

K means within-point scatter deviation

—Elements of Statistical Learning Chapter 14 Reading Note

Shuai

December 29, 2013

The overall within-point dissimilarity can be replaced with the summation of dissimilarity between each point in the cluster and the cluster mean, meaning:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i')=k} \|x_i - x_{i'}\|^2 \quad (1)$$

$$= \sum_{k=1}^K N_k \sum_{C(i)=k} \|x_i - \bar{x}_k\|^2 \quad (2)$$

where, there are K clusters; $C(i) = k$ means the label given to sample i is k; N_k means the overall number of points in cluster k; x_i means sample i.

In this doc, detailed proof will be presented. During the proof, norm will be just written as square.

For expression 1:

For clarity, we replace $\sum_{C(i)=k} \sum_{C(i')=k}$ with $\sum_i \sum_j$.

$$\sum_{C(i)=k} \sum_{C(i')=k} \|x_i - x_{i'}\|^2 = \sum_i \sum_j \|x_i - x_{i'}\|^2 \quad (3)$$

$$= \sum_i \sum_j (x_i^2 + x_j^2) - \sum_i \sum_j x_i x_j \quad (4)$$

$$= N_k \sum_i x_i^2 + N_k \sum_j x_j^2 - 2 \sum_i \sum_j x_i x_j \quad (5)$$

$$= 2(N_k \sum_i x_i^2 + \sum_i \sum_j x_i x_j) \quad (6)$$

For expression 2:

For clarity, we replace $\sum_{C(i)=k}$ with \sum_i .

$$\sum_{C(i)=k} \|x_i - \bar{x}_k\|^2 = \sum_i \|x_i - \bar{x}_k\|^2 \quad (7)$$

$$= \sum_i (x_i^2 + \bar{x}_k^2) - \sum_i x_i \bar{x}_k \quad (8)$$

$$= \sum_i x_i^2 + N_k \bar{x}_k^2 - \sum_i x_i \bar{x}_k \quad (9)$$

$$= \sum_i x_i^2 + N_k \bar{x}_k^2 - 2N_k \bar{x}_k^2 \quad (10)$$

$$= \sum_i x_i^2 - N_k \bar{x}_k^2 \quad (11)$$

$$= \sum_i x_i^2 - \sum_i x_i \sum_j x_j / N_k \quad (12)$$

$$(13)$$

Since $\sum_i x_i \sum_j x_j = \sum_i \sum_j x_i x_j$, proof is done.