1 Introduction

This project investigates algorithms in unsupervised learning: PCA (Principal Component Analysis), K-means clustering and GMMs (Gaussian Mixture Models).

1.1 Experiments

First, two datasets are chosen. In this experiment, the datasets are the Mushrooms dataset from Kaggle and the Pima Indians Diabetes dataset from Kaggle.

Then, two clustering algorithms (K-means clustering and GMMs via expectation maximization) are run.

Then, the datasets are reduced into fewer dimensions using Principal Component Analysis. The clustering algorithms are re-performed on the reduced dataset.

Then, the original results of the PCA algorithm on the Pima Indians Diabetes dataset are taken, and the neural network is trained on this reduced dataset. To evaluate the accuracy of the neural network, both the training and testing datasets are projected with the dimensionality function that had been generated before.

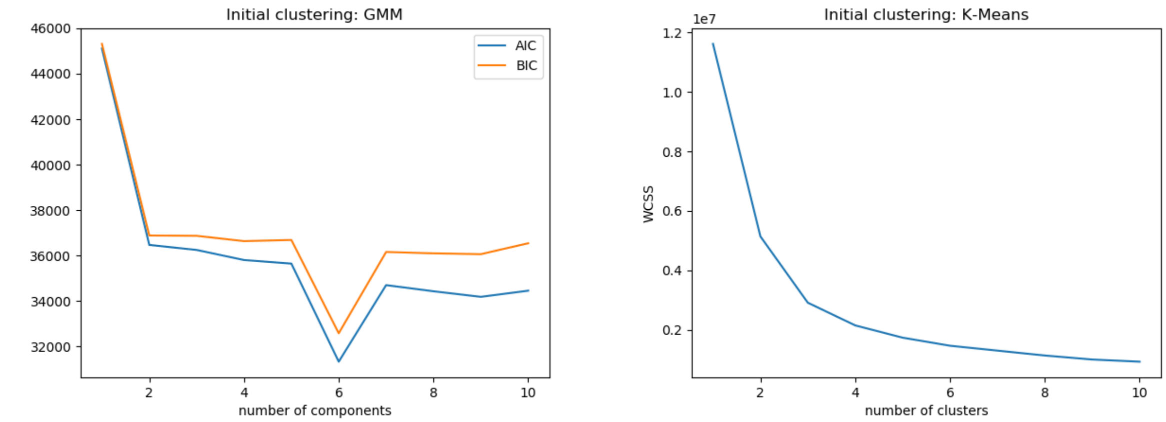
Finally, the training dataset of the Pima Indians Diabetes dataset is clustered using the k-Means and GMM algorithms and reduced to fewer dimensions using the two algorithms. In these specific experiements, the k-Means algorithm reduces the data to the cluster-distance space (sklearn's `transform` function), while the GMM reduces each datapoint to the probabilities of the datapoint being in each cluster (sklearn's `predict_proba` function). Then, with the clustering algorithms used on the training set, the test set is also reduced to those same features. A neural network is then trained on the training datasets produced by the two clustering algorithms.

2 Results and Analysis

2.1 Initial clustering

For each of the two datasets, the GMM and K-means clustering were both run on the training set. To determine the optimal number of cluster, some form of a metric was plotted over the number of clusters. For K-means, this metric was WCSS (within-cluster sums of squares), while metric for GMMs was AIC(Alkaline Information Criterion) and BIC(Bayesian information criterion). Here are the plots generated:

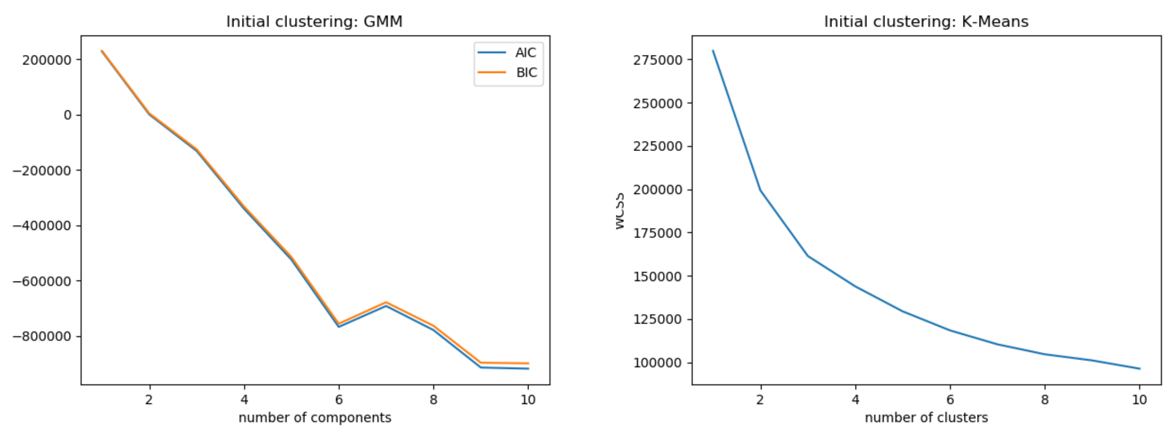
2.1.1 Initial clustering: Pima Indians Diabetes dataset



