Final Project Progress Report

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CSE 546 Machine Learning

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1 Initial Plan

To begin on this project, I sat down with the requirements and wrote down what I had planned to do for each of them, given my knowledge about the problem and what methods were likely to be the best options for each. I will discuss them in the order I decided them, not necessarily the order listed for the assignment. For phase one, I wanted to handle which classifiers I was planning on using, which data normalization techniques works best for each, and what are the dimensionality reduction needs for each classifier

1.1 4 Different Classifiers

I wanted to include 2 classifiers that I felt like had the highest chance of success, and 2 classifiers that I felt like are foundational for Machine Learning which are important for me to get more experience in. As such for the two I felt like would do well, I chose to go with a Multi Layer Perceptron Neural Network (MLPNet for short), and a kernel SVM.

I chose the MLPNet because I feel like since our dataset is described by a feature set created by a CNN, then an MLPNet is the most logical solution since that is likely the most similar achitecture to what the CNN was using to generate the optimal kernel weights for feature generation. I chose the kernel SVM because I'm aware that in the history of Machine Learning, before neural networks and deep learning took over, these models were usually the go-to option and the best performing.

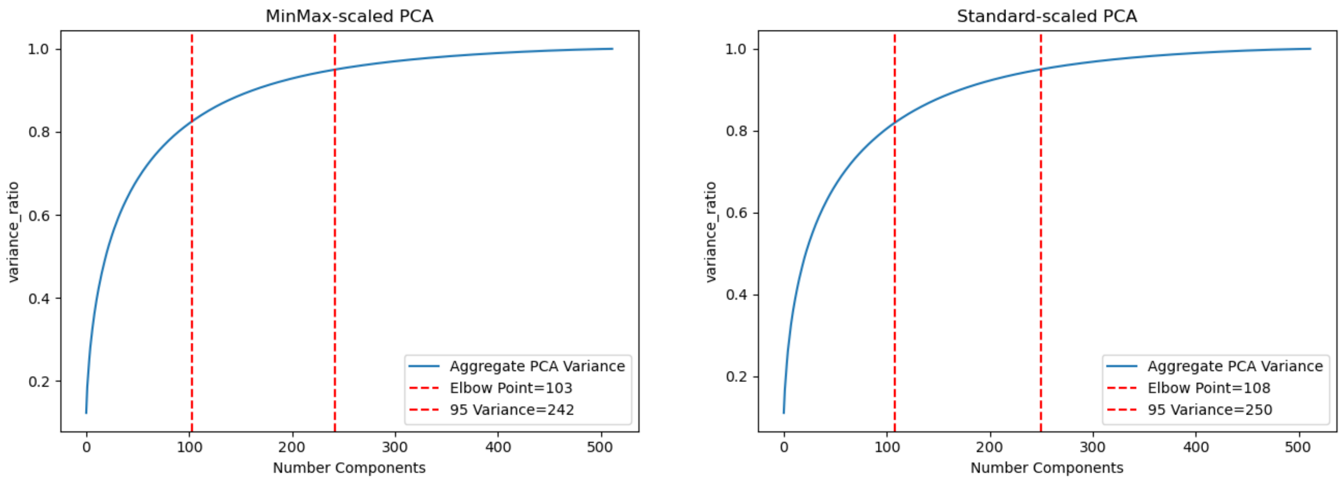
For the two "Foundational" classifiers that I felt I need more experience with, I went with the Gaussian Naive Bayes classifier (GNB), and the Random Forest classifier (RF). I chose the GNB because I think it will provide a good insight on the training data, and give a good baseline from which we can draw conclusions to influence future decisions given it's extreme mathematical grounding. I chose the RF because I'm aware that it is a very popular technique that is utilized often in bioinformatics. In fact, my start in data science was working on improving the classification of central nervous system cancers which was started by a paper which used a random forest classifier on the methylation array data.

1.2 Data Normalization

For the 2 data normalizations required, I picked the standard scaler and the minmax scaler. I chose the standard scaler because it assumes a normal distribution, which the GNB classifier could use well, and everything's nicer when the standard normal distribution is assumed. Secondly, I chose the minmax scaler because I wanted to utilize the SVM and MLPNet classifiers, both of which historically work best and train fastest when the data is scaled between 0 and 1.

