot acquire it as well [7]. Furthermore, there is a strong possibility of hidden variables obscuring algorithmic scores. One such variable would be the impact of the age when a woman had her first child [8].

There is very little room for improvement on the skin data when using KNN, however there are several enhancements that can be made for KNN on the mammography data. First would be to identify other hidden variables and to account for them in the learning process. Another suggestion would be to greatly increase the number of neighbours. Generally, increasing the K-value for this dataset increased the scores. This may have been because more neighbours could have an easier time masking outliers. Finally, perhaps a uniform weight distribution isn’t the best approach for the data. It would be worthwhile testing a different distribution technique such as distance-based tactics to see their impact.

There was a great deal to learn from the experiments. While, the skin data did produce more consistent scores between the training and testing runs, it may not only have been because of the advantage it had in instance count. The type of data available for the mammography learning process could’ve been the larger difference.