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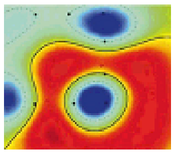

Problem Set 2: Clustering and Expectation-Maximization

Report Machine Learning Lab Course
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Chapter 1

Implementation

This chapter describes the implementation part of the second problem set. There are five assignments in this part: 1) implement *k-means* clustering, 2) implement stepwise optimal *hierarchical agglomerative* clustering, 3) implement a function which given a hierarchical clustering sets up a *dendogram* plot, 4) implement the *EM* algorithm for *Gaussian Mixture Models (GMM)* and 5) implement a function that visualizes the *GMM* for two-dimensional data.

1.1 Assignment 1: K-Means Clustering

In this assignment the *k-means* clustering algorithm should be implemented as follows:

```
mu, r = kmeans(X, k, max_iter=100)
```

The algorithm terminates when the membership and the cluster centers no longer change or after *max_iter* (default value = 100) iteration, depending on which comes first. The implemented function was tested on the test data and passed the test.

1.2 Assignment 2: Hierarchichal Agglomerative Clustering

The task in this assignment is to implement stepwise optimal *hierarchichal agglomerative* clustering with *k-means* criterion as a function. The implemented function was tested on the test data and passed the test.

```
R, kmloss, mergeidx = kmeans_agglo(X, r)
```

1.3 Assignment 3: Dendrogram Plot

The third assignment in the implementation part is to implement a function which given a hierarchical clustering sets up a *dendogram* plot:

```
agglo_dendro(kmloss, mergeidx)
```

The parameters *kmloss* and *mergeidx* correspond to the results of *kmeans_agglo*. The function *scipy.cluster.hierarchy.dendogram* is used to draw the *dendogram* plot.

1.4 Assignment 4: Expectation-Maximization

In this assignment the *EM* algorithm for *Gaussian Mixture Model (GMM)* should be implemented as a function:

```
pi, mu, sigma = em_gmm(X, k, max_iter=100,
                       init_kmeans=False)
```

The parameter *init_kmeans* determines the initialization method. If it is true, then *k-means* is used for the initialization. For random initialization, *k* data points are selected as cluster centers, the prior *pi* of each cluster is set to $1/k$. The sigma of each cluster is the identity matrix. On the other hand, the cluster centers of *k-means* are used for *k-means* initialization. The prior *pi* of each cluster is set to total data points in each cluster divided by total number of data points in the data set. The sigma of each cluster is the covariance matrix of the data points of each cluster.

The algorithm terminates when the maximal number of iterations *max_iter* has been reached or the log likelihood no longer changes (< 0.001)

1.5 Assignment 5: EM Visualization

In the last assignment a function to visualize the *GMM* should be implemented. The figure should show the data as a scatter plot, the mean vectors as red crosses and the covariance matrix as ellipses (centered at the mean).

Chapter 2

Application

In this chapter, the implementations should be applied to three datasets: *2gaussians* dataset, *5gaussians* and *USPS* dataset.

2.1 Assignment 6: *5gaussians* Analysis

In this assignment, the *5gaussians* data set is analyzed. The data set should be clustered using *k-means* and *GMM* for $k = 2, ..., 10$. Figure 2.1 shows the original *5gaussians* data set.

