CS 4641: Unsupervised Learning and Dimensionality Reduction

Bradley Reardon

March 24, 2019

1 Introduction

In this assignment, we are tasked with implementing two clustering algorithms and four dimensionality reduction algorithms, and seeing how they perform when applied both separately and together on two data sets. In addition, we'll take a focus on comparing these results to those of previous assignments when run on the same data sets. For comparison, all tests run for the purpose of this report will run each algorithm over 500 iterations, with a fixed seed to ensure reproducibility across tests.

1.0.1 Car data set

The Car Evaluation Database was created in June, 1997 by Marko Bohanec. It contains 1728 instances and 6 attributes. The purpose of this database is to attempt to classify a car as an unacceptable, acceptable, good, or very good choice based on factors including cost of ownership, comfort, and safety. Full details about the data set can be found at the source link below. Note that the instances of this data set completely cover the attribute space, making it an interesting problem for testing overfitting.

Source: https://archive.ics.uci.edu/ml/datasets/car+evaluation

1.0.2 Breast Cancer Wisconsin data set

The Breast Cancer Wisconsin data set was donated to the UCI Machine Learning Repository in 1992, and contains data from one doctor's clinical cases, gathered from January 1989 to November 1991. In total, there are 699 instances signifying information about breast tumors such as clump thickness, uniformity in shape and size, and other screening factors. Data points are identified by two classes – benign or malignant. The features of the data points are encoded as 9 continuous attributes rating the screening factor from 1 to 10.

Source: https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Original%29

2 Clustering

Clustering algorithms are a method for unsupervised learning which attempt to place a number of instances into clusters based on the closest mean of input attributes to an existing prototype. Because clustering would occur in either 6 or 9 dimensions, the main focus of analysis will be scoring the algorithms for each data set, though visualizations of these clusters do still show interesting information.

2.1 k-means Clustering

2.1.1 Parameter selection

The main parameter for the k-means clustering algorithm is a value k, being the number of clusters that the algorithm will divide the data into. For both data sets, k values of $2, 3, 4, 5, 6$ were tested for best performance. Each run of the algorithm used 20 initializations to ensure that the best possible cluster labelling is chosen for each data set. Smart initialization of clusters using the "k-means++" method ensure initial prototypes outperform random chance.

The car data set did not perform very well in any of the k-means tests, with a maximum silhouette score of 0.119 being reported at a value of $k = 3$. However, the data was known to be separated into 4 output classes, and the completeness of the instances over the attribute space led me to believe that a subset of the data may perform better.

Running the algorithm again with only 500 of the 1728 total instances resulted in better silhouette scores overall, with the best performance occurring at $k = 4$. Figure 1 shows the silhouette plot and cluster visualization for this run.

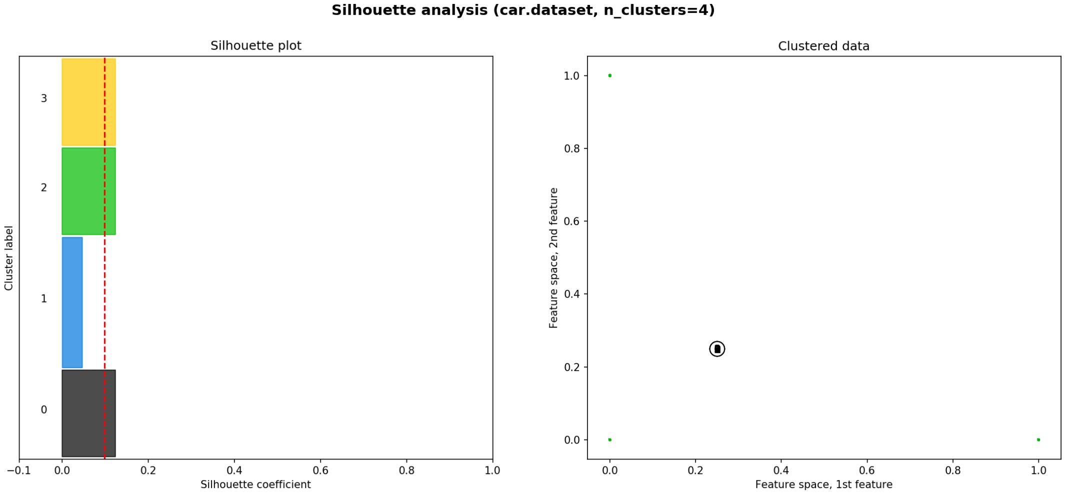


Figure 1: Silhouette plot and clustered data visualization on two features for the car data set.

The breast cancer data set was clustered better, with a best-performing $k = 2$, matching the number of output classes. This resulted in a silhouette score of 0.577, which is much higher than that of the car data set. Figure 2 shows the same visualizations for the cancer data set, which also reveals a very clear separation between the two clusters on the feature spaces for the first two features.

