CSCI 3320: Fundamental of Machine Learning

Programming Assignment 1

Instructor: Prof. John C.S. Lui Due: 23:59 on Sun. Mar. 29, 2020

1 Introduction

k-means clustering is a method of vector quantization. It aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean, serving as a prototype of the cluster. When handling the high-dimensional input data, to make the clustering more efficient, we can apply Principal Component Analysis (PCA) to perform the dimension reduction for the input data. PCA provides a way to create a low dimensional representation of data. This can not only reduce the complexity of the clustering, but also improve the clustering result by the noise reduction. This programming assignment is provided to help you to gain a better understanding of these two methods: we combine these two method with an image data application. More specifically, this programming assignment consists of the following two parts.

- The first part will guide you through a complete version of **Principal Component Analysis (PCA)**. First, you will learn to implement your own PCA, and compare with the scikit-learn programming interface for the PCA task. Then, you will have an idea of solving practical problems with PCA by performing it on the image data.
- The second part is an exercise about *k*-means clustering. The purpose is to help you understand the process of the *k*-means clustering and different performance evaluation metrics. You will also learn the scikit-learn programming interface for *k*-means clustering.

1.1 File Descriptions

To start, you need to download the asgn1.zip file from the course website. In asgn1.zip, we provide the following files for you:

- ex1.py: contains some python scripts for you to learn to implement your own PCA.
- ex2.py: contains some python scripts for you to learn to apply PCA on the image data.
- mnist-subset.zip: contains images of handwritten digits 0, 1, 2, which is a subset of the LeCun's MNIST dataset.
- ex3.py: contains some python scripts for you to learn to perform k-means clustering on the synthetic dataset.

- ex4.py: contains some python scripts for you to learn to perform k-means clustering on the image data.
- t10k-images.idx3-ubyte and t10k-images.idx3-ubyte: contains images of handwritten digits, which is a subset of the LeCun's MNIST dataset.

Note: Please do **not** change filenames (*.py) of files described above.

2 Principal Component Analysis (PCA)

2.1 Implement PCA(20%)

Our first problem is to perform PCA on the created dataset. The purpose is to help you understand details of PCA. Please refer to chapter 6 (Dimension Reduction) of the lecture notes. You need to finish the following tasks:

1. Write Your Own PCA. (10%)

Read lecture notes carefully, and implement your own PCA. You need to complete the function pca(X) in the ex1.py script. The input is the matrix X in which each row represents a sample. The output should be [V, D], where V is a matrix containing all eigenvectors (whose eigenvalues are in a decreasing order) and D should be a column vector containing all eigenvalues (in a descent order). You can compare your result with the one of PCA in the scikit-learn¹.

2. Plot Eigenvalues and POV. (10%)

In ex1.py, we generate a dataset X, which is a 1000×6 matrix. Perform PCA on this matrix and plot all eigenvalues in a decreasing order. Assume the descent ordered eigenvalues are $\lambda_1, \lambda_2, \dots, \lambda_N$. The x-axis should be $1, 2, \dots, N$ (the order of eigenvalues) and y-axis should be the eigenvalues (refer to pages 20 in chapter 6). Use the definition of Proportion of Variance (POV) explained in the lecture notes, plot POV v.s. the order of the eigenvalues (refer to pages 20 in chapter 6).

Note: You need to submit ex1.py in task 2.1. Your ex1.py file should output the result of [V, D] to the prompt and plot the figure of eigenvalues v.s. the order of the eigenvalues and the figure of POV v.s. the order of the eigenvalues. Make sure your python script has no syntax error before submission.

2.2 Perform PCA on Image Data(25%)

In this part, you are required to perform PCA on images of handwritten digits. In asgn1.zip, we provide mnist-subset.zip which is a subset of the LeCun's MNIST dataset containing images of handwritten digits 0, 1, 2. We already provide the code to read images into a

 $^{^{1} \}texttt{http://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html}$

matrix X to represent them in python script ex2.py. Each row of the matrix X represents an image. You are required to finish the following task.

1. Plot the Eigen Images. (10%)

Perform PCA on the matrix X. You can use PCA implemented by yourself or the one provided in scikit-learn. Plot **eigenvectors** corresponding to **the largest 9 eigenvalues**. Combine and save these figures in a single file **eigens_fig.jpg**. We also provide the sample code for presenting **vectors** as an image. For PCA on images data, you can read the example in scikit-learn².

