Machine Learning Course - CS-433

K-Means Clustering

Nov 19, 2020

Last updated on: November 17, 2020

EPFL

Clustering

Clusters are groups of points whose inter-point distances are small compared to the distances outside the cluster.

The goal is to find "prototype" points $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2,, \ldots, \boldsymbol{\mu}_K$ and cluster assignments $z_n \in \{1, 2, \ldots, K\}$ for all $n = 1, 2, \ldots, N$ data vectors $\mathbf{x}_n \in \mathbb{R}^D$.

K-means clustering

Assume K is known.

$$\min_{\mathbf{z}, \boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2$$

$$\text{s.t. } \boldsymbol{\mu}_k \in \mathbb{R}^D, z_{nk} \in \{0, 1\}, \sum_{k=1}^{K} z_{nk} = 1,$$

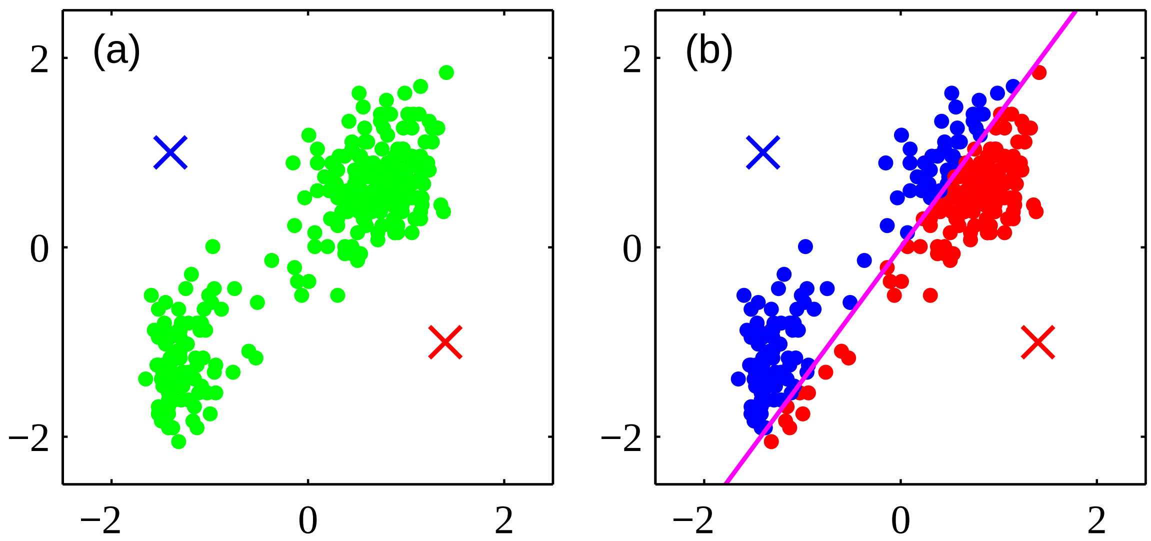
$$\begin{aligned} \text{where } \mathbf{z}_n &= \left[z_{n1}, z_{n2}, \ldots, z_{nK}\right]^\top \\ \mathbf{z} &= \left[\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\right]^\top \\ \boldsymbol{\mu} &= \left[\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K\right]^\top \end{aligned}$$

Is this optimization problem easy?

Algorithm: Initialize $\boldsymbol{\mu}_k \, \forall k$,
then iterate:

1. For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.
2. For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.

Step 1: For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.