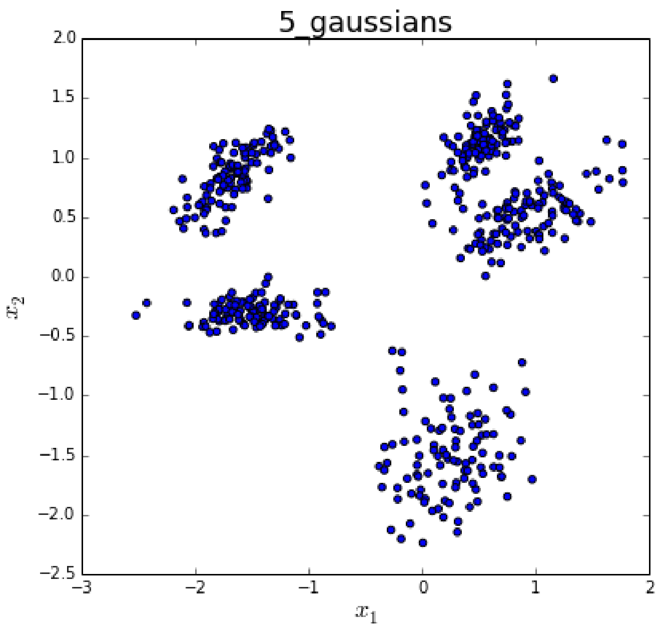

Figure 2.1: *5gaussians* data set

Question 6.1: Do both methods find the five clusters reliably?
K-means finds the five clusters reliably. Since *k-means* can have different result depending on the initialization, it was run 100 times. The loss value from each run was calculated, as depicted in Figure 2.2. The clustering which gives the lowest loss value was then picked and visualized in Figure 2.3.

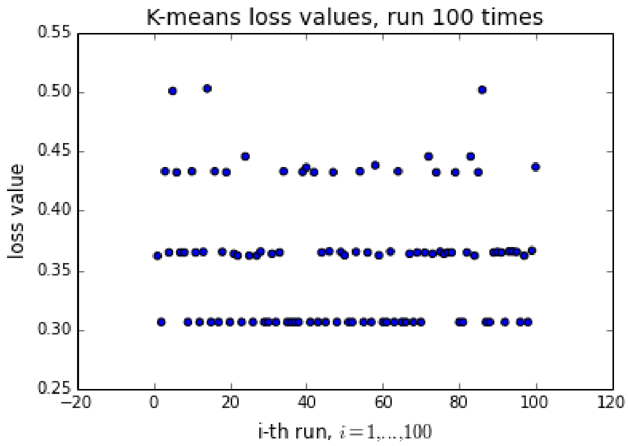

Figure 2.2: Loss values of k-means, run 100 times

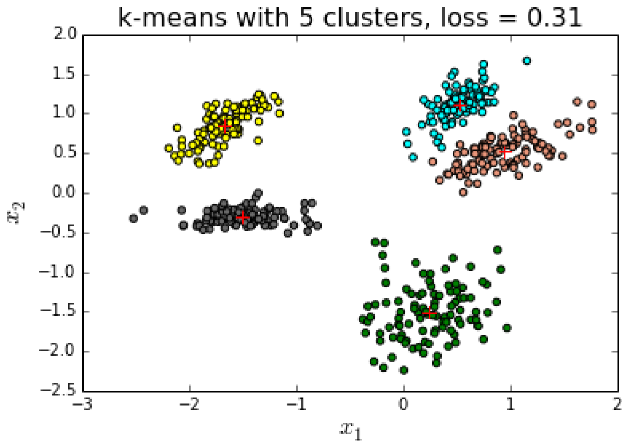

Figure 2.3: k-means clustering with $k = 5$, applied to *5gaussians* data set

GMM with random initialization also finds the five clusters reliably. The same method as *k-means* was applied to *GMM*. It was also run 100 times, but instead of loss value, the log likelihood of each run was calculated, as shown in Figure 2.4. The clustering which gives the highest log likelihood was then picked and visualized in Figure 2.5.