1.3 PCA

I originally planned to be more scientific about my choice of PCA components. I had planned to plot the total variance captured, and find both the elbow point of variance, and the 95 percent variance



(a) MinMax PCA Variance

(b) Standard Scaler PCA Variance

Figure 1: Initial PCA choice experiment

mark. I successfully did both of these experiments as shown in 1, but I quickly discoverd that I could instead pass the desired amount of variance directly to sklearns PCA function.

Once I discovered this, I realized I could include this within a gridsearch so I could see if different classifiers have different dimensionality reduction needs. So, I combined seaching for optimal PCA variance and optimal normalization into the same first experiment, which I will talk more on later.

However, one important takeaway from this is that I can keep 95% of the total variance of the data while cutting my dimensionality by more than half. This is huge for rapid experimentation, and something I will absolutely abuse.

2 Experiment 1

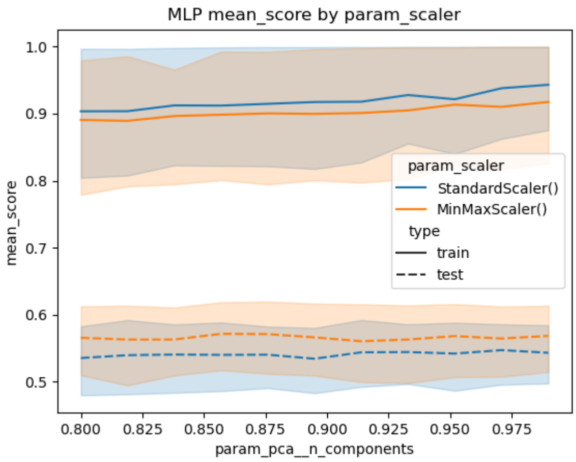
For my first experiment, I used only 1/4 of the data, and quite a large grid search of sparse options for most items. My goal was to discover which scaler worked best, and prod to see what behavior a PCA analysis invokes. Looking at the plots for the PCA variance in 1, I discovered that the elbow point was located close to the 80% variance mark, and that the 95% variance mark would still result in a respectable amount of dimensionality reduction. As such, I locked my PCA search to be between .80 and .96 for all items. I did only use the accuracy metric for these first few experiments since my pre-existing codebase was hardcoded to use only the accuracy metric, and attempting to fix it constituted a larger endeavor than I felt necessary for initial experiments.

2.1 MLPNet

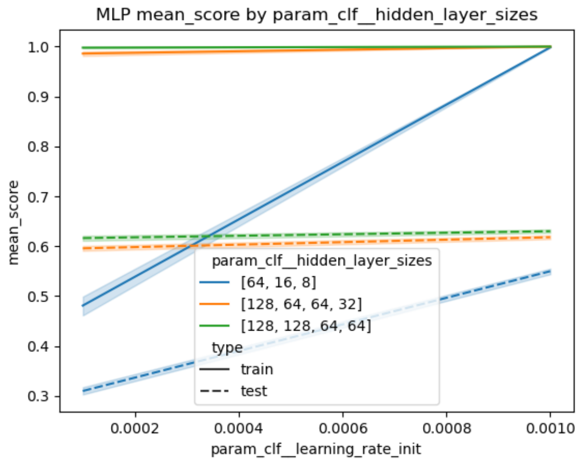
I had 3 major conclusions for the MLPNet which can be shown by these two plots in 2. First, We can see that across the board the minmax scaler appeard to be the correct choice of scaling. Across all metric combinations, the minmax scaler both showed higher validation accuracy, and less over fitting than the standard scaler. So, I locked in the minmax scaler for all future experiments for the MLPNet classifier.

Second, we can see very minimal increase in performance across the PCA search, but we do see some slight improvements once we reach into the 90% variance range. To check this, in the next experiment I cut down my search to be in the 90s with the same amount of points, leading to a tighter search.

Finally, the more advanced network appeared to vastly out perform the simpler one. So, I increased model complexity for subsequent experiments.

