Machine Learning Course - CS-433 K-Means Clustering

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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.

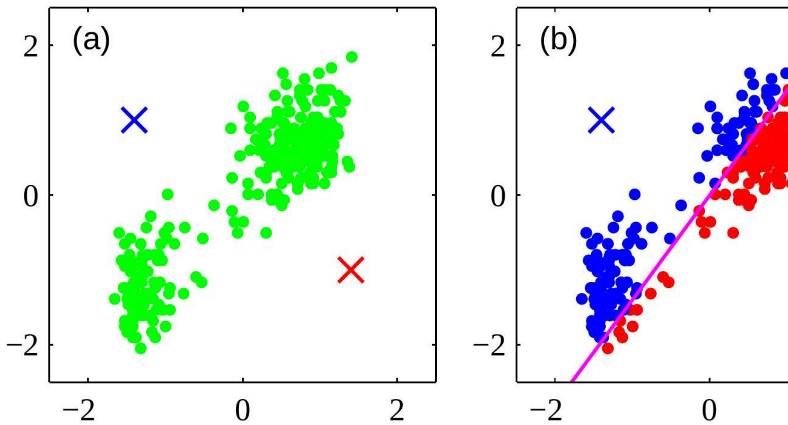
$$\min_{\mathbf{z}, \boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \left\| \mathbf{x}_n - \boldsymbol{\mu}_k \right\|_2^2$$

s.t. $\boldsymbol{\mu}_k \in \mathbb{R}^D, z_{nk} \in \{0, 1\}, \sum_{k=1}^{K} z_{nk} = 1,$
where $\mathbf{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]^\top$

$$\mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N]^\top$$
$$\boldsymbol{\mu} = [\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K]^\top$$

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 $\mathbf{z}$.

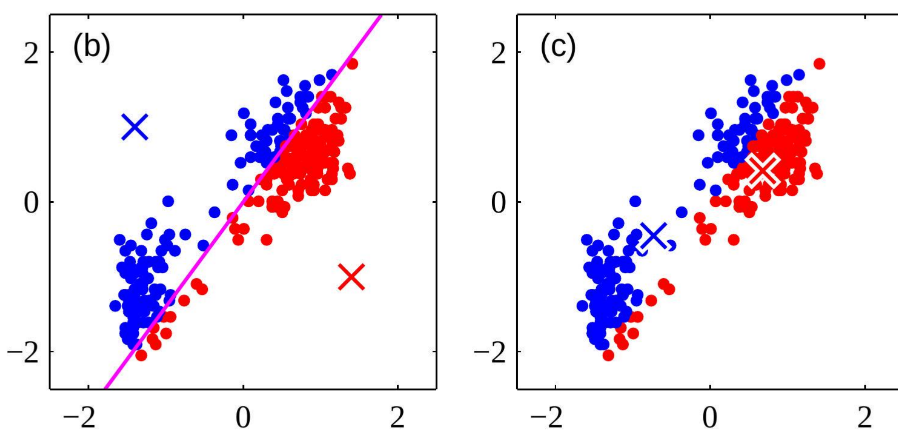


Step 1: For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.

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

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 $\boldsymbol{\mu}$.