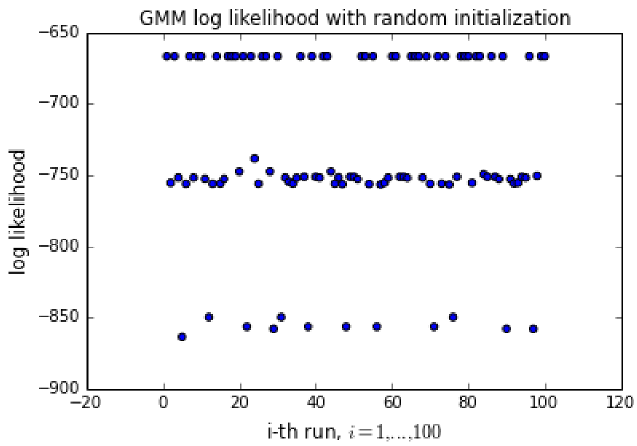

Figure 2.4: Log likelihood of GMM with random initialization, run 100 times

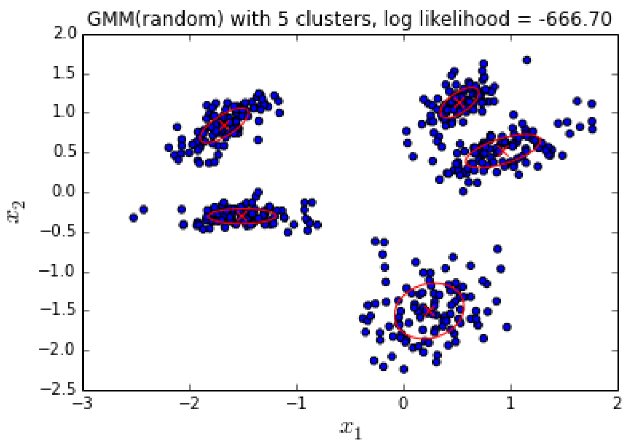

Figure 2.5: GMM clustering with random initialization, $k = 5$, applied to *5gaussians* data set

Finally, *GMM* with *k-means* initialization was utilized. It also finds the five clusters reliably. It was also run 100 times and the log likelihood of each run was calculated. Figure 2.6 and Figure 2.7 depict the log likelihood of each run and the clustering which gives the highest log likelihood, respectively.

As we have seen above, the three methods can find the five clusters reliably, because the *5gaussians* data set is a well-separated data set.

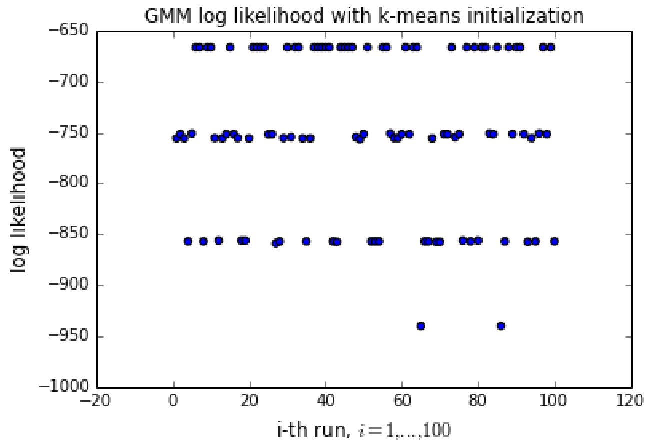

Figure 2.6: Log likelihood of GMM with k-means initialization, run 100 times

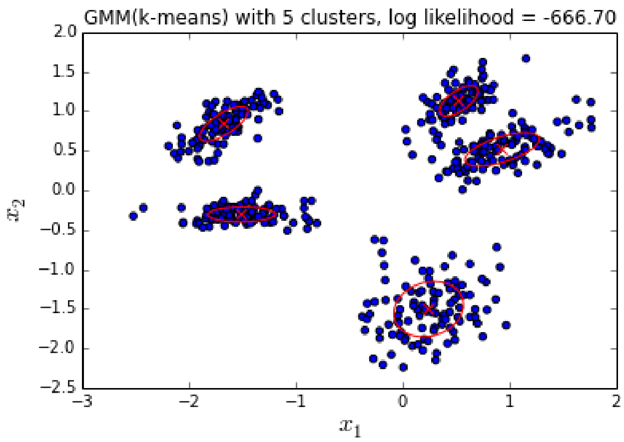

Figure 2.7: GMM clustering with k-means initialization, $k = 5$, applied to *5gaussians* data set

Question 6.2: What role does the initialization of the GMM with a k-means solution play in the number of necessary iterations and the quality of the solution?

The initialization of the *GMM* with a *k-means* solution plays a significant role in the number of necessary iterations until the convergence is reached. *GMM* depends strongly on the initialization. With *k-means* initialization, the *GMM* converged more quickly than random initialization.

GMM was run 100 times with random and k-means initialization to avoid some bad local optima. As we can see from Figure 2.8, *GMM* with random initialization never converged with the number of iterations below 20, whereas *GMM* with k-means initialization converged mostly only with about eight iterations.

On the other hand, the initialization does not play a significant role in the quality of the solution. Both the random and k-means initialization produce almost the same log likelihoods. Figure shows the maximum log likelihoods of both initialization which were run 100 times. Both methods produce almost the same maximum log likelihood, about -666.7011.