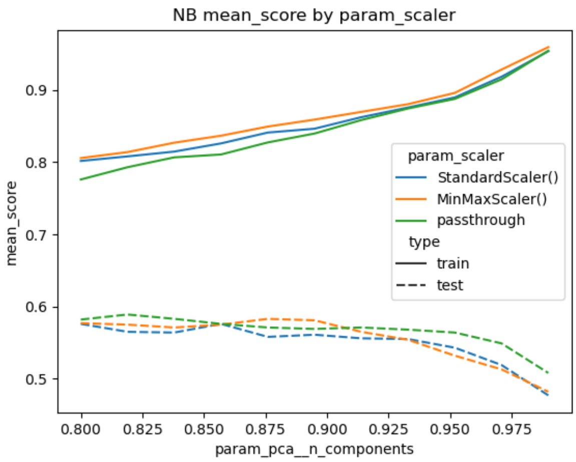


(a) Scaler Choice By PCA

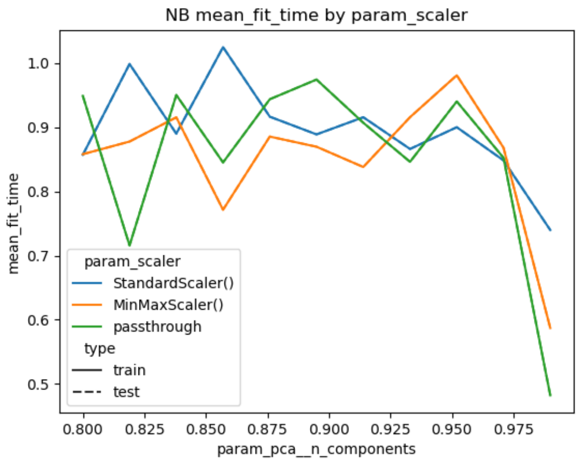


(b) Model Choice by Learning Rate

Figure 2: MLPNet Experiment 1



(a) Scaler Choice By PCA score



(b) Scaler Choice by PCA Train Time

Figure 3: GNB Experiment 1

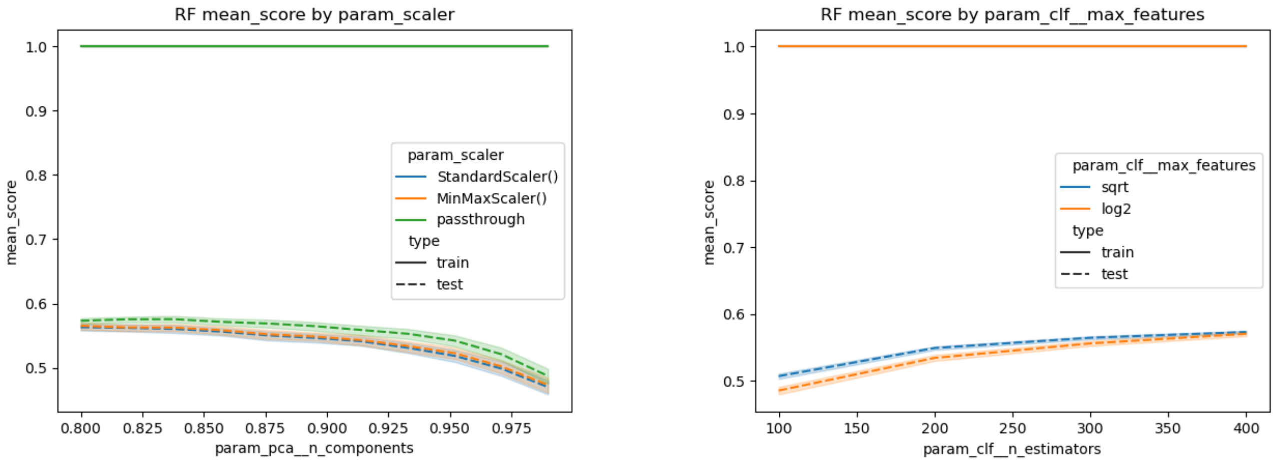
2.2 GNB

The GNB results were the most straightforward. Oddly enough, the MinMax scaler appeared to perform the best, even though one would think a Gaussian-based preprocessing technique would be the best for a Gaussian-based classifier.