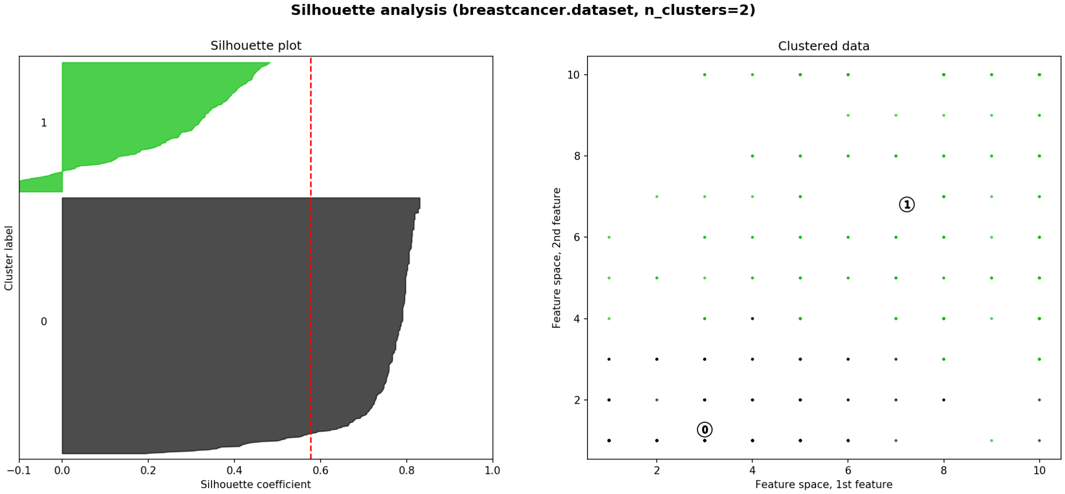
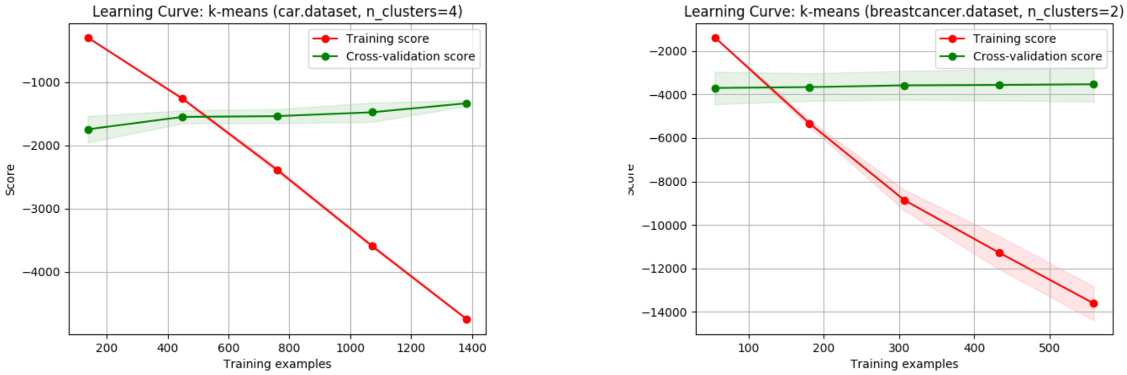


Figure 2: Silhouette plot and clustered data visualization on two features for the cancer data set.

2.1.2 Performance

Using the ideal k values of 4 and 2 for the cancer and car data sets respectively, learning curves were generated to evaluate the peformance over the two data sets. These curves can be found in Figure 3.



(a) Learning curve, car.dataset

(b) Learning curve, cancer.dataset

Figure 3: Learning curves for both data sets, using optimal parameters.

Both data sets seem to converge into clusters reasonably quickly, as shown by the low variance in the cross validation scores. Interestingly though, the variation in the car data set's cross validation score narrows as the proportion of training examples used approaches 100%. The fit times of each test were recorded at 0.102s for the car data, and 0.044s for the cancer data. These running times will be compared to other algorithms and methods in a later section.

Though the cancer data set is clustered better than the car data set by k-means, this same drop in variance is not observed. This suggests to me that the completeness of the instances in the car data had some effect on that outcome. However, this will be looked into further when dimensionality reduction algorithms are applied prior to clustering.

2.2 Expectation Maximization

The expectation maximization algorithm was tested using gaussian mixture models, with negative log-likelihood as the performance metric.

