# 2IMW30 - FOUNDATION OF DATA MINING
## Assignment 1b Report

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(Both students contributed equally in this assignment)

## EXERCISE 1

In this assignment, we implement the k-means algorithm for clustering the input data points. Clustering is considered as a unsupervised machine learning problem, that means there no labels in the data that we need to predict as classification, but it helps us getting some insights about the input data.

We developed four methods for initializing the first K cluster centroids (where K is an input) The first one is just choosing the first K data points to be the centroids, the second method is randomized selections of the initial centroids. the third method is k-means++ and the fourth method is using Gonzales algorithm.

For each method, we run k-means for different values of k 3,4,5 and in randomized methods, we run that 5 times. we visualise the results to get more understanding and learning experience as shown below. In figure 12, we shows the k-means clustering result on the dataset C2.txt with various initialization strategies and different values of $k$.

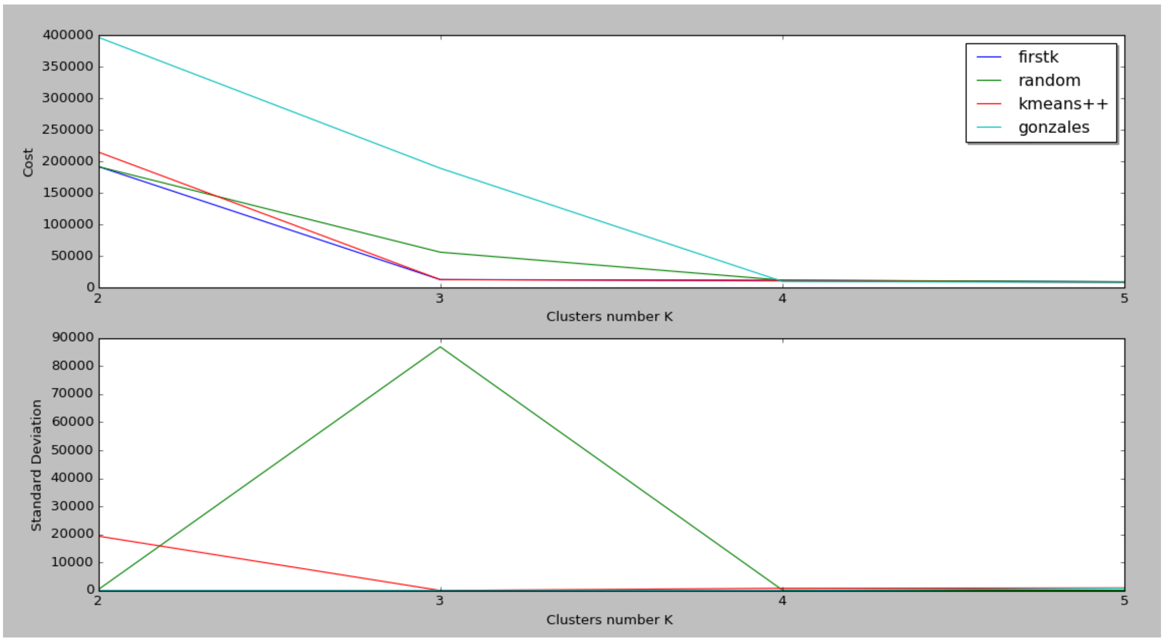


Figure 1: The average costs(top) and average Standard deviations(bottom) of several runs of k-means for different clusters numbers and using different methods of initialization.

The top digram of figure 1 shows the average cost of 5 runs of each method of initialization for k-means for different number of clusters, we can see that Gonzales method has the worst average cost across all the methods for 2 and 3 clusters. Starting of 4, all the method has similar costs on average. The reason for this is the distribution of the data points in the file C2 where we can find an outlier point that's very far of most of the points. this point is always chosen by Gonzales' algorithm as a center of one of the clusters.

The bottom figure shows standard deviation of the costs across all the 5 runs. and we can see the random initialization can have higher standard deviation which means that one or more of the runs can be highly deviated from average of the runs.

Figure 2 shows the convergent rate of k-means algorithm using the first 5 points as the initial centroids, we can see that of course it will be same if run this several times as no randomization exists.

Figure 3 and 4 shows the convergent rate of k-means algorithm of 3 clusters using Gonzales's algorithm centers as the initial centroids, we can see it converged in just one step.

But for 5 clusters Gonzales' algorithm convergent rate was diverse between 1 and 15 steps as in figure 5.

Doing the same for the random method we can see in figures 6 , 7 and 8 that for 3,4 and 5 clusters we can see different rates of convergence in each of the 5 runs per cluster number, that shows k-means algorithm is dependent on the initial centroids.