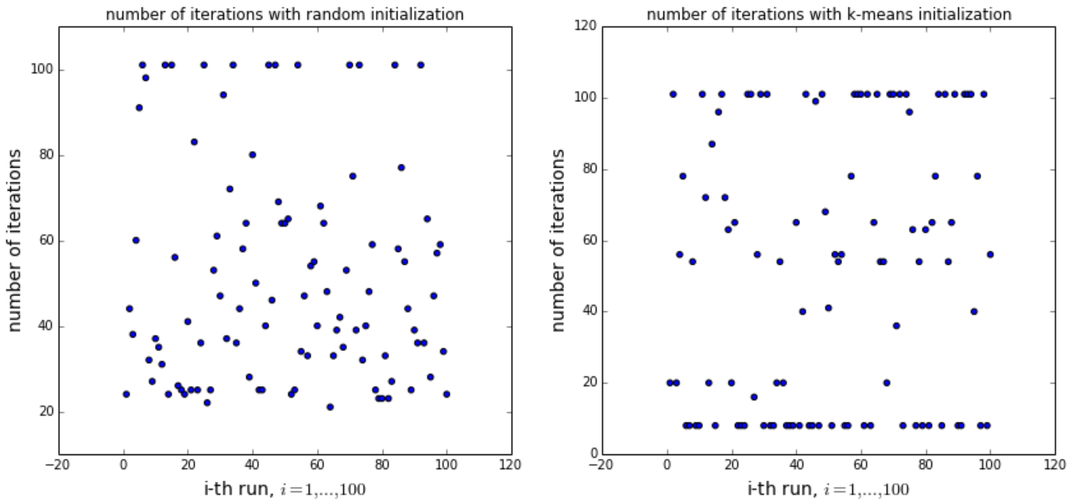

Figure 2.8: Number of iterations of *GMM* ($k = 5$) with random and k-means initialization, run 100 times

Question 6.3: What does the dendogramm of the hierarchical clustering look like and is it possible to pick a suitable value of *k* from the dendogramm?

It is possible to pick a suitable value of *k* from the dendogramm plot. Figure 2.10 shows the dendogramm plot of *kmeans_agglo* with initial clustering $k = 50$. From the plot, we can see that the clusters can actually be divided into five clusters (marked with yellow ellipses). Before the merge of those five clusters, there is no significant increase of the loss values. But after merging those five clusters, the loss values increase significantly.

In this case the difference in iterations seems insignificant. However, as will be seen in the presence of poorly separated data a good choice for our initial guesses can drastically reduce the number of iterations required to obtain convergence

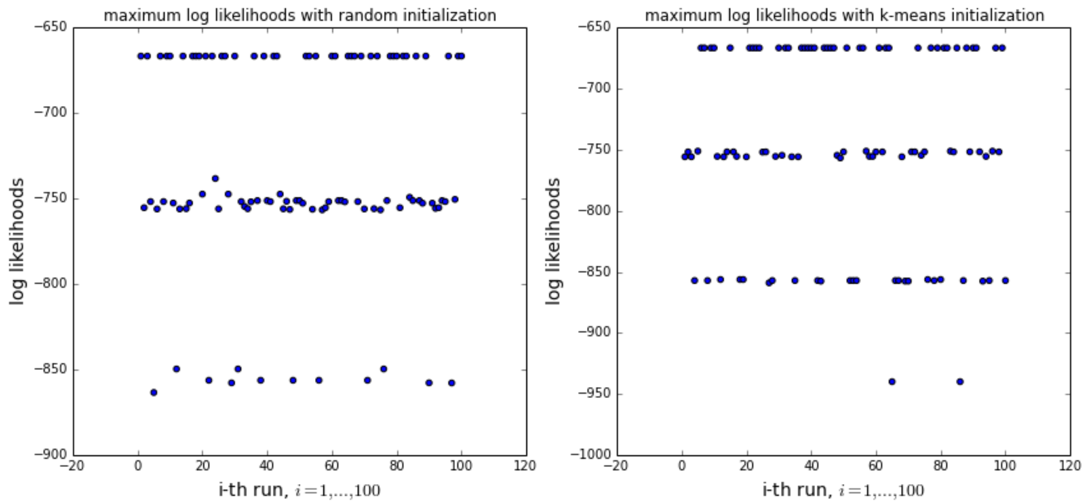

Figure 2.9: Maximum log likelihoods of *GMM* ($k = 5$) with random and k-means initialization, run 100 times