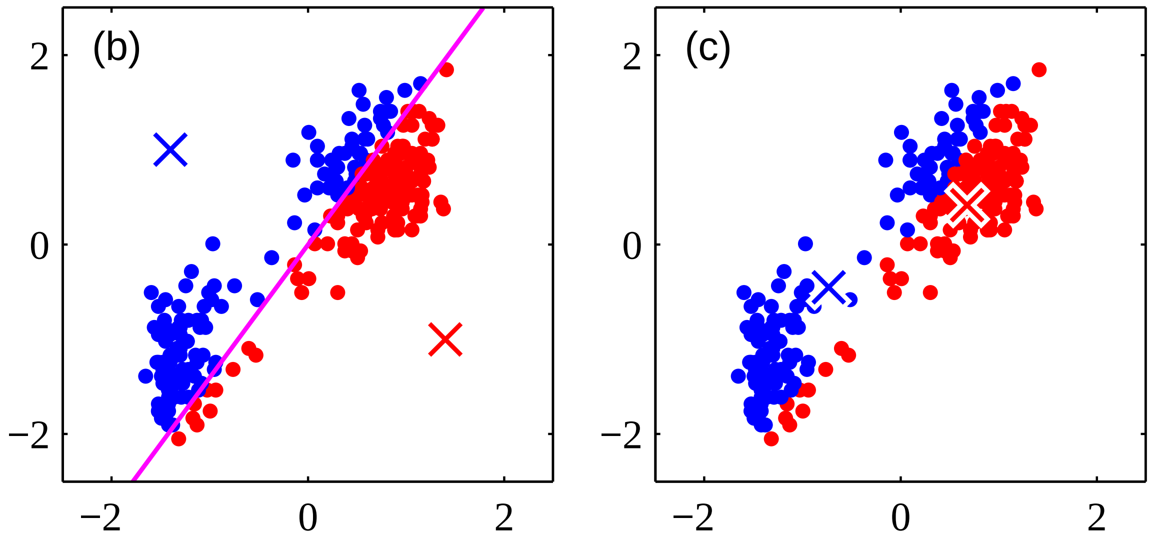


$$z_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_{j=1,2,\ldots K} \|\mathbf{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

Step 2: For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.
Take derivative w.r.t. $\boldsymbol{\mu}_k$ to get:

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$$

Hence, the name 'K-means'.



Summary of K-means

Initialize $\boldsymbol{\mu}_k \, \forall k$, then iterate:

1. For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.

$$z_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

2. For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$$

Convergence to a local optimum is assured since each step decreases the cost (see Bishop, Exercise 9.1).

Coordinate descent

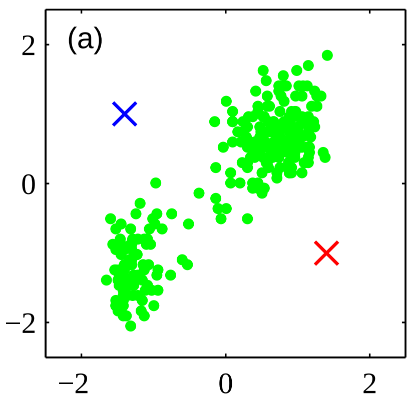
K-means is a coordinate descent algorithm, where, to find $\min_{\boldsymbol{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu})$, we start with some $\boldsymbol{\mu}^{(0)}$ and repeat the following:

$$\mathbf{z}^{(t+1)} := \arg\min_{\boldsymbol{z}} \ \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}^{(t)})$$

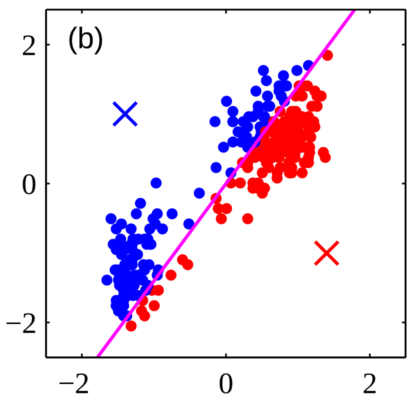
$$\boldsymbol{\mu}^{(t+1)} := \arg\min_{\boldsymbol{\mu}} \ \mathcal{L}(\mathbf{z}^{(t+1)}, \boldsymbol{\mu})$$

