Friday, April 1, 2022 12:26 PM

Problem 1: (5 points) In this problem, you will show that the K-means algorithm is guaranteed to converge to a local minimum. Do this by using the following steps:

(a) Let $\{X_i\}_{i=1}^n$ be observed samples in $\mathbb{R}^p$. Recall the K-means objective

$$\mathcal{L}(\mathcal{W}) = \sum_{k=1}^{K} \frac{1}{|W_k|} \sum_{i,j \in W_k} \|X_i - X_j\|^2.$$

$\mathcal{W} = (W_1, \dots, W_K)$ is a set a clusters, where W_k is the set of i such that X_i is in cluster k. Let $\mathcal{W}^{(t)}$ denote the clusterings after t steps of K-means. Show that

$$\mathcal{L}(\mathcal{W}^{(t+1)}) \leq \mathcal{L}(\mathcal{W}^{(t)})$$

Hint: Rewrite $L(\mathcal{W})$ using the mean vector like we did in class (see Equation 12.18 in Chapter 12 of the ISLRv2 textbook), and show that each step of K-means must decrease the objective.

Homework

$$L(W) = \sum_{k=1}^{K} \frac{1}{|W_k|} \sum_{i,j \in W_k} \overbrace{\|X_i - X_j\|^2}^{\text{euclidean distance}}$$

Textbook

$$\sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

k = clusters (i,j)
p = features

$$\frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{x}_{kj})^2$$

$$\boxed{\begin{gathered} L(W) = \sum_{k=1}^{K} 2 \sum_{i,j \in W_k} \|x_i - x_k\|^2 \\ L(W^{(t+1)}) \leq L(W^{(t)}) \end{gathered}}$$

After each step in $L(W)$ the k-means algorithm will assign an observation to the one with the least euclidean distance, $\|x_i - x_k\|^2$. Such that every step decreases objective.

Algorithm 12.2 decrease objective each step 12.17

Iterate until the cluster assignments stop changing

(a) For each cluster compute cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster

(b) Assign each observation to the cluster whose centroid is closest. (euclidean distance)

12.17

$$\underset{C_1 \cdots C_k}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \underbrace{\sum_{j=1}^{p}}_{\text{vector of p-features}} \overbrace{(x_{ij} - x_{i'j})^2}^{\text{centroid distance}} \right.$$

(b) Argue that the K-means algorithm will eventually exactly converge to a local minimum. *Hint:* Use the fact the the set of possible K-means outcomes is finite.

We know from equation 12.18 that $\|x_i - x_j\|^2$ is the feature minus the cluster mean for said feature used to minimize sum of squared deviations. We know relocating the algorithms can only improve as shown in (a).

This means that as the algorithm runs, clustering will continuously improve until it can nolonger. This is because set of possible K-means outcomes is finite. Meaning it will converge at a local minimum.