2. **Plot POV**. (15%)

Plot POV v.s. the order of eigenvalues as in task 2.1. Save figures in file digit_pov.jpg. You also need to answer that to achieve POV larger than 0.95, how much dimensions should we preserve? Create a file description2.txt to describe your answers and your understanding of the result.

<u>Note:</u> You need to submit the python script ex2.py which includes the implementation of task 2.2. Besides, you also need to submit eigens_fig.jpg, digit_pov.jpg and description2.txt in this task.

3 k-Means Clustering

3.1 k-Means Clustering on the Synthetic Dataset (25%)

Our problem in this task is to perform k-means clustering on the synthetic dataset. The purpose is to help you understand the process of k-means clustering and different performance evaluation metrics. You need to finish the following tasks. Please use ex3.py as your starting point.

1. Creat dataset. (5%)

Please read how we generate the datasets in creat_dataset(), and see what are centers of clusters. Complete creat_dataset() and plot data points in a scatter plot. Use different colors to represent clusters.

2. k-means clustering. (10%)

Complete the function my_clustering(X, y, n_clusters).

- Inputs. Sample points (X, y) and the number of clustering.
- Tasks. Implement the k-means by yourself and cluster samples into n_clusters clusters using your own k-means. Print out all cluster centers. Plot all clusters formed, and use different colors to represent clusters defined by k-means. Draw a marker (e.g., a circle or the cluster id) at each cluster center.

²http://scikit-learn.org/stable/auto_examples/applications/face_recognition.html

• Outputs. Return the following four evaluation metrics: Adjusted Rand index, Mutual Information based scores, V-measure, and Silhouette Coefficient. For details about these metrics, you can read the documentation of scikit-learn ³.

3. Select the number of clusters. (10%)

Plot scores of all four evaluation metrics as functions of n_clusters in a single figure. What's the best number of clusters? Answer this in description3.txt.

Note: You need to submit ex3.py and description3.txt for task 3.1. Your ex3.py script should output cluster centers and values of four evaluation metrics mentioned above. Also, it should plot formed clusters and scores of all four evaluation metrics as functions of n_clusters as mentioned above.

3.2 k-Means Clustering on the Image Dataset (30%)

In this part, we want to cluster images of handwritten digits. In asgn1.zip, we provide two input files t10k-images.idx3-ubyte and t10k-labels.idx1-ubyte. They are subsets of the LeCun's MNIST dataset containing images of handwritten digits. You are required to finish the following tasks. Please use ex4.py as your starting point.

1. Load the dataset. (5%)

We provide codes to load images and their labels into a matrix X and a label vector y to represent them in python script ex4.py. Each row of the matrix X represents an image. What are the number of samples and the number of features? Answer them in description4.txt.

2. **PCA**. (5%)

Perform PCA on the matrix X (requirement: $POV \ge 0.9$).

3. k-means clustering. (10%)

Complete my clustering mnist(X, y, n clusters).

- Inputs. Sample points (X, y) and the number of clustering n clusters.
- Tasks. Cluster images into n_clusters clusters using the k-means implemented by yourself or the one provided in scikit-learn. Plot centers of clusters as images and combine these images in a single figure.
- Outputs. Return the following evaluation metrics: Adjusted Rand index, Mutual Information based scores, V-measure, and Silhouette Coefficient.

4. What is the best number of clusters? (10%)

Plot scores of all four evaluation metrics as functions of n_clusters. In description4.txt, briefly describe the figure you see. Feel free to state your insights about what you see.

http://scikit-learn.org/stable/modules/clustering.html#clustering-performance-evaluation

 $^{^3}$ Section 2.3.9 in

<u>Note:</u> You need to submit ex4.py and description4.txt for task 3.2. Your ex4.py script should output values of all four evaluation metrics. It should also plot centers of clusters and scores of all four evaluation metrics as functions of n_clusters.

4 Submission

Instructions for the submission are as follows. Please follow them carefully.

- 1. Make sure you have answered all questions in your report.
- 2. Test all your Python scripts before submission. Any script that has syntax error will not be marked.
- 3. Zip all the required files into a single zipped file named <student-id>_asgn1.zip, where <student-id> should be replaced with your own student ID. e.g., 1155012345_asgn1.zip. Please do not change the filenames of the python scripts. The following is the checklist for you:
 - ex1.py
 - ex2.py
 - ex3.py
 - ex4.py
 - eigens fig.jpg
 - digit_pov.jpg
 - description2.txt
 - description3.txt
 - description4.txt
- 4. Submit the zipped file <student-id>_asgn1.zip to CUHK Blackboard System no later than 23:59 on Sun. Mar. 29, 2020.