In this dataset, a clear "elbow" can be seen at two clusters for the GMM, and there is a slight "elbow" at three clusters for the K-means.

The gmm graph has an unintuitive dip at k = 6. However, this could have just been due to randomness; there is no striking behavior seen in the final experiment in the plot for the neural network when k = 6.

2.1.2 Initial clustering: Mushrooms dataset



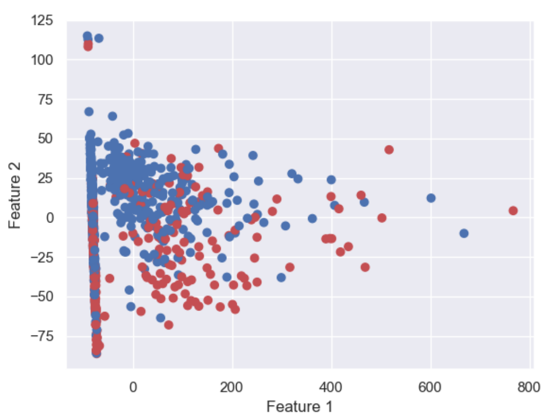
These two graphs look quite different. The plot for Gaussian Mixture Models has a much sharper elbow, implying that this model does much better when given a higher number of clusters compared to a low number, unlike k-Means, which would run in the least cost manner when running it with a smaller number of components.

A reasonable explanation for this disparity is that K-means is sensitive to outliers and would put them in a separate cluster by [3] and thus would need more clusters to minimize its cost.

2.2 PCA

PCA was run on a couple of the datasets. To make the datasets easy to visualize, the PCA was run such that the data was to be split into two components. Here are the results of the PCA that was performed:

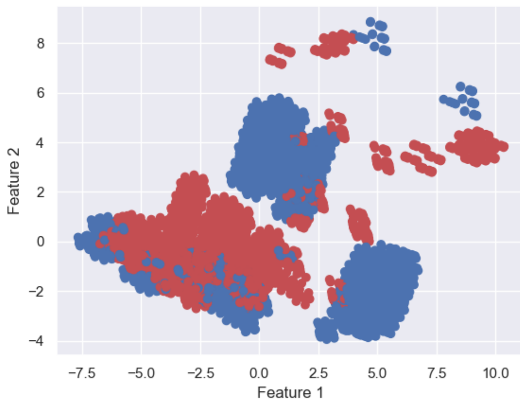
2.2.1 PCA: Pima Indians Diabetes dataset



When considering the visualization of the data reduced to two dimensions, it can clearly be seen that there are two different regions, the vertical region in the left hand side and the larger region in the right hand side.

The regions in this data do not align with their labels; for each region, one half consists of cases of diabetes, and the other half consists of cases without diabetes.

2.2.2 PCA: Mushrooms dataset

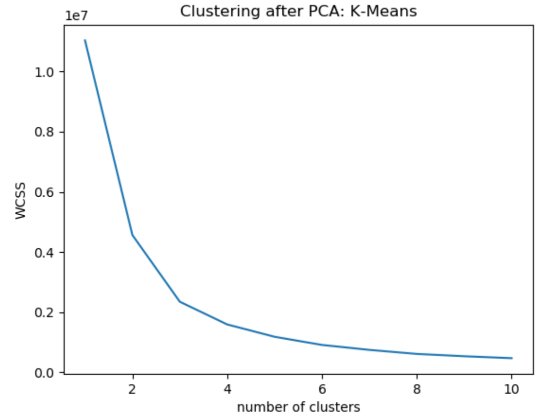


In this two-dimensional projection of the Mushrooms dataset, we can see clear candidates for clusters. There are two blue regions. Also, there is an overlap of blue and red in the bottom left corner. In addition to those main components, there are some outlying red and blue distributed around the upper right portion of the graph.

