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2. Limitations of the K Means
Algorithm

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2. Limitations of the K Means Algorithm

Limitations of the K Means Algorithm



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Limitations of the K-Means Algorithm I

1/1 point (graded)

Remember that the K-Means Algorithm is given as below:

1. Randomly select z_1, \dots, z_K

2. Iterate

1. Given z_1, \dots, z_K , assign each data point $x^{(i)}$ to the closest z_j , so that

$$\text{Cost}(z_1, \dots, z_K) = \sum_{i=1}^n \min_{j=1, \dots, k} \|x^{(i)} - z_j\|^2$$

2. Given C_1, \dots, C_K find the best representatives z_1, \dots, z_K , i.e. find z_1, \dots, z_K such that

$$z_j = \operatorname{argmin}_z \sum_{i \in C_j} \|x^{(i)} - z\|^2 = \frac{\sum_{i \in C_j} x^{(i)}}{|C_j|}$$

where $|C_j|$ is the number of points in C_j .

Which of the following are **false** about K-Means Algorithm? Please choose all those apply.

☐ C_1, \dots, C_K found by the algorithm is always a partition of $\{x_1, \dots, x_n\}$

☒ It is always guaranteed that the K representatives $z_1, \dots, z_K \in \{x_1, \dots, x_n\}$

☐ The algorithm may output different C_1, \dots, C_K and z_1, \dots, z_K depending on the initialization of line 1

☐ Line 2.2 of the algorithm (Given C_1, \dots, C_K find the best representatives z_1, \dots, z_K ...) finds the cost-minimizing representatives z_1, \dots, z_K .



Solution:

It is not guaranteed that $z_1, \dots, z_K \in \{x_1, \dots, x_n\}$, because as in line 2.2 of the algorithm above, z_1, \dots, z_K are given by

$$z_j = \frac{\sum_{i \in C_j} x^{(i)}}{|C_j|}$$

There is no guarantee that the centroid of all $x^{(i)}$ in a cluster will itself belong to $\{x_1, \dots, x_n\}$. Depending on the application context, such as when clustering Google News articles, it can be problematic that a representative of a clustering is not an actual datapoint.

The other 3 choices are true:

- Clustering always outputs C_1, \dots, C_K that is a partition of $\{x_1, \dots, x_n\}$
- The result of clustering depends on the initialization of z_1, \dots, z_K .
- As we saw in the last lecture, line 2.2 of the algorithm

$$z_j = \frac{\sum_{i \in C_j} x^{(i)}}{|C_j|}$$

minimizes the cost

$$\text{Cost}(C_1, \dots, C_K) = \min_{j=z_1, \dots, z_K} \sum_{j=1}^k \sum_{i \in C_j} \text{dist}(x^{(i)}, z_j)$$

where the distance function $\text{dist}(x^{(i)}, z_j)$ is the squared euclidean distance function $\|x^{(i)} - z_j\|^2$.

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i Answers are displayed within the problem

Limitations of the K-Means Algorithm II

2/2 points (graded)

Suppose we have a 1D dataset drawn from 2 different Gaussian distribution $\mathcal{N}(\mu_1, \sigma_1^2), \mathcal{N}(\mu_2, \sigma_2^2)$ where $\mu_1 \neq \mu_2$. The dataset contains n data points from each of the two distributions for some large number n .

Define **optimal clustering** to be the assignment of each point to the more likely Gaussian distribution given the knowledge of the generating distribution.

Consider the case where $\sigma_1^2 = \sigma_2^2$, would you expect a 2-means algorithm to approximate the optimal clustering?

☒ Yes

☐ No



Now if $\sigma_1^2 \gg \sigma_2^2$, would you expect a 2-means algorithm to approximate the optimal clustering?

☐ Yes

☒ No



Solution:

When $\sigma_1^2 = \sigma_2^2$, the boundary between the 2 optimal clusters is the midpoint between μ_1 and μ_2 . The 2 centroids found by the 2-means algorithm will also be approximately equidistant from this boundary (midpoint between μ_1 and μ_2), and therefore the assignment to clusters will be a similar split around the midpoint.

When $\sigma_1^2 \gg \sigma_2^2$, the boundary between the 2 optimal clusters is closer to one centroid than the other. Since the 2-means algorithm will always have an equidistant split between the two centroids, this behavior cannot be reproduced and thus k-means clustering will erroneously assign more points to the cluster with a smaller variance.

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