Due to the speed of this classifier, and the lack of other hyperparameters to tune, I was able to more densly pack the PCA search for this one. This led to an interesting discovery. For some reason, the scaling options all meet in validation performance at one point, before the minmax scaler proves to be the best for a short while, then the passthrough takes over again as performance degrades at the highest end of pca variance.

One thing I found interesting, was that this classifier did not show the usual improvements in fit time when the dimensionality was lower. In fact, they saw remarkable improvements to fit times as the PCA approached maximum dimensionality.

Regardless, the GNB is serving it's purpose for me. I can see that the baseline accuracy should be greater than about .6, and I can see that the linear separability of classes does indeed improve if given even the slightest amount of dimensionality reduction.



(a) Scaler Choice By PCA score

(b) Feature choice by N Estimators

Figure 4: RF Experiment 1

2.3 RF

For the remaining classifiers, I will more quickly sum up the observations and conclusions as the broader information has already been covered.

For the RF classifier, we see nearly identical performance drop off at high levels of PCA variance that we saw in the GNB classifier, which is good for us because that means we can cut down the PCA to be in the 80s with respect to variance.

We can also see that the classifier behaves the best when we use no normalization, and that the sqrt method of feature selection appears to outpace the log2 method.

It appears that we could use more estimators likely, but I was planning on reserving that and the maximum depth searches for the next iteration of experiments.

2.4 SVM

For our last model, the SVM, I decided to only test for rbf and sigmoid kernels to save time, and it appears that nothing is working at all for this classifier. We are getting moderately better results with the MinMax scaler, but they are still hanging around the .2 accuracy mark.

We are seeing that lower PCA values are moderately better, but that's likely due to the fact that this experiment used only 1/4 of the data.

I can't make any strong conclusions for the SVM yet, but I will lock in the MinMax scaler as the best option, while also lowering Gamma since it appears like lower was better.

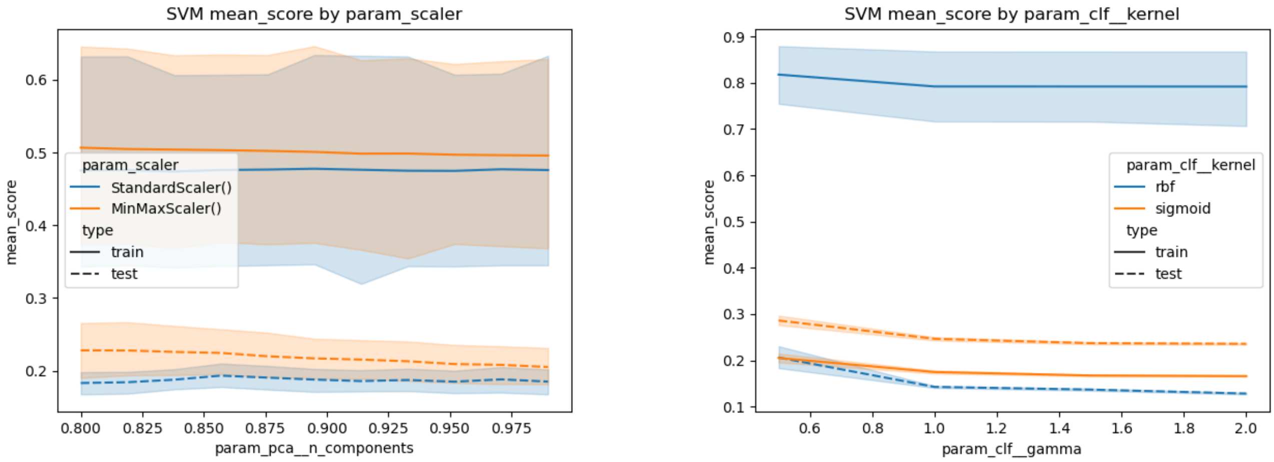
3 Experiment 2

For this experiment, I'm still sticking with only looking at accuracy, but my goal is to tighten my searches a bit and confirm I'm moving in the right direction from Experiment 1. I'm moving on to use half of the data for this instead of 1/4 of the data.

