K-means

Group 04:

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Introduction

K-means algorithm is used in the solution of the clustering problem. It aims to partition *n* given data points (or observations) into *k* different clusters. This algorithm dates back to 1957 by Stuart Lloyd and 1965 by E. W. Forgy.

Programming setup

Python (version 3) was used as a programming language for this assignment. It was chosen for it's ease of use and comprehensive list of available packages which could simplify the development of the program. Package-management system **pip** allowed us to use the following packages:

1. NumPy – library which supports multi-dimensional arrays and matrices and also provides the functions to operate on them. We also used it as a tool to import data from TXT and CSV files.
2. Scikit-learn – machine learning library which gave us the ability to calculate the Normalized Mutual Information score.
3. Matplotlib – plotting library which was used by us to visualize the clustering result.

Project structure

The project has the following structure:

1. kmeans.py – main class, where the data is read, processed, metrics are calculated, execution time is measured, and the results are presented.
2. setup.py – class which is required for setuptools working.
3. init_strategies.py – class which describes different techniques for the initial definition of clusters in k-means algorithm.
4. update_strategies.py – class where different algorithms to update cluster's centroids are described.

5. mq_run_script.py – separate script which is used for MacQueen update strategy.
6. experiment.py – benchmark tool which is used for calculation the average results among 100 runs.

Initialization techniques

Our team has implemented three different algorithms for initial definition of clusters in k-means algorithm:

1. Random initialization – given *n* data points, we choose random *k* among them and define them as our cluster centroids.
2. Farthest point initialization – first point is selected randomly, second one is chosen with the largest distance to the first one, third point has the largest distance to two previous points and so on, until all *k* clusters are defined.

Updating techniques

We have developed two algorithms for updating the clusters:

1. Lloyd algorithm – cluster centroids are updated after all point's affiliation with clusters are recalculated.
2. MacQueen algorithm – cluster centroids are updated after every single one recalculation of point's cluster membership.

Dataset description

Two datasets were used in our k-means implementation:

1. Skin Segmentation Data Set – RGB values from face images of various age, race groups and genders. They are taken from FERET and PAL databases. 50859 instances are skin samples, and 194198 are non-skin samples (artificially generated values).
2. HTRU2 Data Set - a sample of pulsar candidates collected during the High Time Resolution Universe Survey. There are 8 continuous variables describing each instance in dataset. 1639 instances are real pulsar examples and 16259 are fake.

Metrics

For the evaluation of the results, two metrics were used:

1. **Normalized Mutual Information (NMI)** measures the similarity between two labels of the same data. If $|U_i|$ is the number of samples in cluster

U_i, and $|V_j|$ is the number of samples in cluster V_j, their mutual information equals

$$MI(U,V) = \sum_{i=1}^{|U|} \sum_{j=1}^{|V|} \frac{|U_i \cap V_j|}{N} \log \frac{N|U_i \cap V_j|}{|U_i||V_j|}$$

Then, mutual information is normalized.
NMI score has values between 0 and 1, where 0 means “no mutual information” and 1 mean “perfect correlation”.
Ideal k-means algorithm would provide the result with NMI score equals 1.

2. **Within-cluster sum of squares (WCSS)** is the sum of squared deviations from each observation and the cluster centroid. If ($\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_n$) is the set of observations, and $\mathbf{S} = \{S_1, S_2, …, S_k\}$ are the clusters with $\boldsymbol{\mu}_i$ - the mean of points in S_i, then WCSS is:

$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2 = \underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{k} |S_i| \operatorname{Var} S_i$$

The lower the metric, the better, because it means that the cluster is more compact.

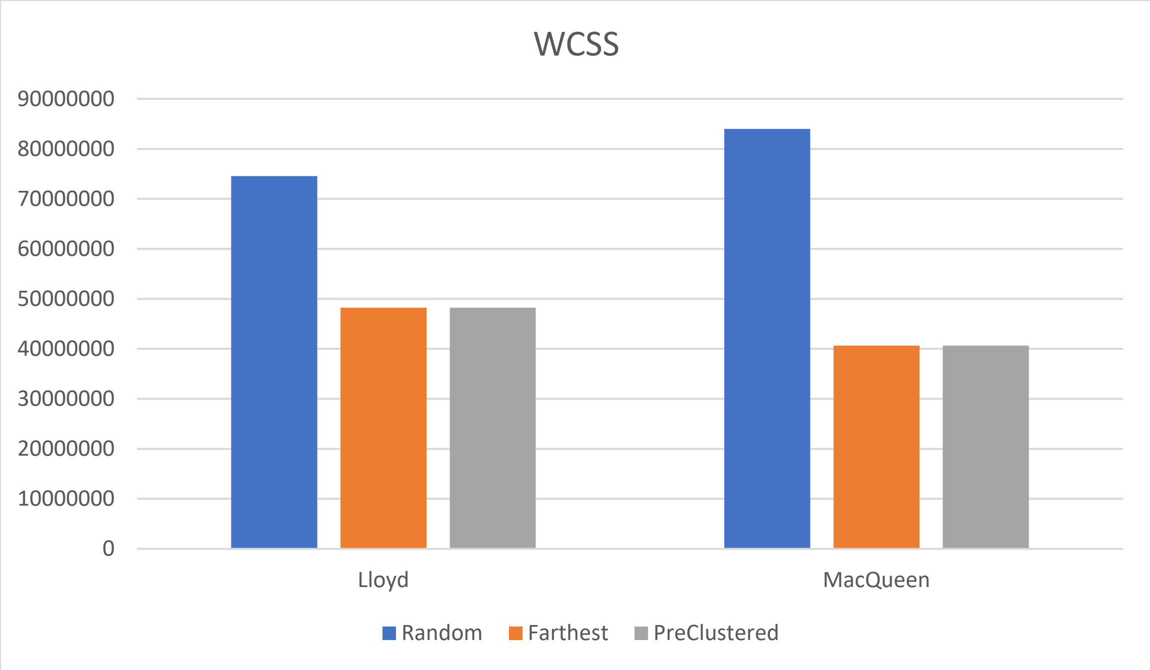
Result of k-means algorithm

We evaluated six possible combinations of k-means algorithm (three initialization strategies multiply by two update strategies) regarding to the HTRU2 dataset. The result metrics (NMI and WCSS) are presented in tables below:

WCSS	Random	Farthest	PreClustered
Lloyd	74544592,5012591	48229826,3875866	48229826,3875866
MacQuee	84000670,7533754	40670318,7237643	40670318,1221059

NMI	Random	Farthest	PreClustered
Lloyd			
MacQueen			

Let’s visualize results:



Conclusion

If we compare different algorithms by using WCSS metric, we may notice that MacQueen update strategy performs better than Lloyd, because the resulting clusters are more compact. Comparing different initialization algorithms, we conclude that random initialization leads to worst results, while “Farthest” and “PreClustered” have better performance, but their score is identical.