ISYE 6740 Homework 1

1 Clustering [25 points]

Given m data points x^i, $i = 1, \ldots, m$, K-means clustering algorithm groups them into k clusters by minimizing the distortion function over $\{r^{ij}, \mu^j\}$

$$J = \sum_{i=1}^{m} \sum_{j=1}^{k} r^{ij} \|\mathrm{x}^i - \mu^j\|^2,$$

where $r^{ij} = 1$ if x^i belongs to the j-th cluster and $r^{ij} = 0$ otherwise.

1. (10 points) Prove (using mathematical arguments) that using the squared Euclidean distance $\|\mathrm{x}^i - \mu^j\|^2$ as the dissimilarity function and minimizing the distortion function, we will have

   $$\mu^j = \frac{\sum_i r^{ij} \mathrm{x}^i}{\sum_i r^{ij}}.$$

   That is, μ^j is the center of j-th cluster.

2. (5 points) Prove (using mathematical arguments) that K-means algorithm converges to a local optimum in finite steps.

3. (10 points) Calculate k-means by hands. Given 5 data points configuration in Figure 1. Assume $k = 2$ and use Manhattan distance (a.k.a. the ℓ_1 distance: given two 2-dimensional points (x_1, y_1) and (x_2, y_2), their distance is $|x_1 - x_2| + |y_1 - y_2|$). Assuming the initialization of centroid as shown, after one iteration of k-means algorithm, answer the following questions.

   (a) Show the cluster assignment;

   (b) Show the location of the new center;

   (c) Will it terminate in one step?

2 Image compression using clustering [25 points]

In this programming assignment, you are going to apply clustering algorithms for image compression. Your task is implementing the clustering parts with two algorithms: *K-means* and *K-medoids*. **It is required you implementing the algorithms yourself rather than calling from a package.**

K-medoids

In class, we learned that the basic K-means works in Euclidean space for computing distance between data points as well as for updating centroids by arithmetic mean. Sometimes, however, the dataset may work better with other distance measures. It is sometimes even impossible to compute arithmetic mean if a feature is categorical, e.g, gender or nationality of a person. With K-medoids, you choose a representative data point

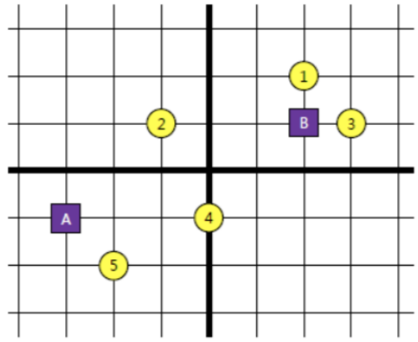


Figure 1: K-means.

for each cluster instead of computing their average. Please note that K-medoid is different from generalized K-means: Generalized K-means still computes centre of a cluster is not necessarily one of the input data points (it is a point that minimizes the overall distance to all points in a cluster in a chosen distance metric).

Given m data points $\mathrm{x}^i (i = 1, \ldots, m)$, K-medoids clustering algorithm groups them into K clusters by minimizing the distortion function $J = \sum_{i=1}^{m} \sum_{j=1}^{k} r^{ij} D(\mathrm{x}^i, \mu^j)$, where $D(\mathrm{x}, \mathrm{y})$ is a distance measure between two vectors x and y in same size (in case of K-means, $D(x, y) = \|\mathrm{x} - \mathrm{y}\|^2$), μ^j is the center of j-th cluster; and $r^{ij} = 1$ if x^n belongs to the k-th cluster and $r^{ij} = 0$ otherwise. In this exercise, we will use the following iterative procedure:

- Initialize the cluster center μ^j, $j = 1, ..., k$.
- Iterate until convergence:
  - Update the cluster assignments for every data point x^i: $r^{ij} = 1$ if $j = \arg\min_j D(\mathrm{x}^i, \mu^j)$, and $r^{ij} = 0$ otherwise.
  - Update the center for each cluster j: choosing another representative if necessary.

There can be many options to implement the procedure; for example, you can try many distance measures in addition to Euclidean distance, and also you can be creative for deciding a better representative of each cluster. We will not restrict these choices in this assignment. You are encouraged to try many distance measures as well as way of choosing representatives (e.g., ℓ_1 norm).

Formatting instruction

Input

- `pixels`: the input image representation. Each row contains one data point (pixel). For image dataset, it contains 3 columns, each column corresponding to Red, Green, and Blue component. Each component has an integer value between 0 and 255.
- `k`: the number of desired clusters. Too high value of K may result in empty cluster error. Then, you need to reduce it.

Output

- `class`: cluster assignment of each data point in pixels. The assignment should be 1, 2, 3, etc. For $k = 5$, for example, each cell of class should be either 1, 2, 3, 4, or 5. The output should be a column vector with `size(pixels, 1)` elements.

- `centroid`: location of k centroids (or representatives) in your result. With images, each centroid corresponds to the representative color of each cluster. The output should be a matrix with K rows and 3 columns. The range of values should be [0, 255], possibly floating point numbers.