I will more succinctly discuss the results and conclusions for this experiment since much of the justification for my choices will stay the same.

3.1 MLPNet

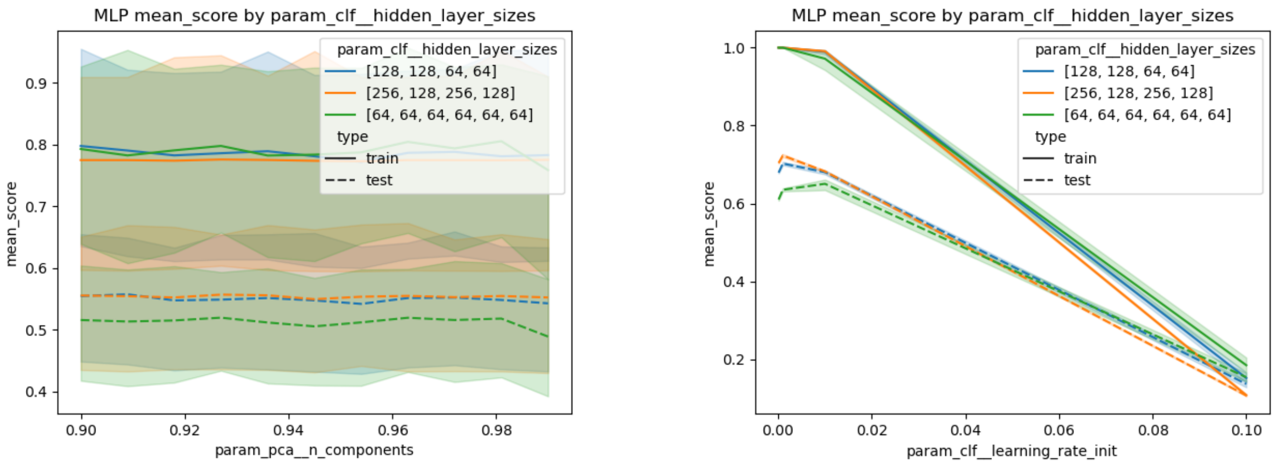
We can see that PCA had little influence on the performance of the models across, regardless of model complexity. As such, I'm likely going to keep it on the higher side for now since we will be adding more data as we progress, and the trend appears to be that more complex models work better.