2.3 Clustering after PCA

The two datasets were clustered with the two algorithms after the PCA dimensionality reduction algorithms were run on them.

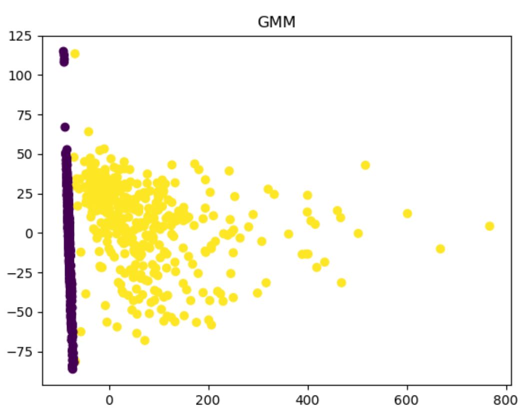
2.3.1 Clustering after PCA: Pima Indians Diabetes dataset

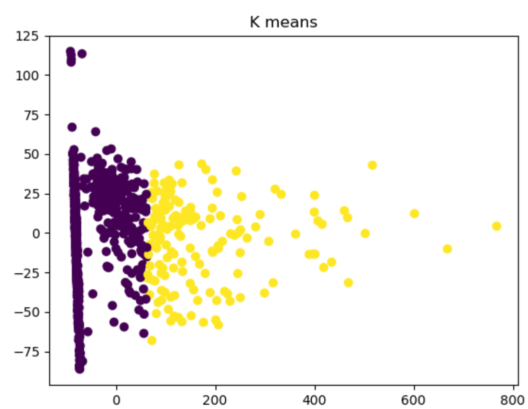


This plot still has a slight dip at k = 6, but it is much smaller than the dip that was created before PCA. Still, there is not any clear information that can be obtained from this dip.

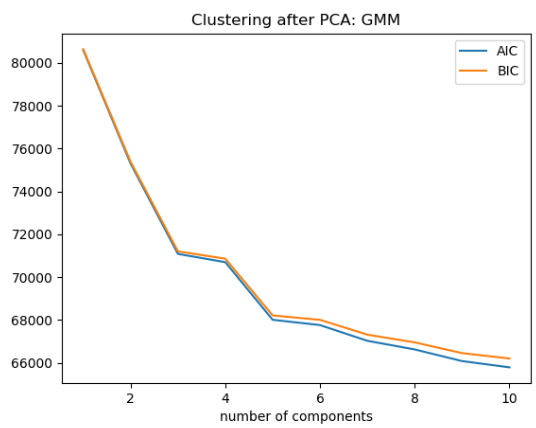
Aside from the dip, the graphs seem similar to the ones created before the PCA algorithm had been run (an elbow at 2 clusters for the GMM and at 3 clusters for the PCA).

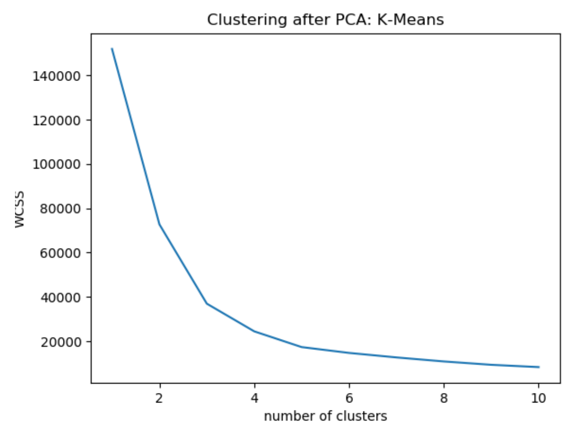
Here are images of the clustering algorithms on the 2-dimensional data.





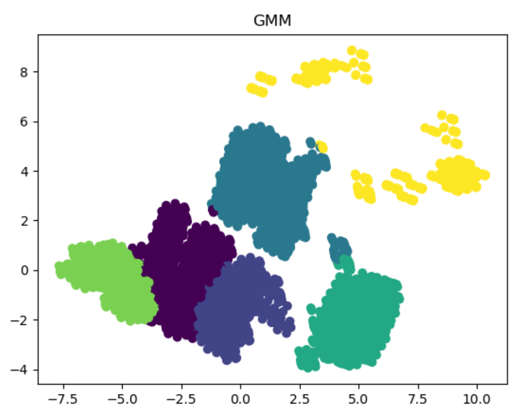
2.3.2 Clustering after PCA: Mushrooms dataset

