MLT Week-3

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Contents

Abstract

The week commences with an introduction to the concept of clustering and a comprehensive examination of the K-means algorithm, a crucial element within the topic. The week also delves into the constraints of the K-means approach and offers potential remedial measures to address such limitations.

1 Introduction to Clustering

Clustering is a method of unsupervised machine learning that groups similar objects into clusters, discovering structure in data for exploratory analysis or as a pre-processing step for other algorithms.
Our objective is to group n datapoints into k clusters.
Notation:

$$\{x_1, x_2, \ldots, x_n\} \qquad x_i \in \mathbb{R}^d$$

$$\{z_1, z_2, \ldots, z_n\} \qquad z_i \in \{1, 2, \ldots, k\}$$

Objective Function:

$$F(z_1, z_2, \ldots, z_n) = \sum_{i=1}^{n} ||x_i - \mu_{z_i}||_2^2$$

where

$$\mu_k = \frac{\sum_{i=1}^{n} x_i \cdot \mathbf{1}(z_i = k)}{\sum_{i=1}^{n} \mathbf{1}(z_i = k)}$$

Goal:

$$\min_{\{z_1, z_2, \ldots, z_n\}} \sum_{i=1}^{n} ||x_i - \mu_{z_i}||^2$$

Unfortunately, finding a solution manually is an NP-Hard problem due to the existence of k^n possibilities. As a result, alternative approaches must be considered to address this challenge.

2 K-means Clustering (Lloyd's Algorithm)

Lloyd's Algorithm, also known as the k-means algorithm, is a widely used and straightforward method for clustering that divides a dataset into K pre-determined clusters by iteratively computing the mean distance between the points and their cluster centroids.

2.1 The Algorithm

The algorithm is as follows:

Step 1: Initialization
Assign $z_1^0, z_2^0, \ldots, z_n^0$ where $z_i^0 \in \{1, 2, \ldots, k\}$. The approach on how to initialize them is discussed later.

Step 2: Compute Means

$$\mu_k^t = \frac{\sum_{i=1}^{n} x_i \cdot \mathbf{1}(z_i^t = k)}{\sum_{i=1}^{n} \mathbf{1}(z_i^t = k)} \qquad \forall k$$

Step 3: Reassignment Step

$$z_i^{t+1} = \arg\min_k ||x_i - \mu_k^t||_2^2 \qquad \forall i$$

Step 4: Loop until Convergence
Repeat steps 2 and 3 until convergence for t iterations.

2.2 Fact regarding Lloyd's Algorithm

Lloyd's Algorithm, also known as K-means, is guaranteed to converge to a solution. While the converged solution may not be the optimal one, it has been observed to produce acceptable clustering results in practice.

3 Convergence of K-means Algorithm

The objective function strictly reduces after each reassignment.

$$F(z_1^{t+1}, z_2^{t+1}, \ldots, z_n^{t+1}) \leq F(z_1^t, z_2^t, \ldots, z_n^t)$$

And as there are only finite number of reassignments possible, the algorithm must converge.
Alternate Explanation: K-means algorithm converges because it is an iterative procedure that minimizes the sum of squared distances between points and their cluster centroids, which is a convex function with a global minimum. The algorithm will reach the convergence point, guaranteed to exist, under mild assumptions on the initial cluster means, making it a reliable tool for clustering.

4 Nature of Clusters Produced by K-means

Let μ_1 and μ_2 be the centroids of the clusters C_1 and C_2 respectively.
For C_1,

$$||x - \mu_1||^2 \leq ||x - \mu_2||^2$$
$$\therefore x^T(\mu_2 - \mu_1) \leq \frac{||\mu_2||^2 - ||\mu_1||^2}{2} \qquad \forall x$$

The cluster regions are known as half-spaces or Voronoi regions.

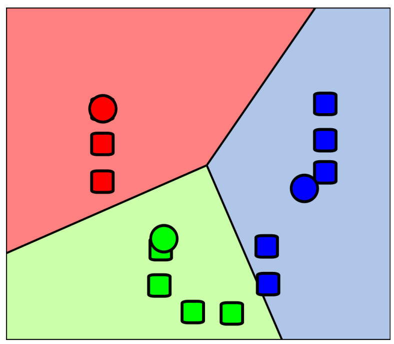
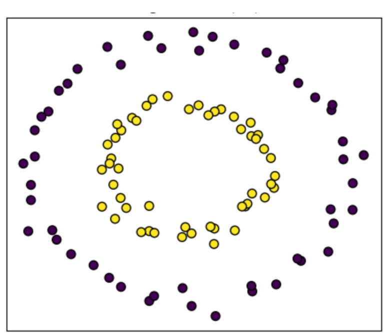


Figure 1: Voronoi regions for three clusters

But what if the dataset is as follow:



The standard k-means algorithm may not perform well when the underlying clusters in the dataset have a non-linear structure. In such cases, alternative methods such as Kernel K-means or Spectral Clustering can be employed to improve clustering accuracy. However, the intricacies of these methods will not be covered in this session.

5 Initialization of Centroids and K-means++

One possible way to initialize the centroids is to randomly assign datapoints from the dataset as centroids.
The other method is K-means++.

5.1 K-means++

The premise is to select centroids that are as far as possible from each other.

- Step 1: Choose μ_1^0 randomly from the dataset.
- Step 2: For $l \in \{2, 3, \ldots, k\}$, choose μ_l^0 probablistically proportional to score(S) where S is,

  $$S(x) = \min_{\{j=1,2,\ldots,l-1\}} ||x - \mu_j^0||^2 \qquad \forall x$$

  The probabilistic aspect of the algorithm provides an expected guarantee of optimal convergence in K-means. The guarantee is given by,

  $$\mathbb{E}\left[\sum_{i=1}^{n} ||x_i - \mu_{z_i}||^2\right] \leq O(\log k)\left[\min_{\{z_1,z_2,\ldots,z_n\}} \sum_{i=1}^{n} ||x_i - \mu_{z_i}||^2\right]$$

  where $O(\log k)$ is a constant of order $\log k$.
- Step 3: Once the centroids are determined, we proceed with Lloyd's Algorithm.

6 Choice of K

A pre-requisite of K-means is k or the number of clusters. But what if k is unknown? If k is choosen to be equal to n,

$$F(z_1, z_2, \ldots, z_n) = \sum_{i=1}^{n} ||x_i - \mu_{z_i}||^2 = 0$$

But we don't want as many clusters as datapoints. Therefore, k needs to be as small as possible. We do this by penalizing large values of k.

$$\arg\min_k \left[\sum_{i=1}^{n} ||x_i - \mu_{z_i}||^2 + \text{Penalty}(k)\right]$$

Two common criteria for making the above argument:

- Akaike Information Criterion: $\left[2K - 2\ln(\hat{\mathcal{L}}(\theta^*))\right]$
- Bayesian Information Criterion: $\left[K\ln(n) - 2\ln(\hat{\mathcal{L}}(\theta^*))\right]$

Details for the same will be discussed in future lectures.

7 Credits

- Professor Arun Rajkumar: The content as well as the notations are from his slides and lecture.