For kmeans++ we ran the algorithm 5 times for each different clusters number to visualize the convergence rate as in figures 9 , 10 and 11. We can that the rates are also diverse across diffrent runs but on average k-means converge in less number of steps due to the intelligence of kmeans++ and choosing the initial centroids.

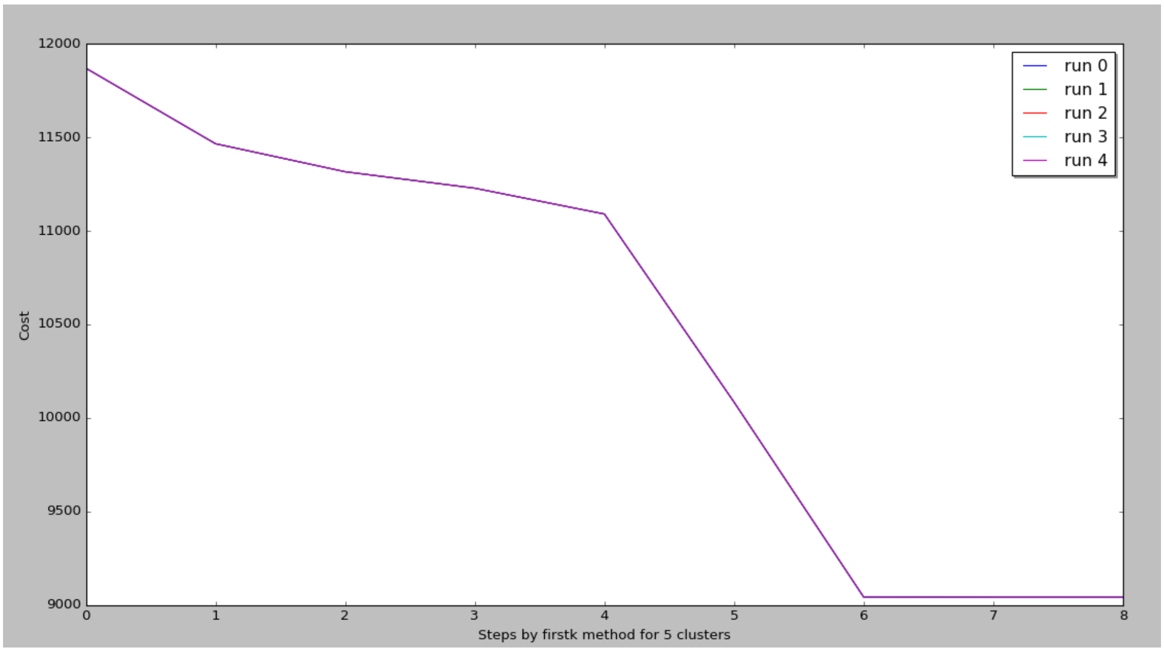


Figure 2

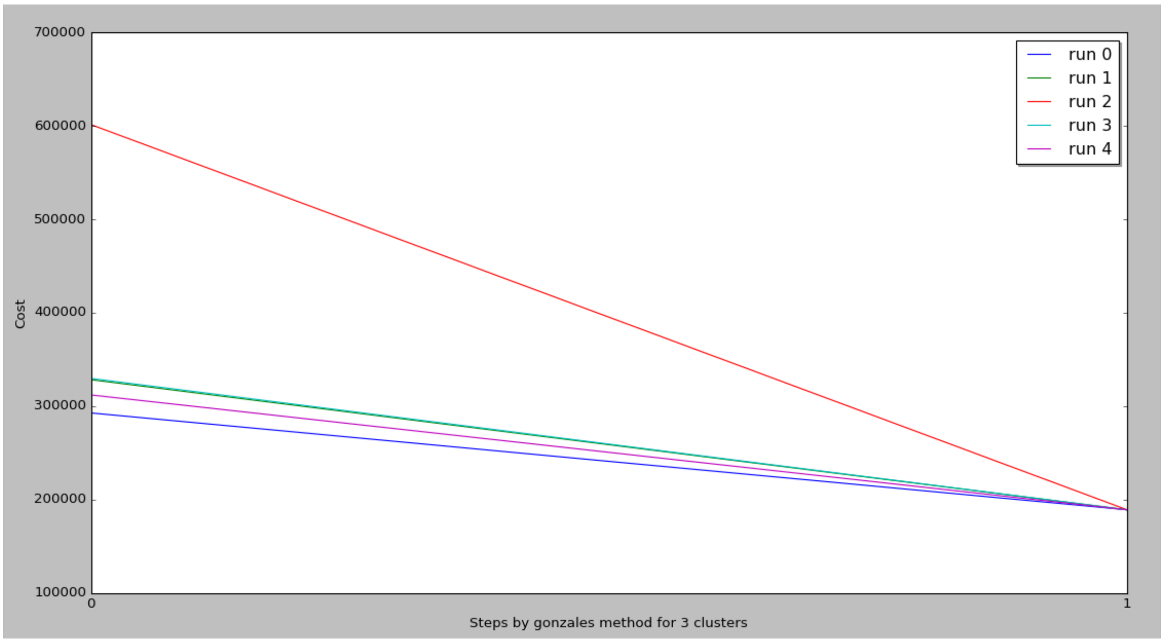


Figure 3

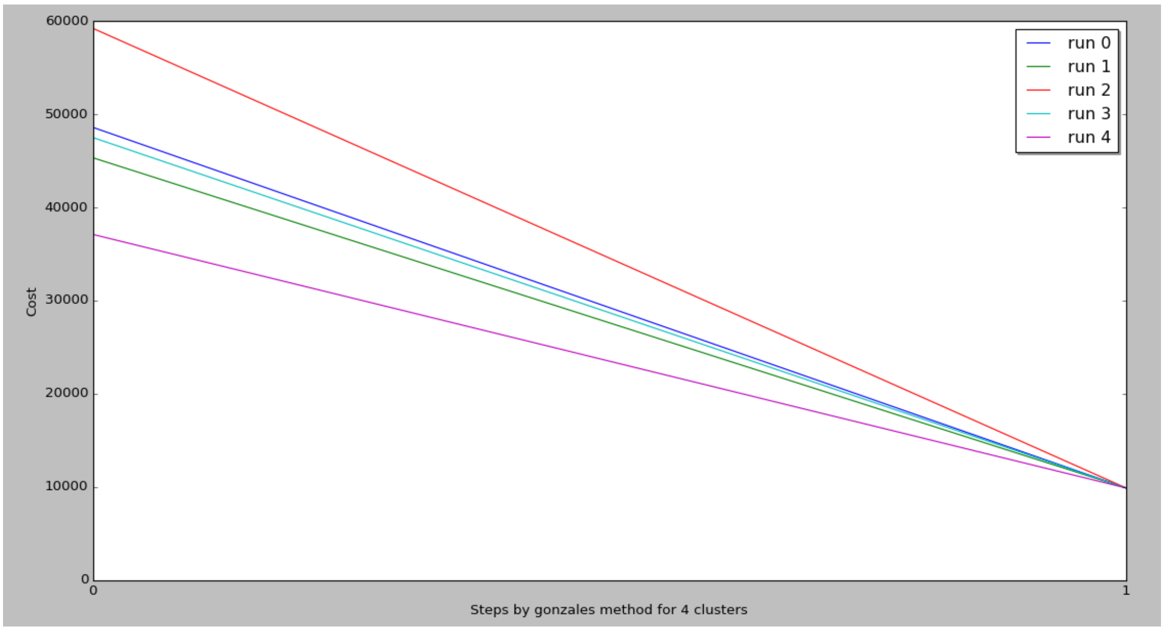


Figure 4