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

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

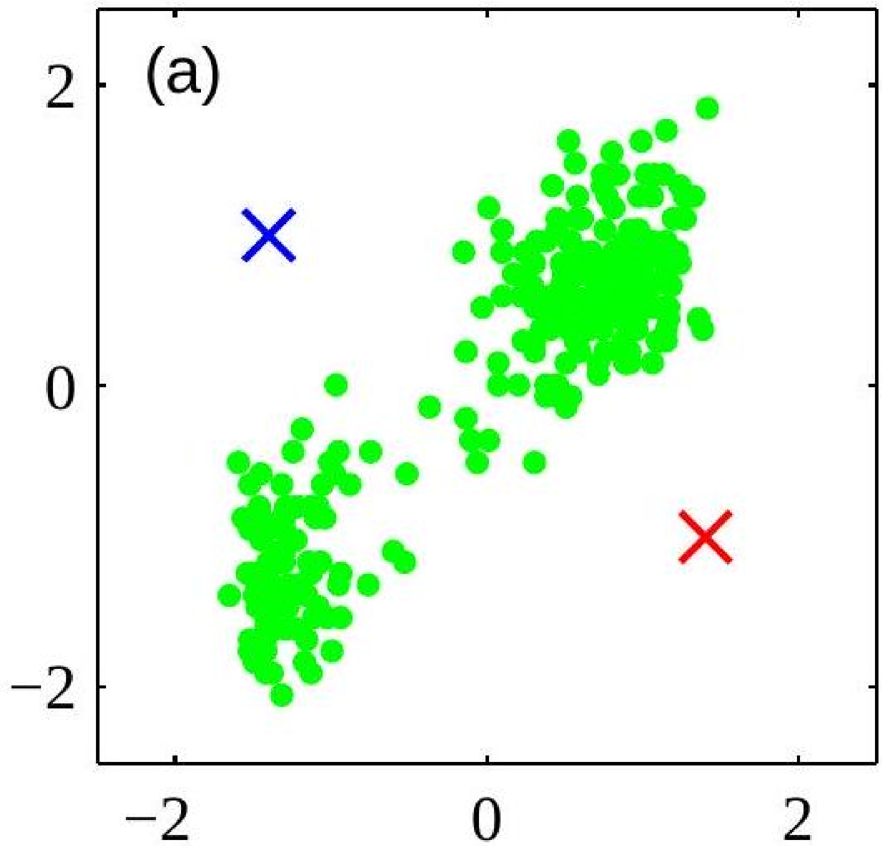
K-means is a coordinate descent algorithm, where, to find $\min_{\boldsymbol{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu})$, we start with some $\boldsymbol{\mu}^{(0)}$ and repeat the following:

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

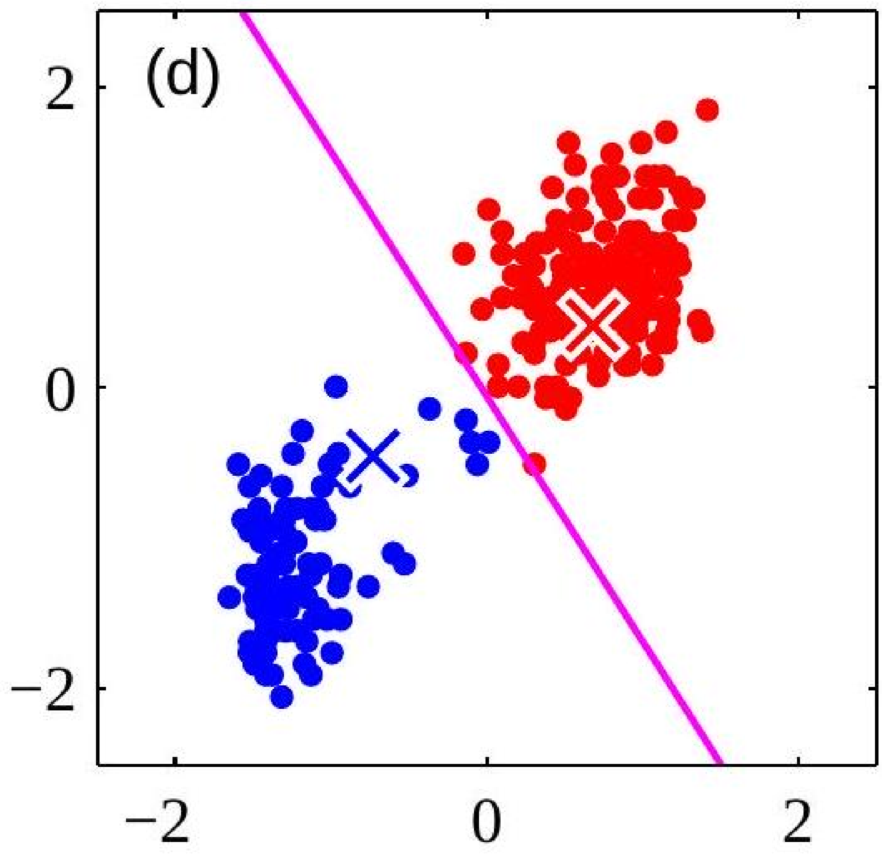
$\boldsymbol{\mu}^{(t+1)} := \arg\min_{\boldsymbol{\mu}} \mathcal{L}\left(\mathbf{z}^{(t+1)}, \boldsymbol{\mu}\right)$