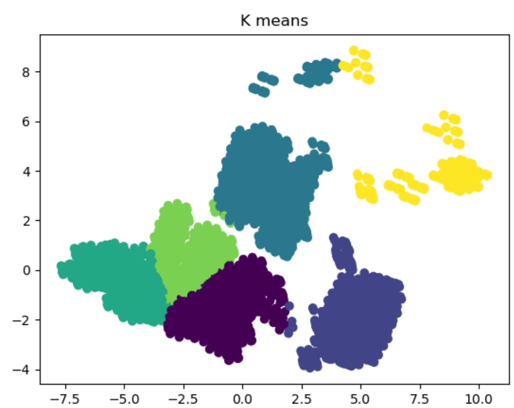




The above two graphs seem quite similar to each other. This is unlike how they were before PCA, where the GMM had an elbow at a much larger number of clusters compared to the GMM.

Here are images of the clustering algorithms on the 2-dimensional data.



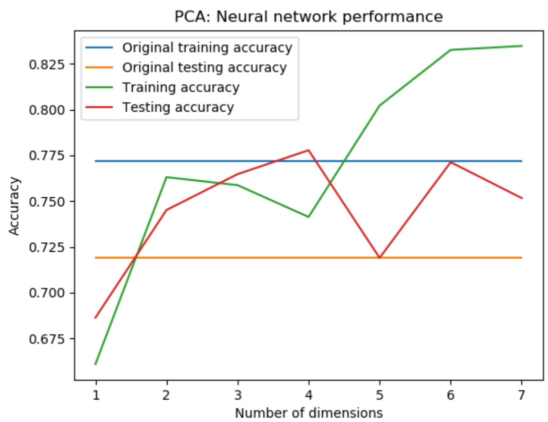


2.4 Training a neural network after PCA

The Pima Indians dataset was split such that 60 percent of it was training data and 20 percent was testing data.

Cross-validation was not necessary, since the objective here is not to produce the best neural network possible, but to rather observe and analyze the similarities in the neural network performance based on how the dimensions are reduced. Cross-validation adds an overcomplication which detracts from the main purpose of these experiments.

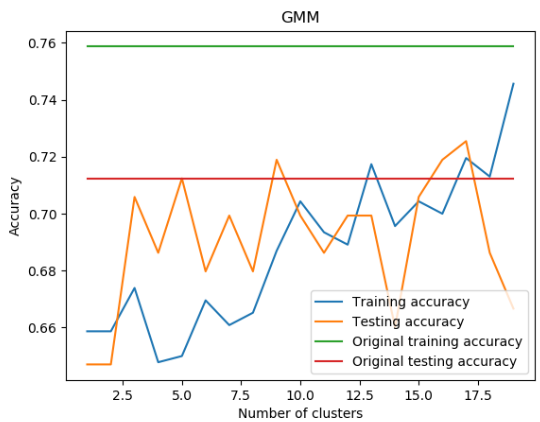
Here is a plot of the accuracy of the neural network (training and testing) with respect to the number of principal components generated in the PCA algorithm:

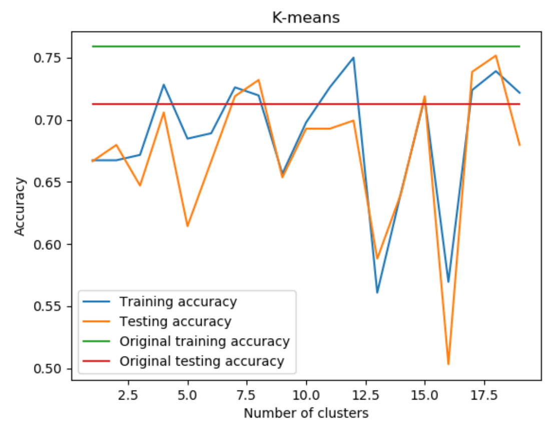


2.5 Clustering for dimensionality reduction

The Pima Indians diabetes was split into a training and testing set (60 percent training and 20 percent testing).

Then, the GMM and the k-Means algorithm were each used to reduce the dimensions of the data for the Pima Indian Diabetes dataset. For each number of clusters, a neural network was trained to produce a mapping from the reduced data to labels. Here are the results for the training and testing accuracies:





3 Sources

[1] https://www.kaggle.com/uciml/pima-indians-diabetes-database

[2] https://www.kaggle.com/uciml/mushroom-classification

[3] https://people.eecs.berkeley.edu/ jordan/courses/294-fall09/lectures/clustering/slides.pdf