(a) Scaler Choice By PCA score

(b) Kernel choice by Gamma

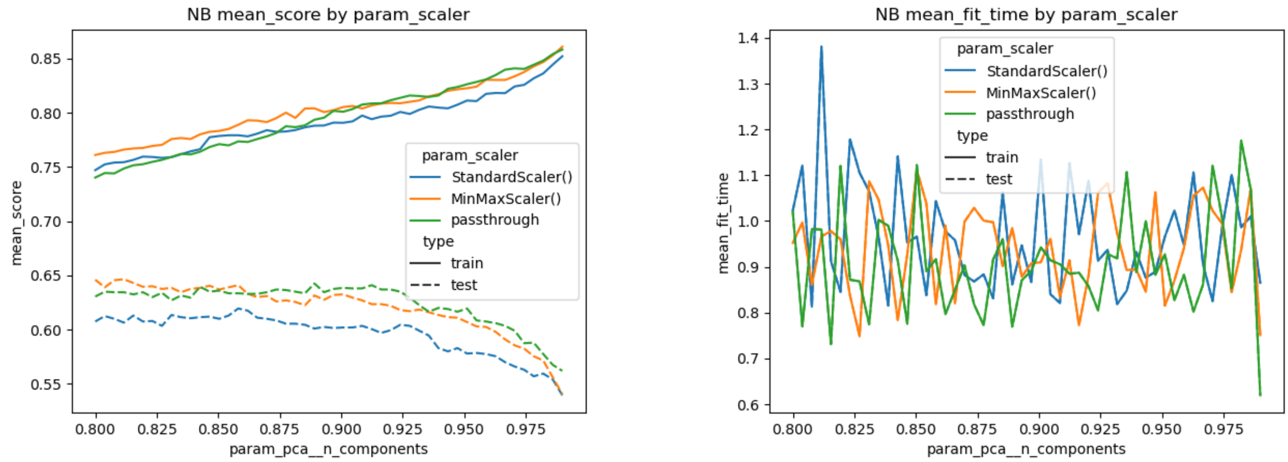
Figure 5: SVM Experiment 1



(a) Effect of PCA on Performance

(b) Effect of Learning Rate on Performance

Figure 6: MLPNet Experiment 2



(a) Scaler Choice By PCA score (b) Scaler Choice by PCA Train Time

Figure 7: GNB Experiment 2

Learning rate was the highest driver of performance, with a nearly linear relationship between performance and value, and very little variance denoted by the lightly colored region. Thus, low learning rate still wins out.

3.2 GNB

Results are almost identical to before, even with the increased data size. I'm expecting a large jump in performance once I use KMeans projections due to the centroid-based nature of the method.

3.3 RF

Higher estimators are better, for sure. The changes I made seemed to have given improvement and no new surprises when we doubled the amount of data. For this experiment, since I'd locked in what scaler I'm using I decided to plot the PCA variance vs. the number of estimators as a heat map, particularly due to the density of the search.

This plot challenges my previous thought that lower PCA was better, since it appears like there's a general improvement just before 90%. I will move my search window to be centered at 90% in the future.

3.4 SVM

In this experiment, we can start to see the rbf kernel pull ahead of the sigmoid kernel in some areas, but not by enough to justify locking in our choice. We are going to have to stick with both of them for now, but I'm expecting the rbf kernel to start to pull ahead once we enter cluster transformations into the mix in the next steps.

Looking at the contour plot of PCA vs. gamma, I think it's pretty clear that low gamma and higher PCA variance appear to have the edge in the gridsearch. So, I'm going to keep PCA high, and gamma low.

4 What Remains

I've mostly expanded my analysis pipeline to include other forms of scoring. I do still have to work the kinks out of a couple of the more automated parts, but I expect to have that done long before you read this. This has been the biggest hurdle so far, but I expect to be over it soon.