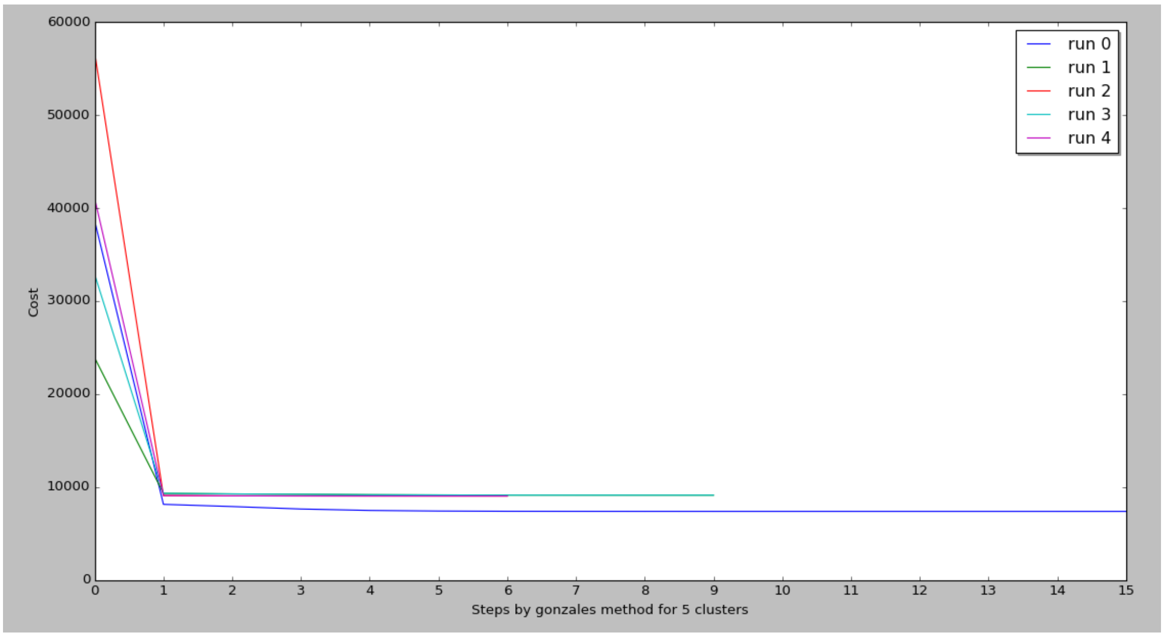


Figure 5

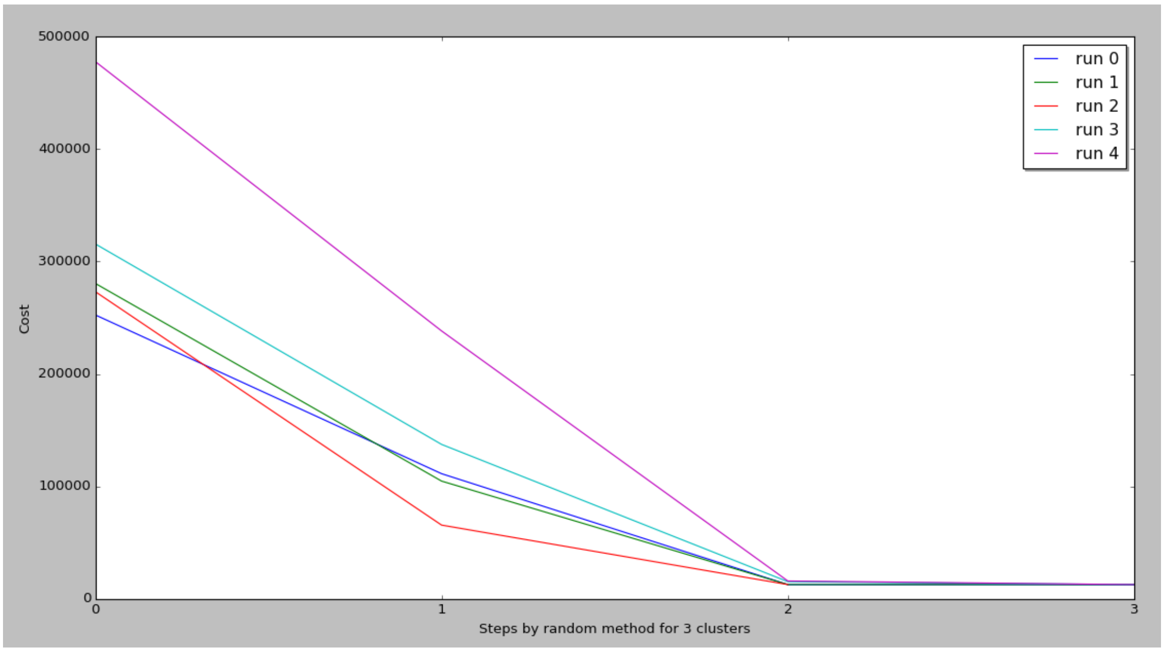


Figure 6: random5clusters

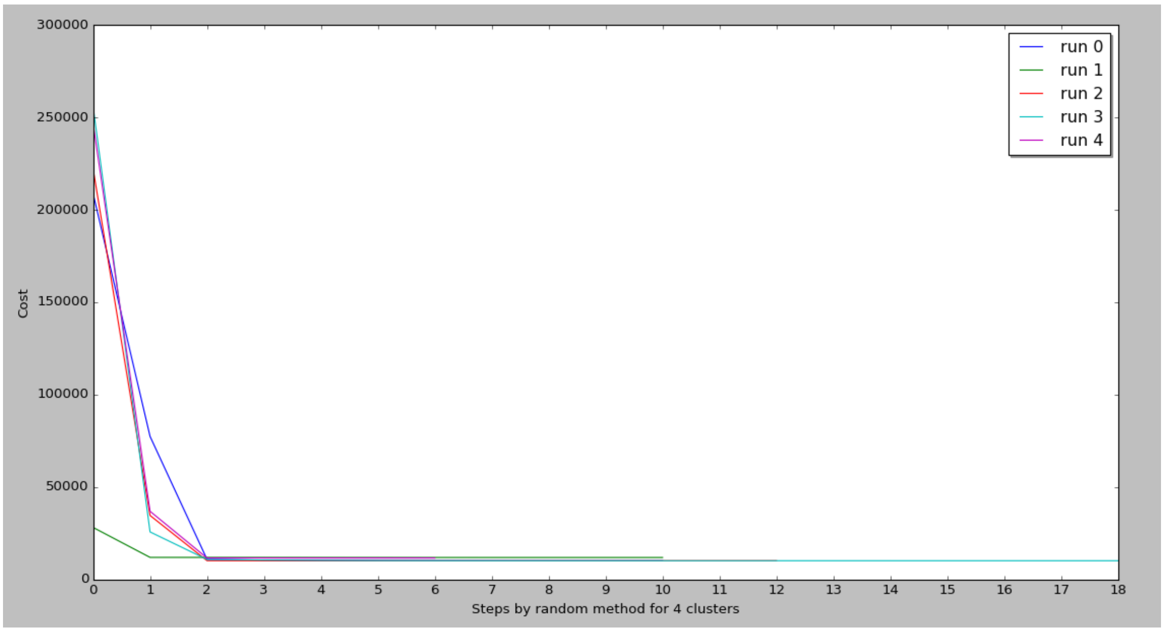