Hand-in

Both of your code and report will be evaluated. Upload them together as a zip file. In your report, answer to the following questions:

1. (5 points) Within the k-medoids framework, you have several choices for detailed implementation. Explain how you designed and implemented details of your K-medoids algorithm, including (but not limited to) how you chose representatives of each cluster, what distance measures you tried and chose one, or when you stopped iteration.

2. (10 points) Attach a picture of your own. We recommend size of 320×240 or smaller. Run your k-medoids implementation with the picture you chose, as well as two pictures provided (beach.bmp and football.bmp), with several different K. (e.g, small values like 2 or 3, large values like 16 or 32) What did you observe with different K? How long does it take to converge for each K? Please write in your report.

3. (5 points) Run your k-medoids implementation with different initial centroids/representatives. Does it affect final result? Do you see same or different result for each trial with different initial assignments? (We usually randomize initial location of centroids in general. To answer this question, an intentional poor assignment may be useful.) Please write in your report.

4. (5 points) Repeat question 2 and 3 with k-means. Do you see significant difference between K-medoids and k-means, in terms of output quality, robustness, or running time? Please write in your report.

Note

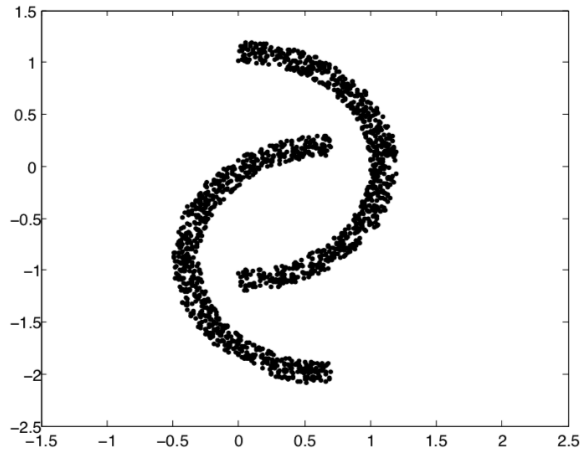
- You may see some error message about empty clusters when you use too large k. Your implementation should treat this exception as well. That is, do not terminate even if you have an empty cluster, but use smaller number of clusters in that case.

- We will grade using test pictures which are not provided. We recommend you to test your code with several different pictures so that you can detect some problems that might happen occasionally.

- If we detect copy from any other student's code or from the web, you will not be eligible for any credit for the entire homework, not just for the programming part. Also, directly calling built-in functions or from other package functions is not allowed.

3 Spectral clustering [25 points]

1. (10 points) For the following data (two moons), give one method that will successfully separate the two moons? Explain your rationale.



2. (15 points) Political blogs dataset.

   We will study a political blogs dataset first compiled for the paper Lada A. Adamic and Natalie Glance, "The political blogosphere and the 2004 US Election", in Proceedings of the WWW-2005 Workshop on the Weblogging Ecosystem (2005). The dataset `nodes.txt` contains a graph with $n = 1490$ vertices ("nodes") corresponding to political blogs. Each vertex has a 0-1 label (in the 3rd column) corresponding to the political orientation of that blog. We will consider this as the true label and try to reconstruct the true label from the graph using the spectral clustering on the graph. The dataset `edges.txt` contains edges between the vertices. You may remove isolated nodes (nodes that are not connected any other nodes).

   (a) (10 points) Assume the number of clusters to be estimated is $k = 2$. Using spectral clustering to find the 2 clusters. Compare the clustering results with the true labels. What is the false classification rate (the percentage of nodes that are classified incorrectly). **It is required you implementing the algorithms yourself rather than calling from a package.**

   (b) (5 points) You might observe the performance is not as good as you expected (given that there is no coding bugs). What do you think might be the reason for the not-so-good performance, due to the discrepancy from "theory" and "application"? Please write in your report.

4 PCA: Food consumption in European area [25 points]

The data `food-consumption.csv` contains 16 countries in the European area and their consumption for 20 food items, such as tea, jam, coffee, yoghurt, and others. There are some missing data entries: you may remove the rows "Sweden", "Finland", and "Spain". The goal is to perform PCA analysis on the data, i.e., find a way to perform linear combinations of features across all 20 food-item consumptions, for each country. If we extract two principal components, that means we use two singular vectors that correspond to the largest singular values of the data matrix, in combining features.

1. (5 points) Write down the set-up of PCA for this setting. Explain how the data matrix is set-up in this case (e.g., each dimension of the matrix correspond to what.) Explain in words how PCA is performed in this setting.

2. (5 points) Suppose we aim to find top k principal components. Write down the mathematical optimization problem involved for solving this problem. Explain the procedure to find the top k principal components in performing PCA.

3. (7 points) Find the top two **principal direction vectors (i.e., the eigenvectors of C)** for the dataset and plot them (plot a value of the vector as a one-dimensional function). Describe do you see any pattern. You may either use a package or write your own code.

4. (8 points) Now project each data point using the top two principal component vectors (thus now each data point will be represented using a two-dimensional vector). Draw a scatter plot of two-dimensional reduced representation for each country. What pattern can you observe? You may use use a package or write your own code.