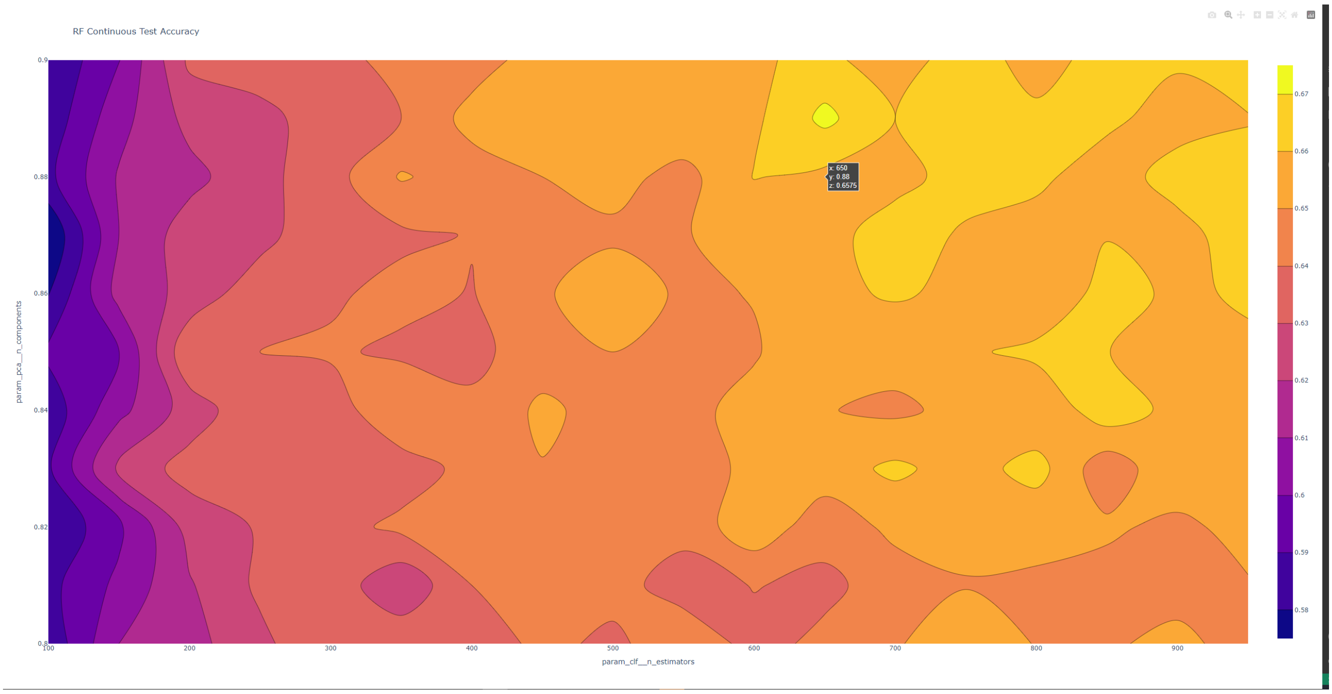
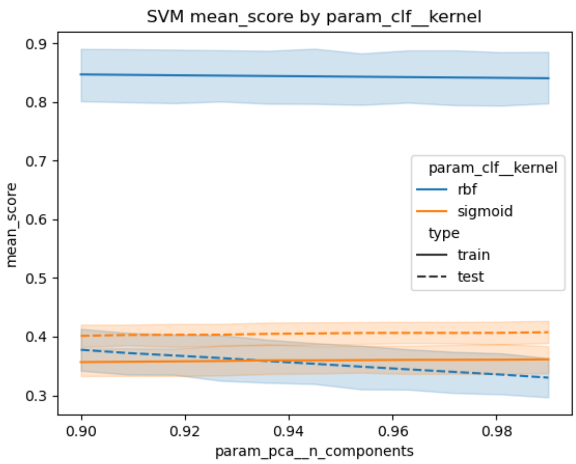


Figure 8: Contour Plot of Variance vs. N Estimators

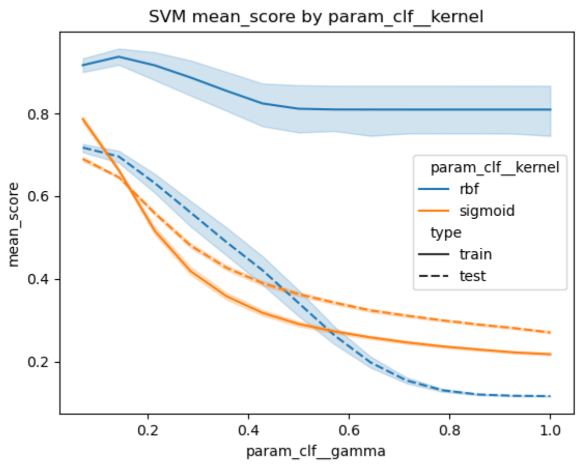
For the cluster mapping requirement, I have decided to go a bit more hands-on for this. I ran KMeans clustering for a number of clusters ranging from 1 to 520, and calculated the gross cluster purity of the clusters. This basically means that for each cluster, I count how many of the samples are correctly grouped in a cluster where their class matches the majority of classes in that cluster. The result of this experiment is in 10.

My goal for this is to use the clusters as dimensionality reduction, so that is why I am not going to go above 520 clusters. As we can see in the plot, we quickly approach a an area where it begins to taper off around 60-100 clusters, and becomes almost linear beyond that. However, since running the cluster analysis to generate these is quite time consuming (unlike PCA) I plan on only using 2 different cluster transformations whcih are 100, and 200 clusters to meet the minimum requirement for the assignment. If I have time and see the benefit, I might do more.

I have not begun yet on the ensemble methods, but I plan to use the best performing item from each of the 4 different classifiers, and ensuring that at least 2 models use the kmeans transformations in order to ensure we have good variance of our classifiers.