2.2.1 Parameter selection

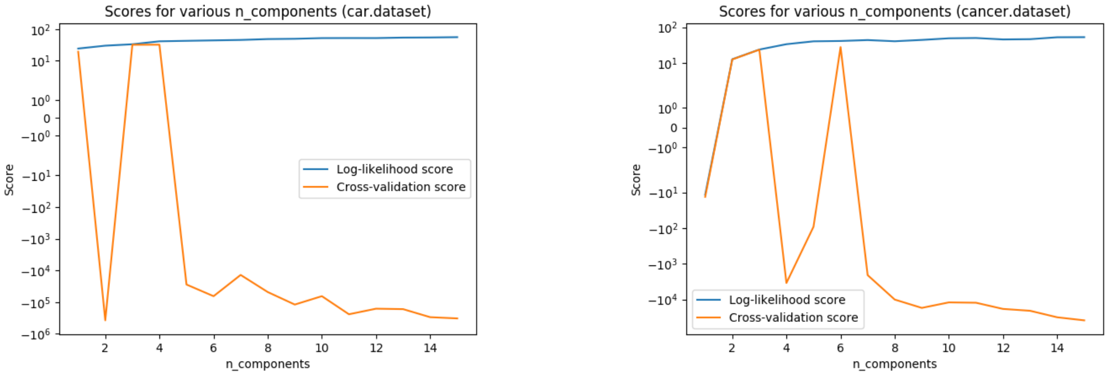
Expectation maximization, in this implementation, takes one main parameter, which is the number of "components". Each algorithm was tested for best performance with between 1 and 15 components inclusive, as shown in Figure 4 on the next page.

In this case, the goal was to find the lowest number of components which resulted in the best scoring, as higher numbers of components increase running time. To satisfy this requirement, the car data set was chosen to have 4 components, while the cancer data set performed better with 3.

2.2.2 Performance

The learning curves for both data sets using expectation maximization are shown in Figure 5 on the following page.

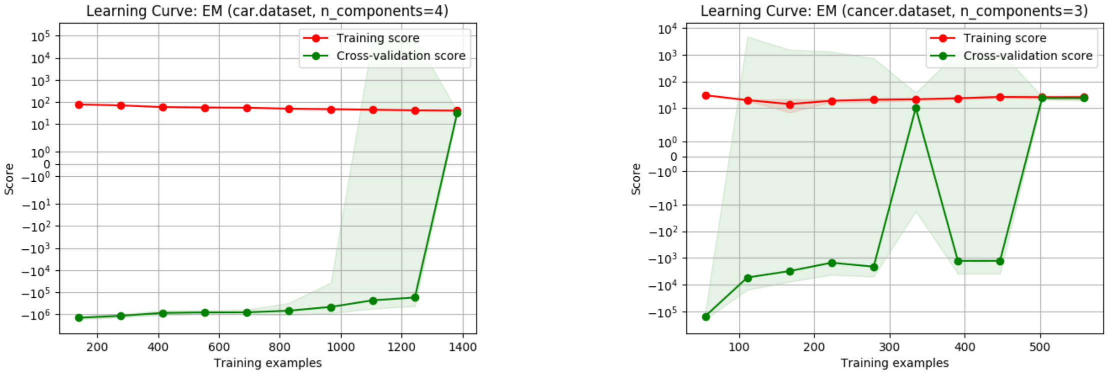
The fit times for these classifiers were 0.025s for the car data, and 0.027s for the cancer data. Interestingly enough, both data sets have high variance in their cross validation scores at least at some point during training. In addition, the cancer data set seemes to have had its cross-validation score converge with the training scores at the end of training. This result will be discussed further after attempting dimensionality reduction.



(a) Scores, car.dataset

(b) Scores, cancer.dataset

Figure 4: Log-likelihood of classifiers for both data sets with varying n_components.



(a) Learning curve, car.dataset

(b) Learning curve, cancer.dataset

Figure 5: Learning curves for both data sets, using optimal parameters.

3 Dimensionality Reduction

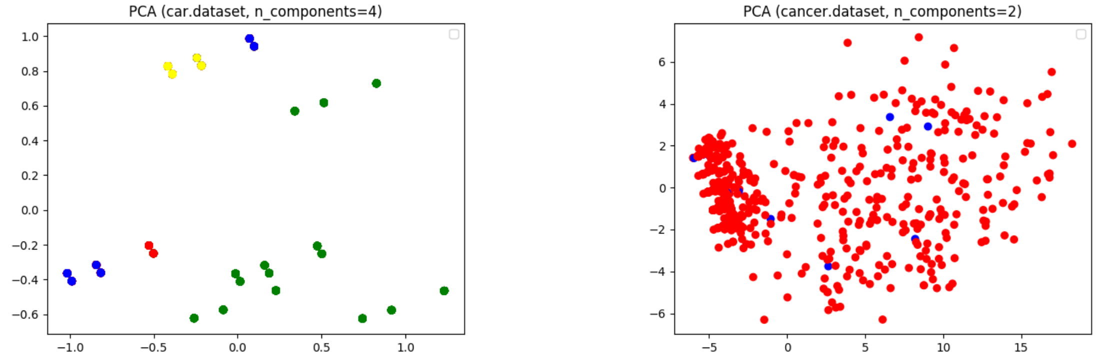
We will now evaluate dimensionality reduction algorithms, which are used for feature selection and to consolidate high-dimension datasets into data more easily digestible by machine learning algorithms. Note that with higher numbers of components, the dimensionality of the algorithm outputs is too high for 2D or 3D visualizations to be sufficient. As such, we will evaluate much of the performance of each algorithm on how it assists a clustering algorithm or a neural network in the next sections. This section will focus on identifying which dimensionality reduction algorithms are effective in clustering the data alone.