Figure 7: random5clusters

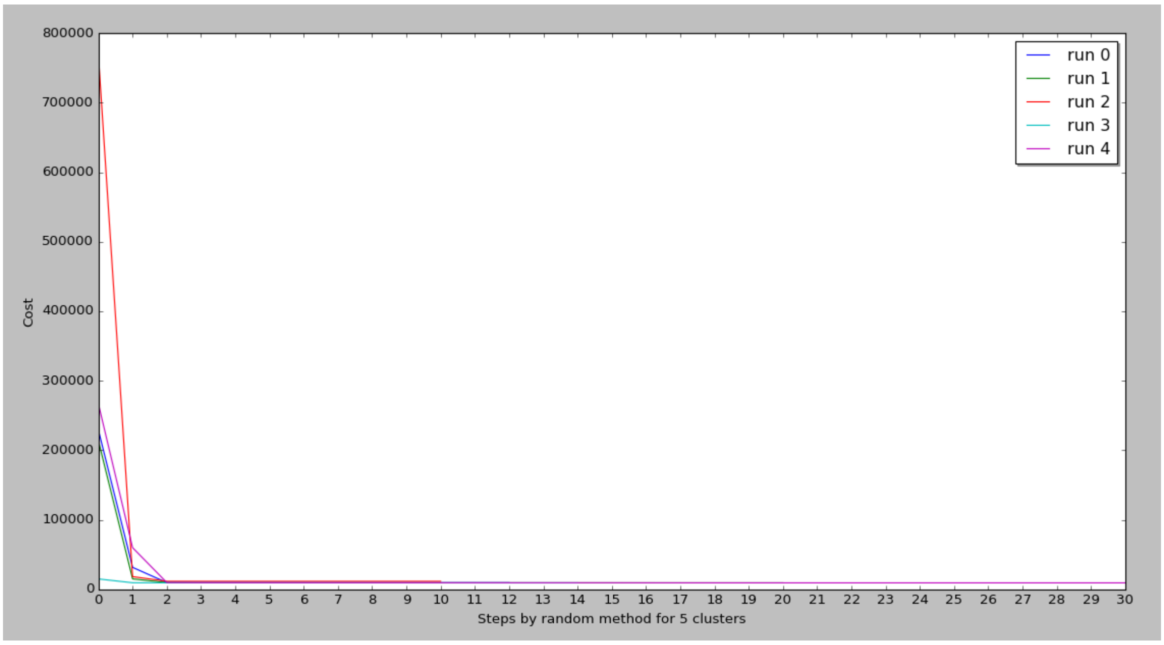


Figure 8: random5clusters

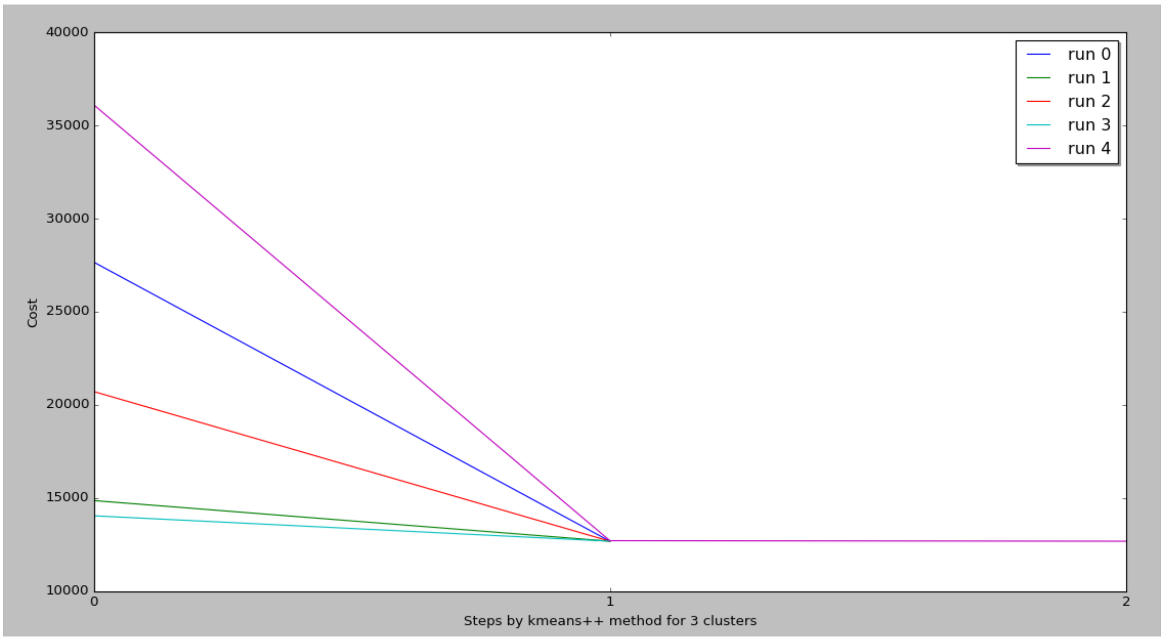


Figure 9: kmeans++3clusters