Examples

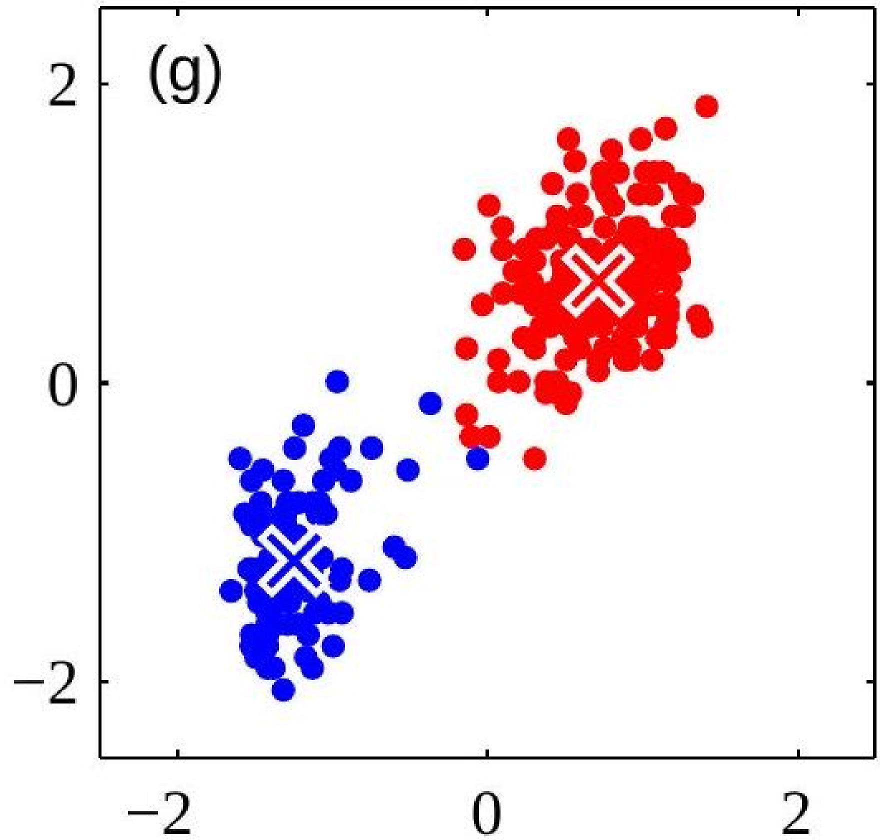
K-means for the "old-faithful" dataset (Bishop's Figure 9.1)