3.1 PCA

Figure 6 on the next page shows the best-found configuration for PCA to maximize clustering apparent on the first two feature spaces. Interestingly, the cancer data set did not have any variation in PCA dimensionality reduction across the first two features of the data set. Due to the high-dimensionality of PCA with larger numbers of components, it is difficult to show the effectiveness of the PCA algorithm at higher numbers of components.

As such, the car data set showed the most apparently clustering on two features with 4 components, whereas the cancer data set did not show any change in clustering on the first two features after adding more components.

TODO something more about variance/statistics from PCA



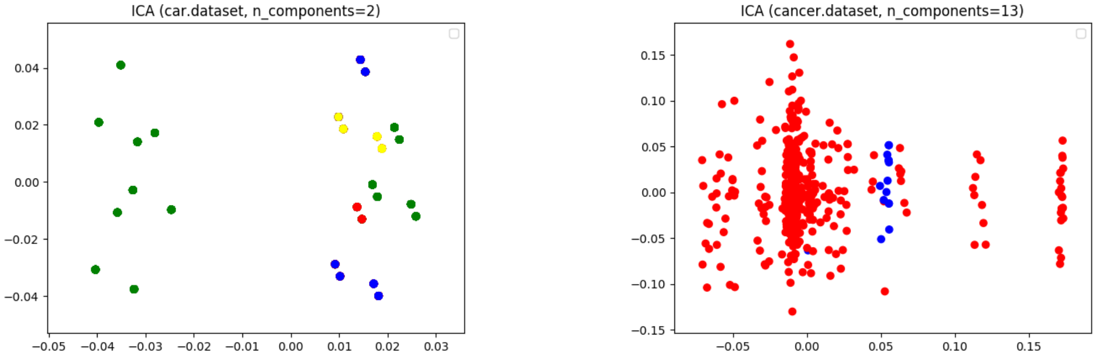
(a) PCA, car.dataset

(b) PCA, cancer.dataset

Figure 6: PCA plots for both data sets.

3.2 ICA

The ICA algorithm resulted in similar clustering to that of the PCA algorithm for the car data set, while clustering the cancer data into narrower bands that more effectively produced a cluster of blue points signifying the malignant tumor class. In this case, the number of components specified had a large effect on the plots of both data sets. The plots for the ICA algorithm can be seen in Figure 7.



(a) ICA, car.dataset

(b) ICA, cancer.dataset

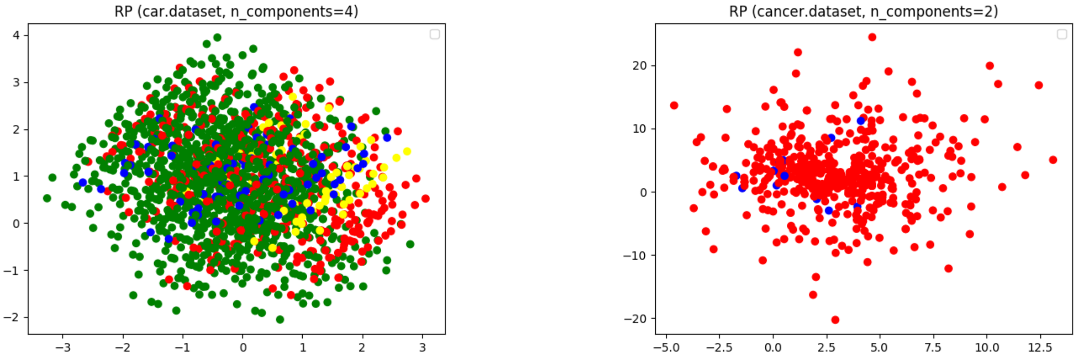
Figure 7: ICA plots for both data sets.

3.3 Randomized Projections

Unlike PCA and ICA, a run of randomized projections using the gaussian random projection algorithm from scikit-learn did not result in any meaningful clustering of either data set when plotted on two features, as shown in Figure 8 on the next page. The effectiveness of this algorithm on the data will be further evaluated when combined with another learner, such as a clustering algorithm or neural net.

3.4 TODO pick feature selection algo??

TODO



(a) RP, car.dataset

(b) RP, cancer.dataset

Figure 8: RP plots for both data sets.

4 Conclusion

TODO