CS5011W: Introduction to Machine Learning
Assignment 1
Course Instructor : Arun Rajkumar.
Release Date : March -03, 2022
Submission Date: On or before 5 PM on March 27 ,2022

SCORING: There are two questions in this assignment each with 4 sub questions. Each sub-question carries 12.5 points. The points will be decided based on the clarity and rigour of the report provided and the correctness of the code submitted.

DATASETS The data-set for both the questions is the same and is in a csv file titled Dataset.csv.

WHAT SHOULD YOU SUBMIT? You should submit a zip file titled 'Solutions_rollnumber.zip' where rollnumber is your institute roll number. Your assignment will NOT be graded if it does not contain all of the following:

- A text file titled 'Details.txt' with your name and roll number.
- A PDF file which includes explanations regarding each of the solution as required in the question. Title this file as 'Report.pdf'
- Clearly named source code for all the programs that you write for the assignment .

CODE LIBRARY: You are expected to code all algorithms from scratch. You cannot use standard inbuilt libraries for **algorithms**. You are allowed to use libraries for plotting, for Eigenvector computations, etc. You can use either Python or Matlab or C.

GUIDELINES: Keep the below points in mind before submission.

- Plagiarism of any kind is unacceptable. These include copying text or code from any online sources. These will lead to disciplinary actions according to institute guidelines.
- Any graph that you plot is unacceptable for grading unless it labels the x-axis and y-axis clearly.
- Don't be vague in your explanations. The clearer your answer is, the more chance it will be scored higher.

LATE SUBMISSION POLICY You are expected to submit your assignment on or before the deadline to avoid any penalty. Late submission incurs a penalty of points equal to 10 times the number of days your submission is late by. Any late submission post 3 days of the deadline would not be graded and will fetch 0 points.

QUESTIONS

(1) You are given a data-set with 1000 data points each in $\mathbb{R}^2$.

i. Write a piece of code to run the PCA algorithm on this data-set. How much of the variance in the data-set is explained by each of the principal components?

ii. Study the effect of running PCA without centering the data-set. What are your observations? Does Centering help?

iii. Write a piece of code to implement the Kernel PCA algorithm on this dataset. Use the following kernels :

A. $\kappa(x, y) = (1 + x^T y)^d$ for $d = \{2, 3\}$

B. $\kappa(x, y) = \exp \frac{-(x-y)^T(x-y)}{2\sigma^2}$ for $\sigma = \{0.1, 0.2, \ldots, 1\}$

Plot the projection of each point in the dataset onto the top-2 components for each kernel. Use one plot for each kernel and in the case of (B), use a different plot for each value of σ.

iv. Which Kernel do you think is best suited for this dataset and why?

(2) You are given a data-set with 1000 data points each in $\mathbb{R}^2$.

i. Write a piece of code to run the algorithm studied in class for the K-means problem with $k = 4$. Try 5 different random initialization and plot the error function w.r.t iterations in each case. In each case, plot the clusters obtained in different colors.

ii. Fix a random initialization. For $K = \{2, 3, 4, 5\}$, obtain cluster centers according to K-means algorithm using the fixed initialization. For each value of K, plot the Voronoi regions associated to each cluster center. (You can assume the minimum and maximum value in the data-set to be the range for each component of $\mathbb{R}^2$).

iii. Run the spectral clustering algorithm (spectral relaxation of K-means using Kernel-PCA) $k = 4$. Choose an appropriate kernel for this data-set and plot the clusters obtained in different colors. Explain your choice of kernel based on the output you obtain.

iv. Instead of using the method suggested by spectral clustering to map eigenvectors to cluster assignments, use the following method: Assign data point i to cluster ℓ whenever

$$\ell = \arg \max_{j=1,\ldots,k} v_i^j$$

where $v^j \in \mathbb{R}^n$ is the eigenvector of the Kernel matrix associated with the j-th largest eigenvalue. How does this mapping perform for this dataset?. Explain your insights.