Clustering

Task: Find clusters/subgroups in a dataset $S = \{x_1, \dots, x_n\} \in \mathbb{R}^p$.

- Samples within subgroup similar/homogeneous
- Samples in different subgroups "distant"/heterogeneous from each other.

Ex:
- Customers of a company → grouping for targeted marketing.
- Biology: Find groups of genes.

Q:
- What notion of similarity?
- Precise definition?

Note: Fundamentally different from classification problems!

"**Unsupervised Learning**":
No subset of data with "correct" classification/grouping available.

k-means clustering: [Steinhaus '56, Lloyd '57]

Given n points $x_1, \dots, x_n \in \mathbb{R}^p$, find k centroids $c_1, \dots, c_k \in \mathbb{R}^p$ and a partition $\Gamma_1 \cup \Gamma_2 \cup \dots \cup \Gamma_k = \{1, \dots, n\}$ $(\Gamma_i \cap \Gamma_j = \emptyset \text{ if } i \neq j)$ such that

$$F\left(\{c_i\}_{i=1}^k, \{\Gamma_i\}_{i=1}^k\right) := \sum_{j=1}^{k} \sum_{i \in \Gamma_j} d(x_i, c_j)$$

"k-means objective" (*)

is minimized, where $d : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ is a "distance" function

Ex: 1. $d(x,y) = \|x-y\|_2^2$ "squared Euclidean" ← by default in

2. $d(x,y) = \|x-y\|_1$. "k-median".

Observation: K-means with is NP-hard for $k \geq 2$. [Drineas et al. '04].

Lloyd's algorithm (often called "k-means"):

Input: $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^p$, desired nr. of clusters k

1. Initialize $c_1, \dots, c_k \in \mathbb{R}^p$.
   - a) randomly among the $\{x_i\}_{i=1}^n$
   - or b) k-means++ : fancier

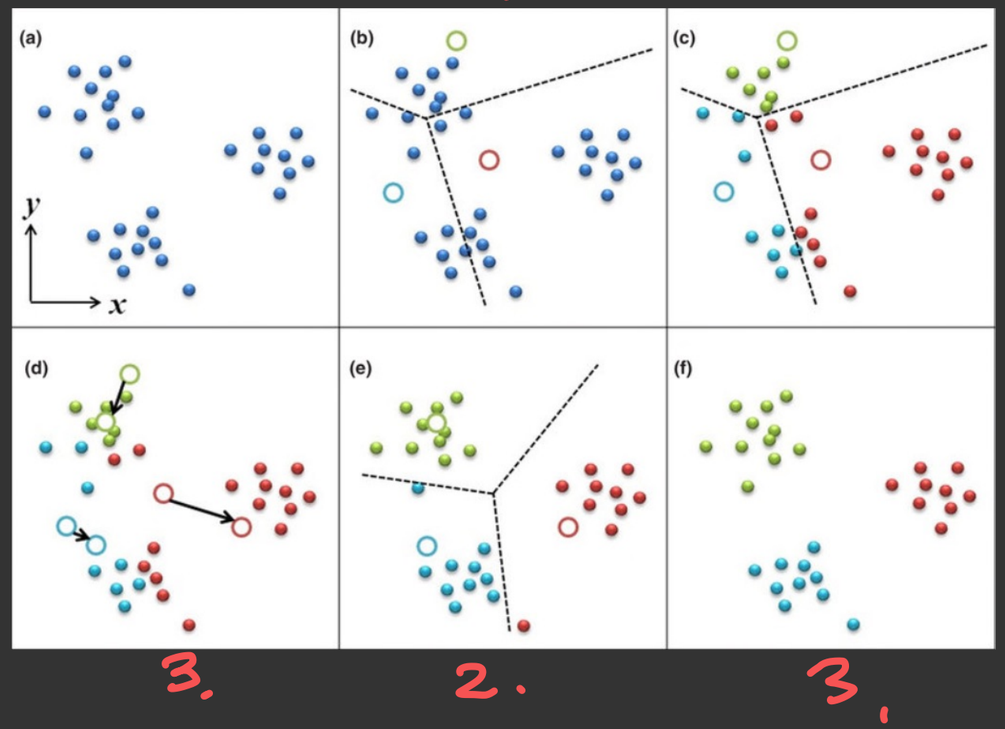
Repeat until convergence:

2. $\forall i = 1, \dots, n$: Assign $x_i \in$? if c_j is closest centroid to x_i among $\{c_\ell\}_{\ell=1}^k$

3. Update $\forall j = 1, \dots, k$:

$$c_j = \underset{c \in \mathbb{R}^k}{\operatorname{argmin}} \sum_{i \in \text{?}} d(x_i, c) = \frac{1}{|\text{?}|} \sum_{i \in \text{?}} x_i$$

(if $d(\cdot,\cdot) = \|\cdot - \cdot\|_2^2$)



- Finds local optimum of (*)
- Works well for "convex" clusters

To consider:

- How to choose nr. of clusters k?
- Which distance to choose (geometry of underlying space...)?
- Initialization: If prior knowledge available, → might be better than random.
  - Needs a lot of pairwise distances. If $n >> 10^5$ or so, slow → "Minibatch KMeans"

Other clustering methods:

- Spectral Clustering: Based on laplacian of similarity graph.
- Hierarchical Clustering: Creates trees