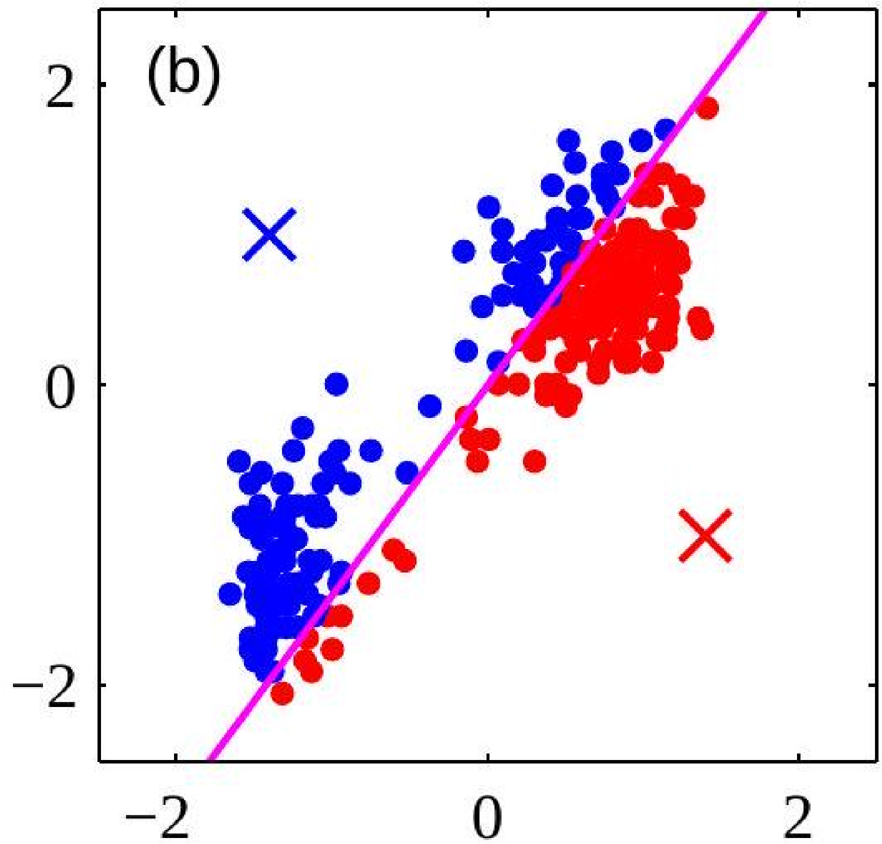
(e) Iteration 0



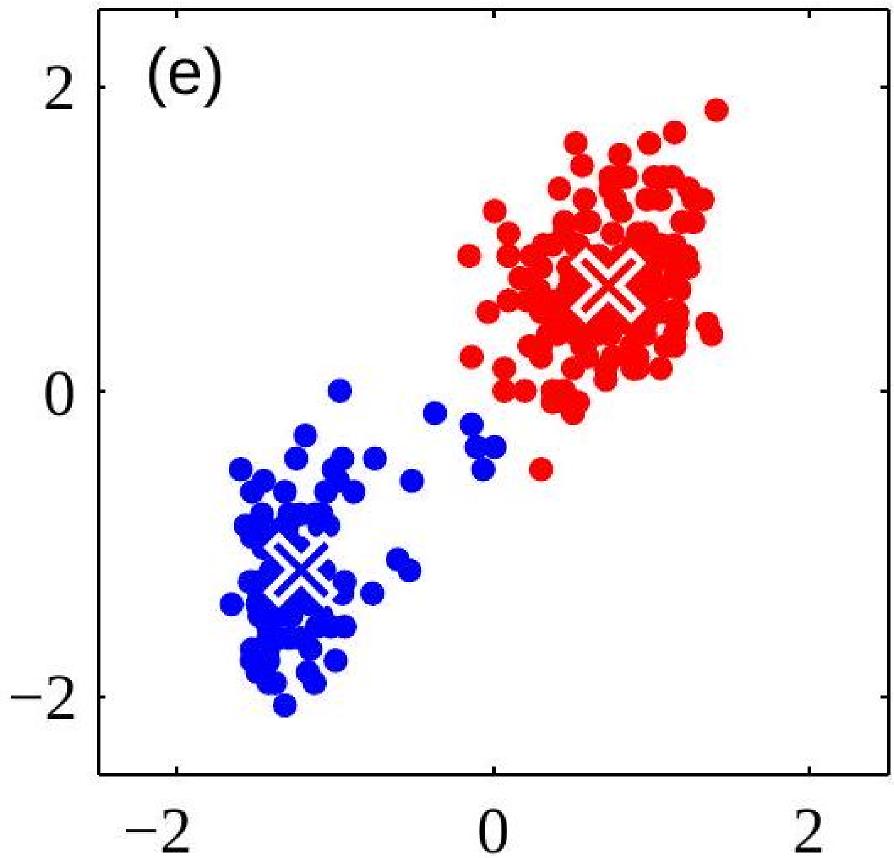
(h) Iteration 2



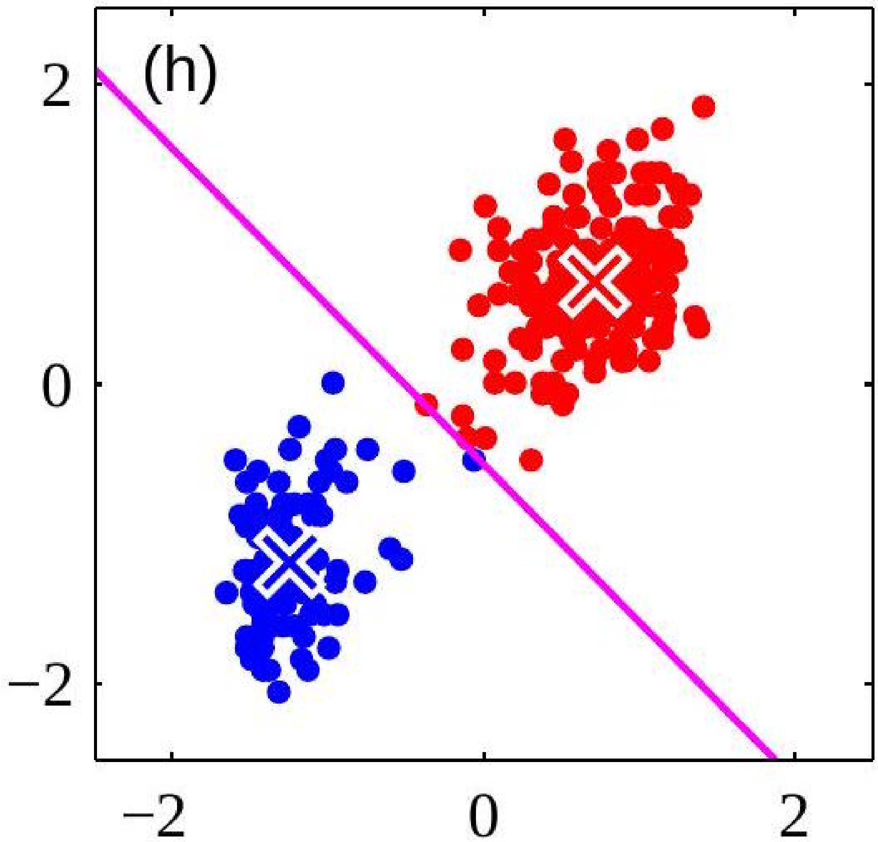