Examples

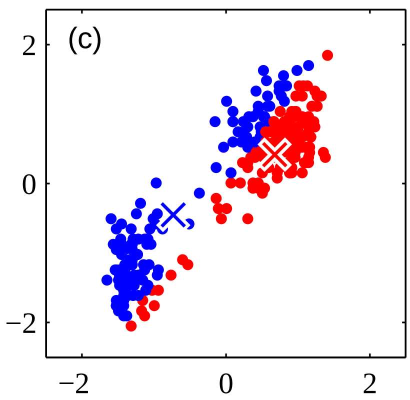
K-means for the “old-faithful” dataset (Bishop’s Figure 9.1)



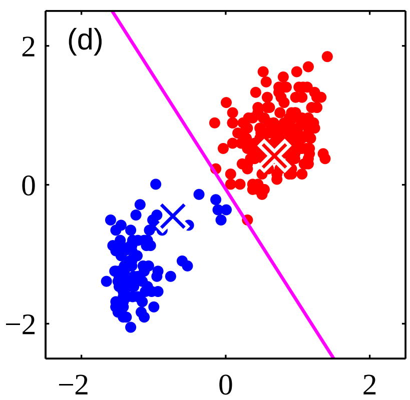
(e) Iteration 0



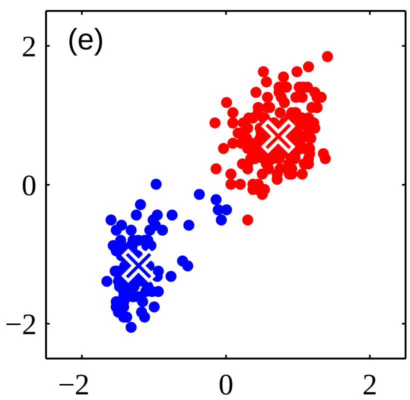
(f) Iteration 1



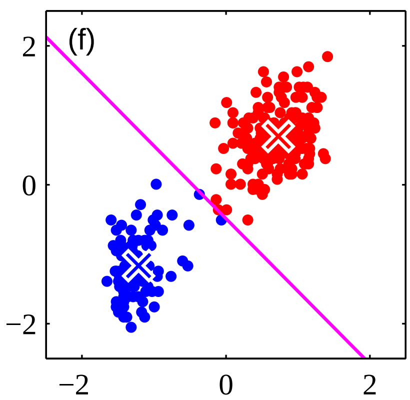
(g) Iteration 1



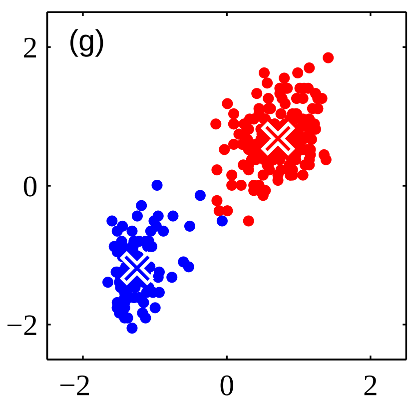
(h) Iteration 2



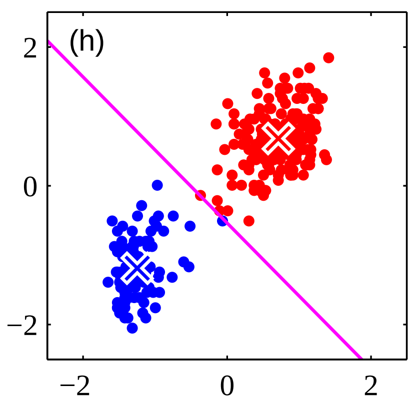
(i) Iteration 2



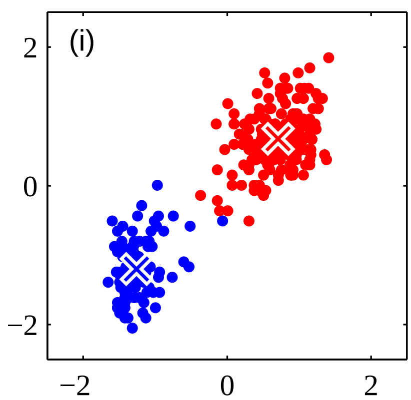
(j) Iteration 3



(k) Iteration 3

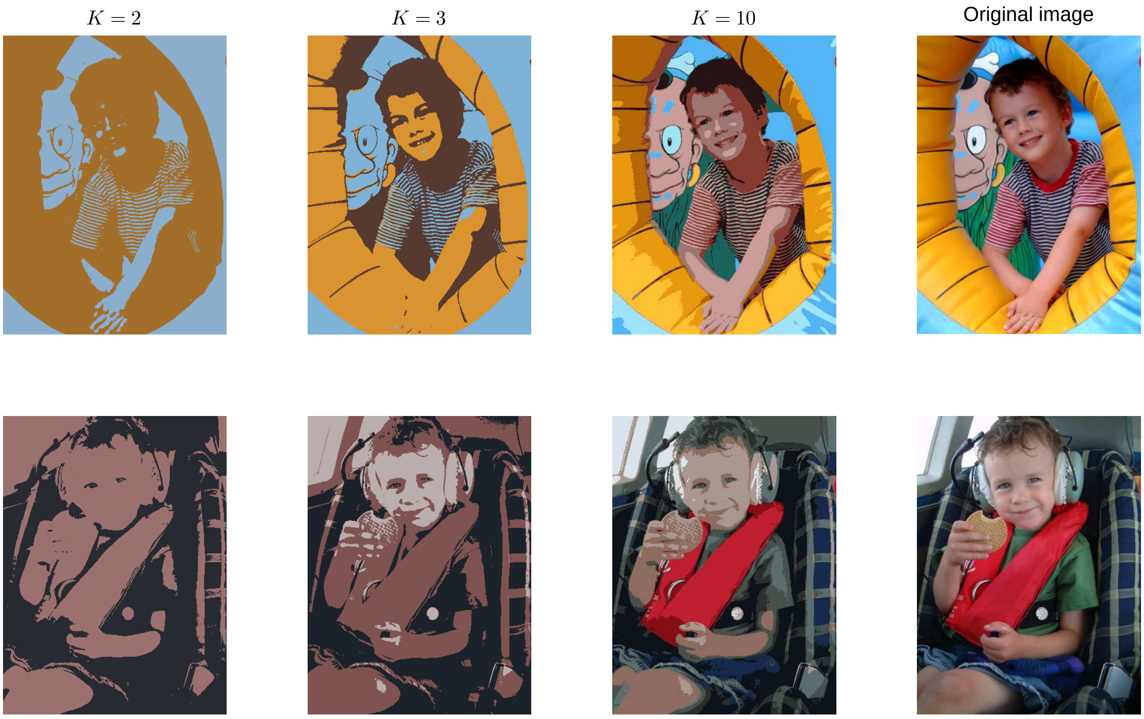


(l) Iteration 4



(m) Iteration 4

Data compression for images (this is also known as vector quantization).



Probabilistic model for K-means

K-means as a Matrix Factorization

Recall the objective

$$\min_{\mathbf{z},\boldsymbol{\mu}} \ \mathcal{L}(\mathbf{z},\boldsymbol{\mu}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2$$

$$= \|\mathbf{X}^\top - \mathbf{M}\mathbf{Z}^\top\|_{\mathsf{Frob}}^2$$

$$\text{s.t. } \boldsymbol{\mu}_k \in \mathbb{R}^D,$$

$$z_{nk} \in \{0,1\}, \ \sum_{k=1}^{K} z_{nk} = 1.$$

Issues with K-means

1. Computation can be heavy for large N, D and K.
2. Clusters are forced to be spherical (e.g. cannot be elliptical).
3. Each example can belong to only one cluster (“hard” cluster assignments).