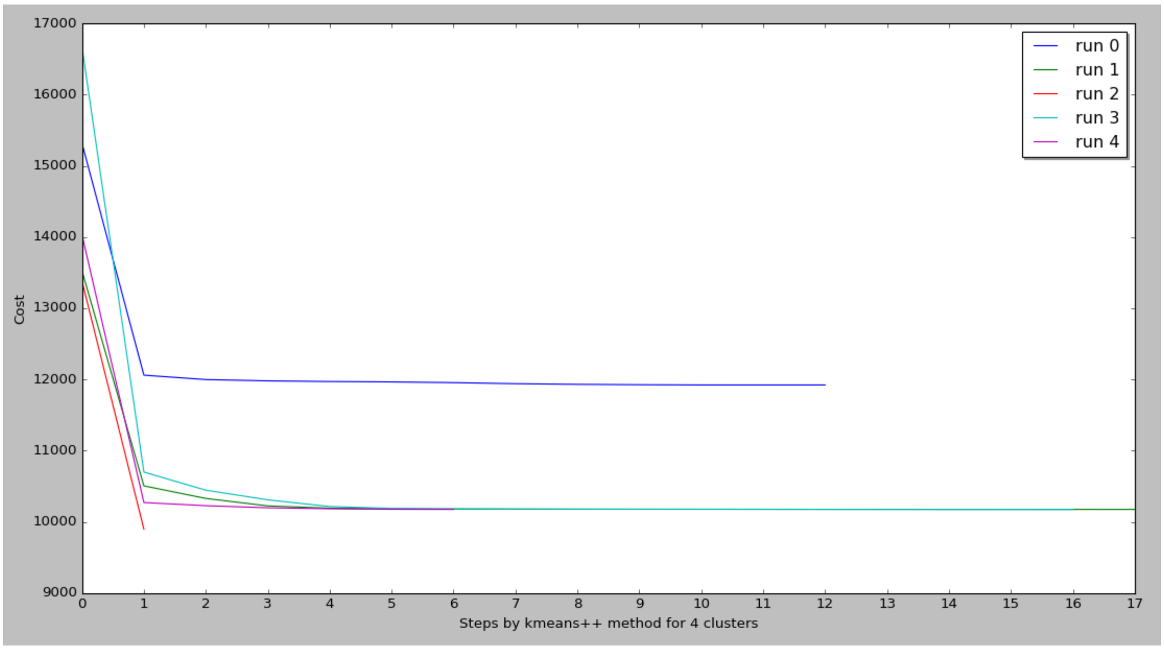


Figure 10: kmeans++3clusters

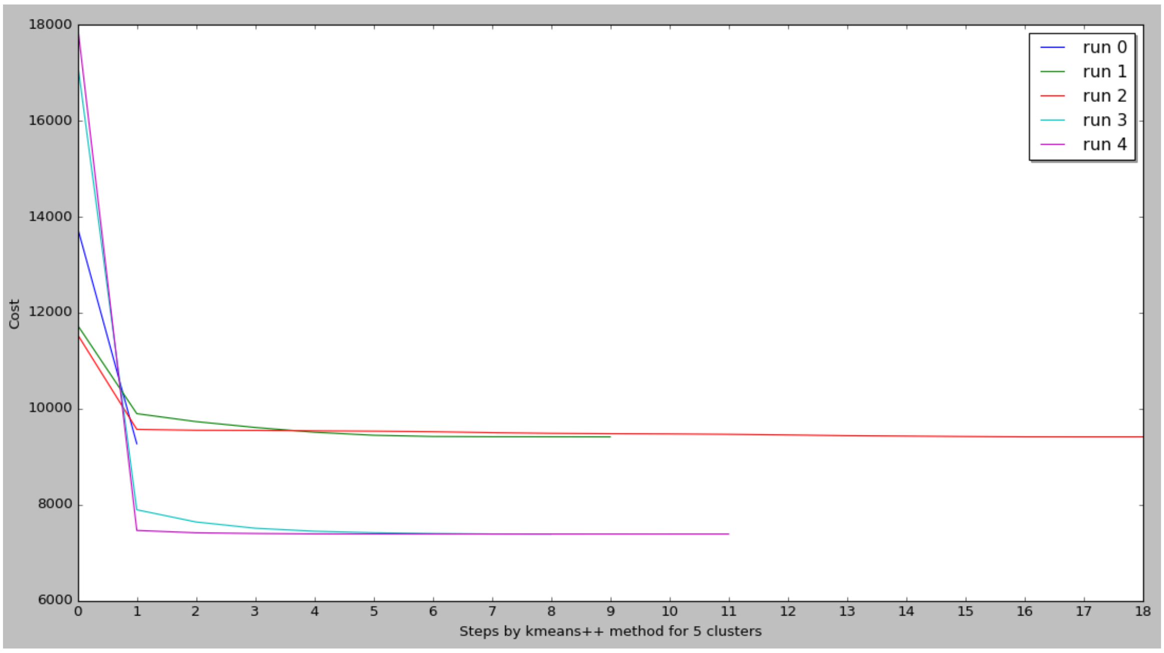
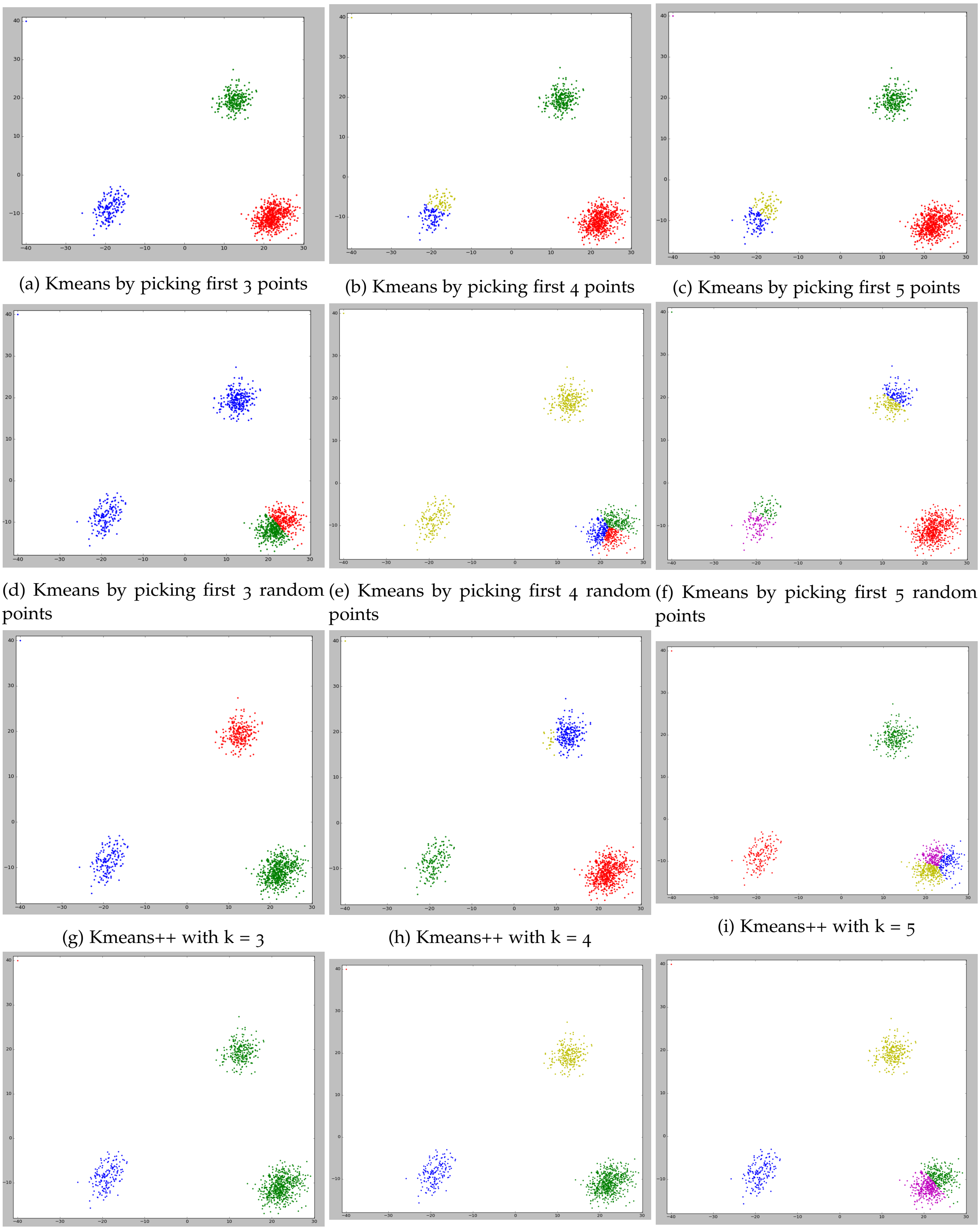