(k) Iteration 3



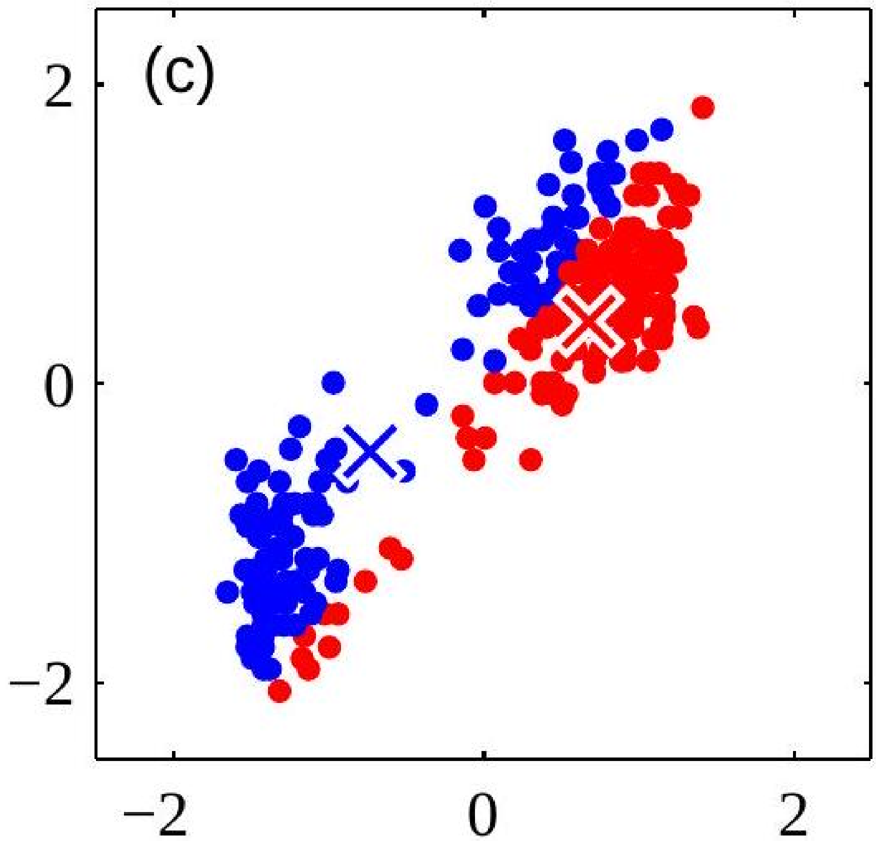
(f) Iteration 1



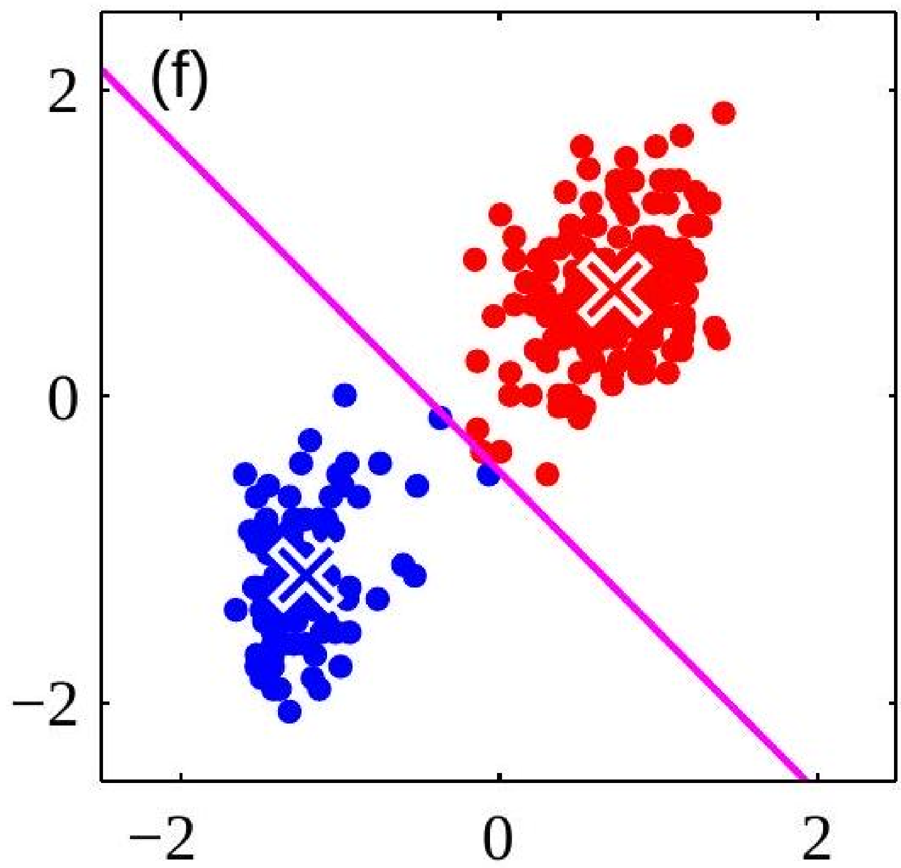
(i) Iteration 2



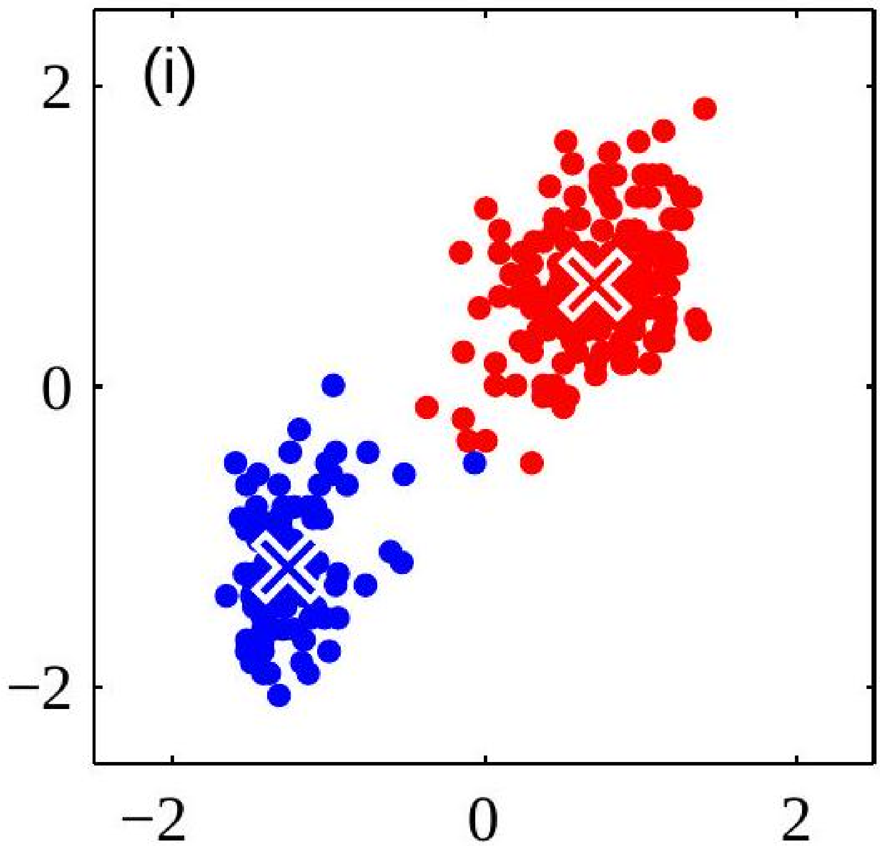
