K-Means Clustering

Introduction to Artificial Intelligence with Mathematics
Lecture Notes

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Unsupervised learning algorithm (no labels)

Clustering

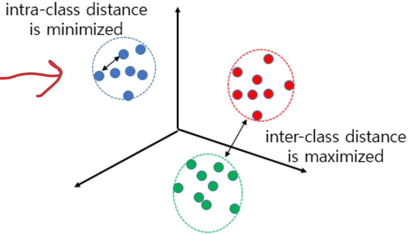
Multiple Clusters

data pts

Clustering is the process of grouping a set of observations into classes of similar observations.

clusters

- high intra-class similarity
- low inter-class similarity different clusters
- It is the most common form of unsupervised learning.
- Note that clustering is subjective.



k-means clustering

data pts

k-means clustering aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean.

- k-means clustering is one of unsupervised learning algorithms.
- It creats a labeling of observations with cluster labels.
- The labels are derived exclusively from the observations.

k-means clustering is described as follows:

For a given set of observations $\{\mathbf{x}_i | \mathbf{x}_i = (x_{i1}, ... x_{ip}), 1 \leq i \leq n\}$,

- if centroids of k clusters are denoted by $\boldsymbol{\mu} = \{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, ..., \boldsymbol{\mu}_k\}$, and partitions are denoted by $\mathcal{C} = \{C_1, C_2, ... C_k\}$, then k-means clustering aims to partition the n observations into $k (\leq n)$ sets $C_1, C_2, ... C_k$ so as to minimize the within-cluster sum of squares (WCSS) (i.e., variance).

prob. function for k-means

Formally, the objective is to find:

data point

centroid

$$J(\mathcal{C}, \boldsymbol{\mu}) := \arg\min_{\mathcal{C}, \boldsymbol{\mu}} \sum_{i=1}^{k} \sum_{\mathbf{x}_j \in C_i} ||\mathbf{x}_j - \boldsymbol{\mu}_i||^2$$

cluster

It seems to be hard to find a solution, but we have a nice heuristic algorithm.

k-means clustering algorithm

1. Let $t = 0$ and start with initial guesses $\boldsymbol{\mu}_1^{(0)}, \boldsymbol{\mu}_2^{(0)}, \cdots, \boldsymbol{\mu}_k^{(0)}$ for cluster centers (centroids).
2. For each observation, find the closest cluster centeroid.

$$C_i^{(t)} = \{\mathbf{x}_l : ||\mathbf{x}_l - \boldsymbol{\mu}_i^{(t)}||^2 \leq ||\mathbf{x}_l - \boldsymbol{\mu}_j^{(t)}||^2,\ \forall j, 1 \leq j \leq k\}$$

Centroids

(Find $\mathcal{C}$ to minimize $J(\mathcal{C}, \boldsymbol{\mu})$ while fixing $\boldsymbol{\mu}$.)

3. Replace each centroid by the average of observations in its partition.

$$\boldsymbol{\mu}_i^{(t+1)} = \frac{1}{|C_i^{(t)}|} \sum_{x_j \in C_i^{(t)}} \mathbf{x}_j$$

(Find $\boldsymbol{\mu}$ to minimize $J(\mathcal{C}, \boldsymbol{\mu})$ while fixing $\mathcal{C}$.)

4. Iterate steps 2 and 3 until convergence (No guarantee but good)

k-means clustering as Expectation Maximization

Let $r_{ij} = 1$ if $\mathbf{x}_j \in C_i$ and $r_{ij} = 0$ if $\mathbf{x}_j \notin C_i$. We then have

$$\begin{aligned} J(\mathcal{C}, \boldsymbol{\mu}) &:= \arg\min_{\mathcal{C},\boldsymbol{\mu}} \sum_{i=1}^{k} \sum_{\mathbf{x}_j \in C_i} ||\mathbf{x}_j - \boldsymbol{\mu}_i||^2 \\ &= \arg\min_{\mathcal{C},\boldsymbol{\mu}} \sum_{i=1}^{k} \sum_{j=1}^{n} r_{ij} ||\mathbf{x}_j - \boldsymbol{\mu}_i||^2. \end{aligned}$$

We want to find $\mathcal{C}$, equivalently r_{ij} and $\boldsymbol{\mu}$ to minimize J.

