

## Exercise 1: Grid search vs random search

(implementation exercise)

## Exercise 2: Implement Multi-dimensional scaling MDS

(implementation exercise)

## Exercise 3: Implement Isomap

(implementation exercise)

## Exercise 4: k-means and kernel k-means

Handwritten mathematical derivations for k-means:

$$\sum_{i \in C_k} \|x_i - m_k\|^2 \leq \sum_{i \in C_k} \|x_i - x_j\|^2, \forall j \in C_k$$

$$\sum \left\langle x_i - \frac{\sum x}{n}, x_i - \frac{\sum x}{n} \right\rangle \leq \sum_{i \in C_k} \langle x_i - x_j, x_i - x_j \rangle$$

$$\sum \left\langle x_i, x_i \right\rangle + \left\langle \frac{\sum x}{n}, \frac{\sum x}{n} \right\rangle - 2 \left\langle x_i, \frac{\sum x}{n} \right\rangle \leq \sum_i \left\langle x_i, x_i \right\rangle + \left\langle x_j, x_j \right\rangle - 2 \left\langle x_i, x_j \right\rangle$$

$$\sum \|x_i\|^2 + \frac{1}{n^2} \langle \sum x, \sum x \rangle - 2 \left\langle x_i, \frac{\sum x}{n} \right\rangle \leq \sum \|x_i\|^2 + \|x_j\|^2 - 2 \langle x_i, x_j \rangle$$

$$\sum \|x_i\|^2 + \|m_k\|^2 - 2 \langle x_i, m_k \rangle \leq \sum \|x_i\|^2 + \|x_j\|^2 - 2 \langle x_i, x_j \rangle$$

(a)

$$\begin{aligned}
 & \sum_i \|x_i\|^2 + \sum_j \|m_K\|^2 - 2 \sum \langle x_i, m_K \rangle \leq \sum \|x_i\|^2 + \sum \|x_j\|^2 - 2 \sum \langle x_i, x_j \rangle \\
 & \sum \|m_K\|^2 - 2 \sum \langle x_i, m_K \rangle \leq \sum \|x_j\|^2 - 2 \sum \langle x_i, x_j \rangle \\
 & n \|m_K\|^2 - 2 (\langle x_1, m_K \rangle + \langle x_2, m_K \rangle + \dots + \langle x_n, m_K \rangle) \\
 & x_1 n + m_K n + x_2 n + m_K n + \dots + x_n n + m_K n + \dots \\
 & \cancel{n \|m_K\|^2} \\
 & n \|m_K\|^2 - 2 \langle \sum x_i, n m_K \rangle \leq \sum \|x_j\|^2 - 2 \sum \langle x_i, x_j \rangle \\
 & n \|m_K\|^2 - 2 \langle n m_K, n m_K \rangle \\
 & n \|m_K\|^2 - 2 n^2 \|m_K\|^2 \leq \langle n m_K, n m_K \rangle - 2 \sum \langle x_i, x_j \rangle \\
 & n \|m_K\|^2 - 2 n^2 \|m_K\|^2 \leq n^2 \|m_K\|^2 - 2 \sum \langle x_i, x_j \rangle
 \end{aligned}$$

$$\begin{aligned}
 & n \|m_K\|^2 - 2 (\langle x_1, m_K \rangle + \langle x_2, m_K \rangle + \dots + \langle x_n, m_K \rangle) \\
 & x_1 n + m_K n + x_2 n + m_K n + \dots + x_n n + m_K n + \dots \\
 & \cancel{n \|m_K\|^2} \\
 & n \|m_K\|^2 - 2 \langle \sum x_i, n m_K \rangle \leq \sum \|x_j\|^2 - 2 \sum \langle x_i, x_j \rangle \\
 & n \|m_K\|^2 - 2 \langle n m_K, n m_K \rangle \\
 & n \|m_K\|^2 - 2 n^2 \|m_K\|^2 \leq \langle n m_K, n m_K \rangle - 2 \sum \langle x_i, x_j \rangle \\
 & n \|m_K\|^2 - 2 n^2 \|m_K\|^2 \leq n^2 \|m_K\|^2 - 2 \sum \langle x_i, x_j \rangle \\
 & n^2 \|m_K\|^2 - 2 \langle n m_K, n m_K \rangle \\
 & n^2 \|m_K\|^2 - 2 n^2 \|m_K\|^2 \leq -n^2 \|m_K\|^2 \Rightarrow n \|m_K\|^2 \leq n^2 \|m_K\|^2
 \end{aligned}$$