

2. Clustering

Describe two datasets of points in \mathbb{R}^2 of 6 points each. One dataset $D_1 = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_6)$ where single-linkage and 2-means-clustering (in terms of the objective function) output 2 clusters of the same sizes (3 points each), and one dataset $D_2 = (\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_6)$, on which the two methods output different clusterings in the following sense: one method outputs a balanced clustering of two clusters of 3 points each and the other one outputs one clusters with only 1 point and another one with 5 points.

(10 marks)

3. k-means clustering

In this question you will implement and experiment with the k -means algorithm.

- (a) Implement the k -means algorithm and include your code in your submission. As always, the data, consisting of n datapoints which are d -dimensional vectors, is given as an $n \times d$ -dimensional matrix. The output of your algorithm should be one n -dimensional vector containing values on $\{1, \dots, k\}$ indicating the cluster assignments of the points. We will work with three ways of initializing the centers. In the first, you will simply set the initial centers by hand. In the second you will choose k datapoints uniformly at random from the dataset as your initial centers. For the third initialization, choose the first center uniformly at random, and then choose each next center to be the datapoint that maximizes the sum of (euclidean) distances from the previous datapoints.
- (b) Load the first dataset `twodpoints.txt`. Plot the datapoints. Which number of clusters do you think would be suitable from looking at the points? Show that, for the number k that you chose by visually inspecting the data, the k -means algorithm can converge to different clusterings depending on the initializations. Show two such instances by plotting the clusterings that k -means produced (use a different color for the points of each cluster) together with the initial centers. In this part, set the initial centers manually.
- (c) Can the above phenomenon also happen if the initial centers are chosen uniformly at random? What about the third way of initializing? For each way of initializing, run the algorithm several times and report your findings.
- (d) From now on, we will work with the third method for initializing cluster centers. Run the algorithm for $k = 1, \dots, 10$ and plot the k -means cost of the resulting clustering (with respect to the last set of centers, which are the means of the output clusters). What do you observe? How does the cost evolve as a function of the number of clusters? How would you determine a suitable number of clusters from this plot (eg in a situation where the data can not be as obviously visualized).
- (e) Repeat the last step (that is, plot the cost as a function of $k = 1, \dots, 10$) for the next dataset `threedpoints.txt`. What do you think is a suitable number of clusters here? Can you confirm this by a visualization?

- (f) Load the UCI “seeds” dataset from the last assignment and repeat the above step. Recall that the task for this dataset is 3-class classification. Remove the last column (which contains the class labels) before the clustering. From how the k -means cost evolves, what seems like a suitable number of clusters for this dataset? How could you use this for designing a simple 3-class classifier for this dataset? What is the empirical loss of this classifier?
- (g) Design a simple (two-dimensional) dataset where the 2-means algorithm with the third initialization method will always fail to find the optimal 2-means clustering. Explain why it will fail on your example or provide plots of the data with initializations and costs that show that 2-means converges to a suboptimal clustering. Discuss what you think is the issue with this initialization method and how it could be fixed.

(4 + 4 + 4 + 4 + 4 + 5 + 5 marks)

IF ANYTHING IS UNCLEAR, COME TO MY OFFICE HOURS OR WRITE ME
EMAILS AND ASK QUESTIONS :)