(a) Kernel Choice By PCA score



(b) Kernel choice by Gamma

(c) Gamma vs. PCA Contour

Figure 9: SVM Experiment 2

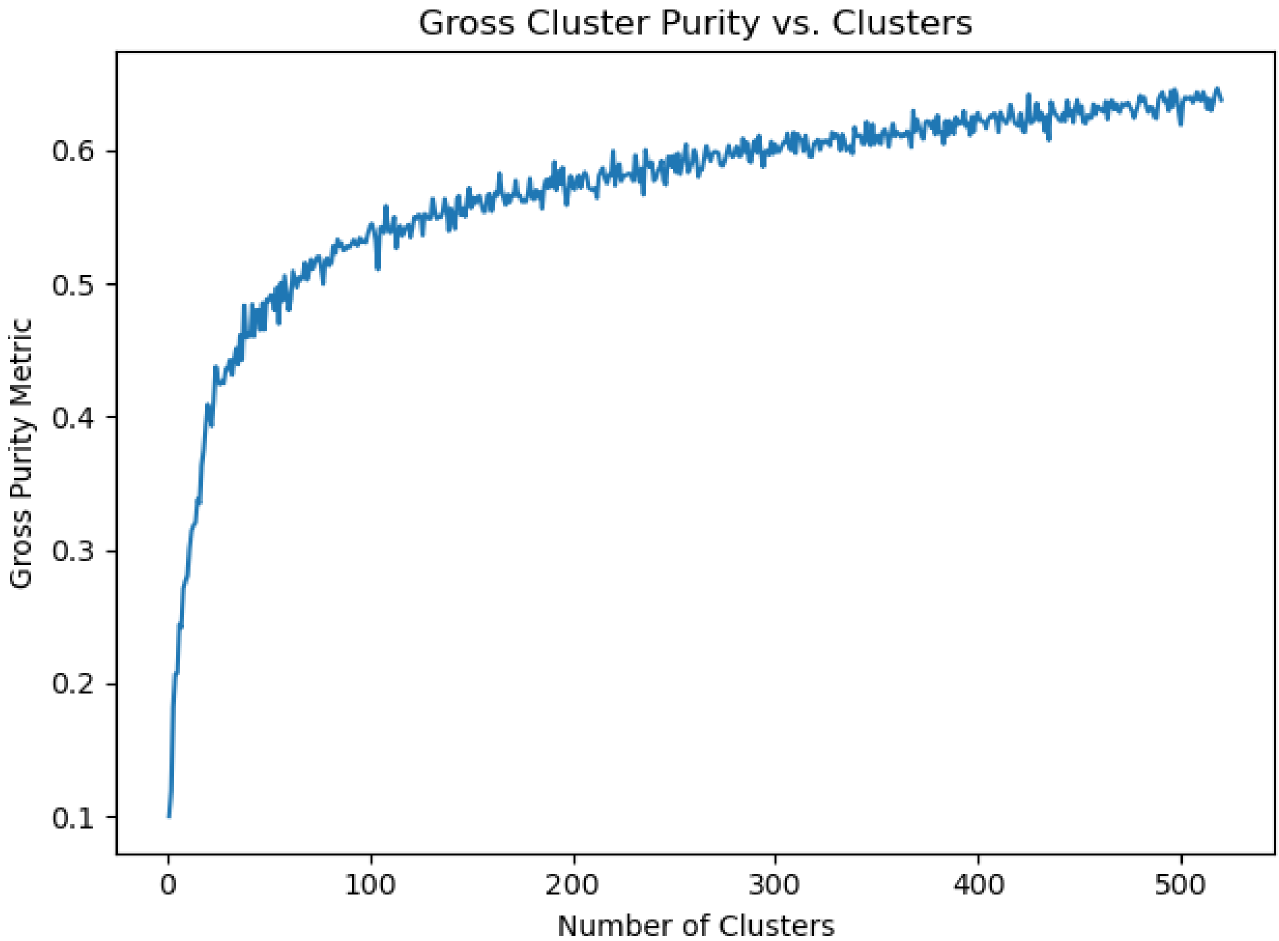


Figure 10: Cluster Analysis