Best values

Step 1: Find r_{ij} to minimize $J(\mathcal{C}, \boldsymbol{\mu})$ while fixing $\boldsymbol{\mu}$. (Expectation)

$$r_{ij} = \begin{cases} 1 & \text{if } i = \arg\min_l ||\mathbf{x}_j - \boldsymbol{\mu}_l||^2 \\ 0 & \text{otherwise.} \end{cases}$$

$x_j \in C_i$

Step 2: Find $\boldsymbol{\mu}$ to minimize $J(\mathcal{C}, \boldsymbol{\mu})$ while fixing r_{ij}. (Maximization)

$$2\sum_{j=1}^{n} r_{ij}(\mathbf{x}_j - \boldsymbol{\mu}_i) = \mathbf{0}$$

Gradient of objective function J wrt μ_i's

$$\boldsymbol{\mu}_i = \frac{\sum_{j=1}^{n} r_{ij}\mathbf{x}_j}{\sum_{j=1}^{n} r_{ij}}$$

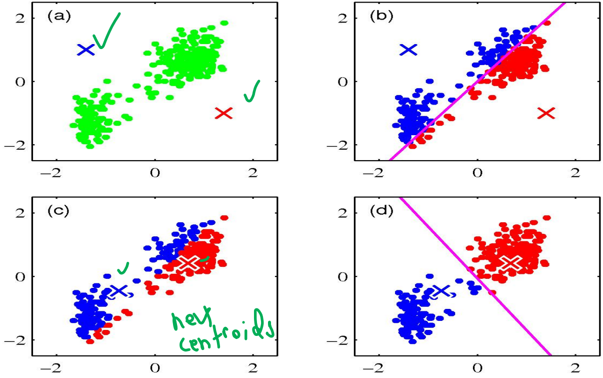
Centroid

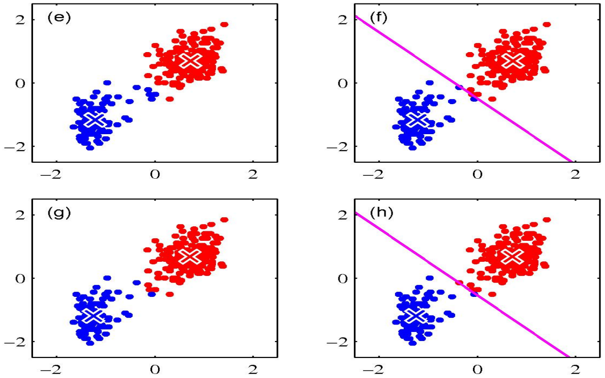
Example:

Christopher M. Bishop, Pattern Recognition and Machine Learning, Springer 2006.

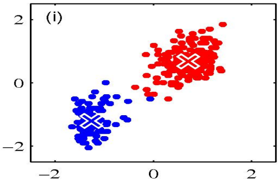
K=2 clusters

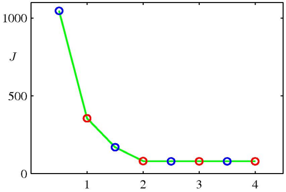
initial centroids





converged





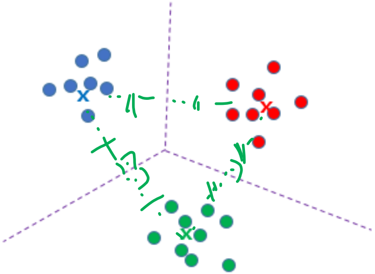
The value of J decreases as we iterate the algorithm as shown above.

cf. blue points (E steps) and red points (M steps)

Expectation

Maximization

When the Euclidean distance is used as a metric, it results in Voronoi cells.



3 boundaries

equilateral triangle

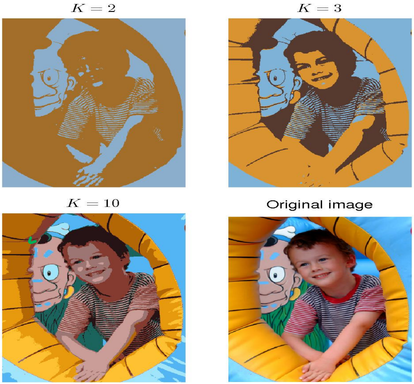
In practice:

- Try many random starting centroids (observations) and choose a solution with the smallest sum of squares
- How to choose the number k of clusters?

Select suitable K

Example: k-means clustering is applied on pixel colour values

- Pixels in each cluster are coloured by cluster mean
- Each pixel (e.g., 24-bit colour value) is represented by the cluster number (e.g., 4 bits for $k = 10$), which is a compressed version.
- This is a good example of vector quantization



3 colors

10 color pixels

Drawbacks of k-means clustering

- The value of k should be given as an input parameter.
- It might converge to a local minumum (not a global minumum).
- Its performance is sensitive to outliers.
- Euclidean distance is used as a metric and variance is used as a measure of cluster scatter, which limits the applicability of the algorithm.