K Means

Clustering

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

  Def.

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

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

  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

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

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

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

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

Limitations

- Makes hard assignments of points to clusters
- Works well only is 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

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