

K Means

Clustering

- Given: N unlabeled examples $\{x_1, \dots, x_N\}$ and number of desired partitions K .
- Goal : Group the examples into K “homogeneous” partitions.

Def.

Given a set of observations $X = \{x_1, x_2, \dots, x_N\} (x_i \in \mathbb{R}^D)$, partition the N observations into K sets ($K \leq N$) $\{\mathcal{C}_k\}_{k=1, \dots, K}$ such that the sets minimize the within-cluster sum of squares:

$$\{\mathcal{C}_k\} = \arg \min_{\{\mathcal{C}_k\}} \sum_{i=1}^K \sum_{x \in \mathcal{C}_i} \|x - \mu_i\|^2$$

where μ is the mean of points in set \mathcal{C}_i .

K Means Algorithm

Algorithm

- (Re)-Assign each example x_i to its closest cluster center (based on the smallest Euclidean distance)

$$\mathcal{C}_k = \left\{ x_i \mid \|x_i - \mu_k\|^2 \leq \|x_i - \mu_{k'}\|^2, \text{ for } \forall k' \neq k \right\}$$

- (\mathcal{C}_k is the set of examples assigned to cluster k with center μ_k) - Update the cluster means

$$\mu_k = \text{mean}(\mathcal{C}_k) = \frac{1}{|\mathcal{C}_k|} \sum_{x \in \mathcal{C}_k} x$$

- Let $z_{i,k}$ be an indicator

$$z_{i,k} = \begin{cases} 1, & x_i \in \mathcal{C}_k \\ 0, & \text{otherwise} \end{cases}$$

- and $z_i = [z_{i,1}, \dots, z_{i,k}]^T$ represents the one-hot encoding of x_i .
- The loss is $L(\mu, X, Z) = \sum_{i=1}^N \sum_{k=1}^K z_{i,k} \|x_i - \mu_k\|^2 = \|X - Z\mu\|^2$
- where $X \in \mathbb{R}^{N \times D}$, $Z \in \mathbb{R}^{N \times K}$, $\mu \in \mathbb{R}^{K \times D}$

Limitations

- Makes hard assignments of points to clusters
- Works well only if the clusters are roughly of equal sizes
- K-means also works well only when the clusters are round-shaped and does badly if the clusters have non-convex shapes

Kernel K Means

- Basic idea: Replace the Euclidean distance/similarity computations in K-means by the kernelized versions

$$\begin{aligned}d(x_i, \mu_k) &= \|\phi(x_i) - \phi(\mu_k)\| \\ \|\phi(x_i) - \phi(\mu_k)\|^2 &= \|\phi(x_i)\|^2 + \|\phi(\mu_k)\|^2 - 2\phi(x_i)^T \phi(\mu_k) \\ &= k(x_i, x_i) + k(\mu_k, \mu_k) - 2k(x_i, \mu_k)\end{aligned}$$