(l) Iteration 4



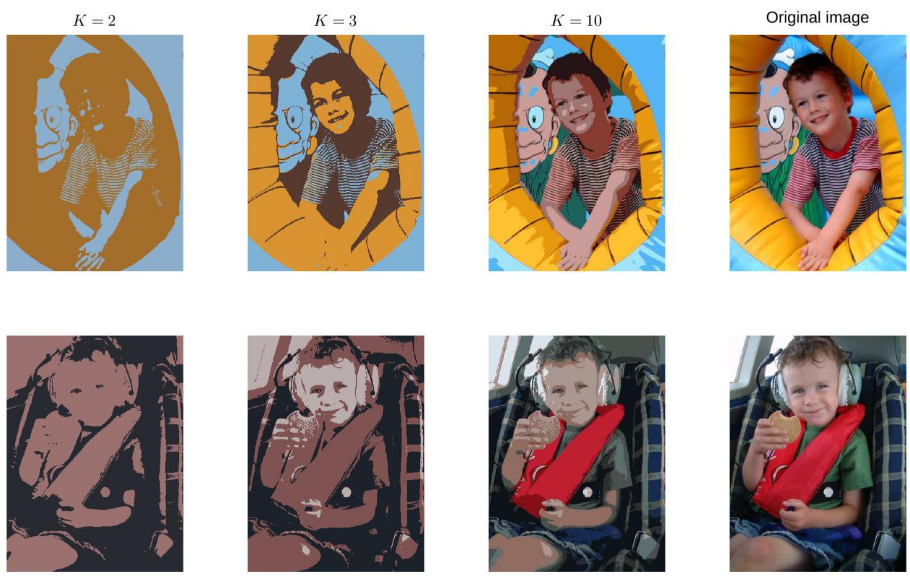
(g) Iteration 1



(j) Iteration 3



(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

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

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

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).