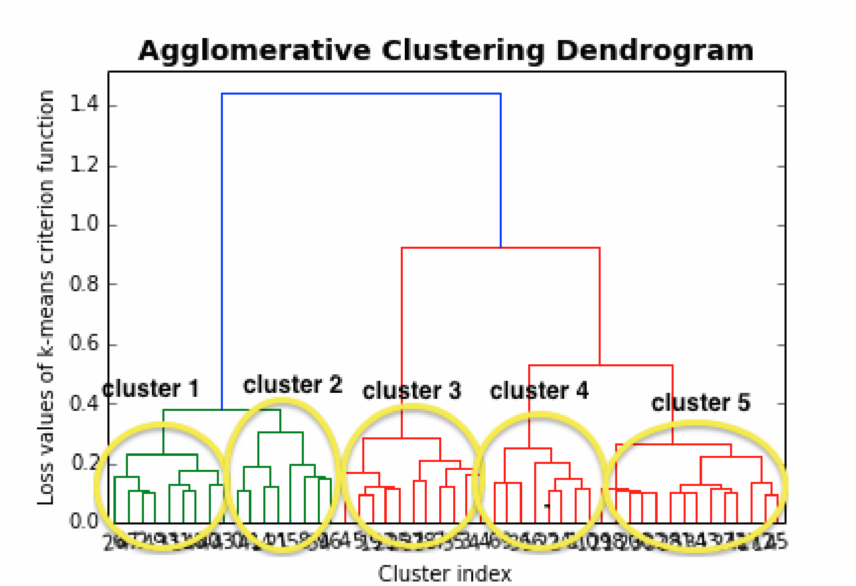

Figure 2.10: Dendogramm plot of the hierarchical clustering with initial clustering $k = 50$

2.2 Assignment 7: *2gaussian* Analysis

In this assignment the *2gaussians* data set should be analyzed with *k-means* and *GMM*. Figure 2.11 show the original *2gaussians* data set.

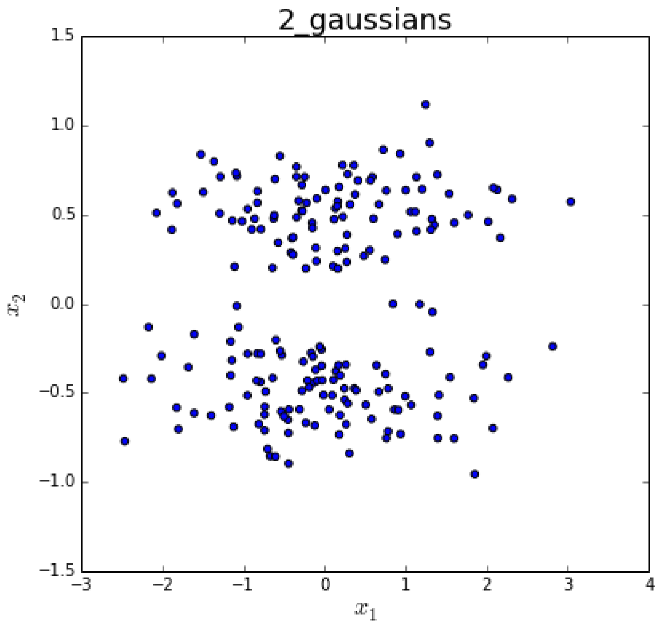

Figure 2.11: *2gaussians* data set

2.3 Assignment 8: *USPS* Analysis

In the last assignment of this problem set, *LLE* has to be applied to noisy *flatroll* data set. Two gaussian noise were added to the data set, with variance 0.2 and 1.8, respectively. After that, both noisy data sets should be unrolled using *knn* with a good value of *k* and a value which is obviously too large. Figure **??** depicts the two noisy images and their resulting embedding. It can be obtained that the noisy data set with big variance(1.8) is not very good unrolled.