Figure 11: kmeans++3clusters



(a) Kmeans by picking first 3 points

(b) Kmeans by picking first 4 points

(c) Kmeans by picking first 5 points

(d) Kmeans by picking first 3 random points

(e) Kmeans by picking first 4 random points

(f) Kmeans by picking first 5 random points

(g) Kmeans++ with k = 3

(h) Kmeans++ with k = 4

(i) Kmeans++ with k = 5

(j) Kmeans using Gonzales algorithm to choose the seeds, k = 3

(k) Kmeans using Gonzales algorithm to choose the seeds, k = 4

(l) Kmeans using Gonzales algorithm to choose the seeds, k = 5

Figure 12: K-means results with different settings

## EXERCISE 2

In this excercise, we are proving that barycenter computed in the update step minimizes the cost function.

Let's first assume that $d = 1$. Then the cost function is

$$\phi(U, b) = \Sigma_{p_i \in U} ||p_i - b||^2$$

The function is minimized when its derivative is 0. In this case, we are considering the changes of the function with respect to the way we choose the center. Thus, we can take the partial derivative with respect to b.

$$\begin{aligned}\frac{d}{d_b}\Sigma_{p_i \in U}||p_i - b||^2 &= \Sigma_{p_i \in U}\frac{d}{d_b}||p_i - b||^2 \\ &= \Sigma_{p_i \in U}2 \cdot ||p_i - b|| \cdot \frac{||p_i - b||}{p_i - b} \cdot (-1) \\ &= 2\Sigma_{p_i \in U}(b - p_i)\end{aligned}$$

The cost function is minimized when

$$\begin{aligned}2\Sigma_{p_i \in U}(b - p_i) &= 0 \\ \Sigma_{p_i \in U}b &= \Sigma_{p_i \in U}p_i \\ b &= \frac{1}{n}\Sigma_{p_i in U}p_i\end{aligned}$$

where $n = |U|$.

The update step also assigns each point to the nearest center, which itself minimizes the total cost because the cost of each point is minimized.

When $d > 1$, the update step in each cluster is independent from the other clusters. Thus, the sum of the costs of each clusters is also minimized when each individual cost is minimized.

Therefore, the update step actually minimizes the cost function.

## EXERCISE 3

In this exercise, we show an example that the cosine distance does not follow the triangle inequality.

Let $p, q$ be 2 vectors where the angle $\alpha$ between them is $\frac{\pi}{2}$, and $r$ be the bisector of that angle. Thus, the angle $\beta$ between $p$ and $r$ and the angle $\gamma$ between $r$ and $q$ are both $\frac{\pi}{4}$. We have:

$$\begin{aligned}dist(p, q) &= 1 - cosine(\alpha) = 1 \\ dist(p, r) + dist(r, q) &= 1 - cosine(\beta) + 1 - cosine(\gamma) \\ &= 2 - \sqrt(2) < 1\end{aligned}$$

which means the cosine distance does not follow the triangle inequality in this case.

This completes the example.

## EXERCISE 4

### *a*

In this exercise, we consider another variant of the clustering problem, the k-median problem. The idea is similar to k-means in the sense that the distance from each point to its center is minimized.

The k-median approach can be more robust against noise because noise does not affect the order of the data, so the medians are not modified if the noise increases. If we use k-means, noise can biase the centroids.

*b*

We use a similar algorithm to k-means, just replace the means by the medians. Thatis, when updating a cluster, we take the point having the medians of the features as coordinates as the new center. This approach is obviously not optimal in term of cost-minimization, as the solution is proven in Exercise 2. So we will experiment the actual cost we get in the set C3.txt.