AI2611 Machine Learning (Spring 2023) Assignment 2

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Problem Prove that the negative loss decreases in the previous K-means algorithm.

Proof Suppose the sample $\hat{\boldsymbol{x}}$ is moved from H_i to H_j. The new centroid of H_i is

$$\hat{\boldsymbol{m}}_i^* = \frac{n_i\boldsymbol{m}_i - \hat{\boldsymbol{x}}}{n_i - 1} = \boldsymbol{m}_i + \frac{n_i\boldsymbol{m}_i - \hat{\boldsymbol{x}}}{n_i - 1} - \boldsymbol{m}_i = \boldsymbol{m}_i + \frac{\boldsymbol{m}_i - \hat{\boldsymbol{x}}}{n_i - 1}$$

Then the updated loss function of H_i is

$$\begin{aligned}
J_i^* &= \sum_{\boldsymbol{x}\in H_i} \|\boldsymbol{x} - \boldsymbol{m}_i^*\|^2 - \|\hat{\boldsymbol{x}} - \boldsymbol{m}_i^*\|^2 \\
&= \sum_{\boldsymbol{x}\in H_i} \left\|\boldsymbol{x} - \boldsymbol{m}_i - \frac{\boldsymbol{m}_i - \hat{\boldsymbol{x}}}{n_i - 1}\right\|^2 - \left\|\frac{n_i}{n_i - 1}(\hat{\boldsymbol{x}} - \boldsymbol{m}_i)\right\|^2 \\
&= \sum_{\boldsymbol{x}\in H_i} \|\boldsymbol{x} - \boldsymbol{m}_i\|^2 + \sum_{\boldsymbol{x}\in H_i} \frac{2}{n_i - 1}(\hat{\boldsymbol{x}} - \boldsymbol{m}_i)^T(\boldsymbol{x} - \boldsymbol{m}_i) \\
&\quad + \sum_{\boldsymbol{x}\in H_i} \frac{1}{(n_i - 1)^2}\|\hat{\boldsymbol{x}} - \boldsymbol{m}_i\|^2 - \frac{n_i^2}{(n_i - 1)^2}\|\hat{\boldsymbol{x}} - \boldsymbol{m}_i\|^2 \\
&= J_i + \frac{2(\hat{\boldsymbol{x}} - \boldsymbol{m}_i)^T}{n_i - 1}\sum_{\boldsymbol{x}\in H_i}(\boldsymbol{x} - \boldsymbol{m}_i) - \frac{n_i^2 - n_i}{(n_i - 1)^2}\|\hat{\boldsymbol{x}} - \boldsymbol{m}_i\|^2 \\
&= J_i - \frac{n_i}{n_i - 1}\|\hat{\boldsymbol{x}} - \boldsymbol{m}_i\|^2
\end{aligned}$$

which indicates that $J_i^* < J_i$. Therefore, the loss of H_i decreases after moving $\hat{\boldsymbol{x}}$ from H_i to H_j.