Clustering

ML Instruction Team, Fall 2022

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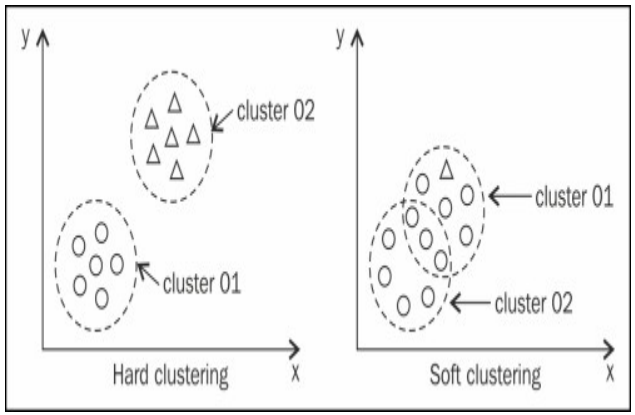
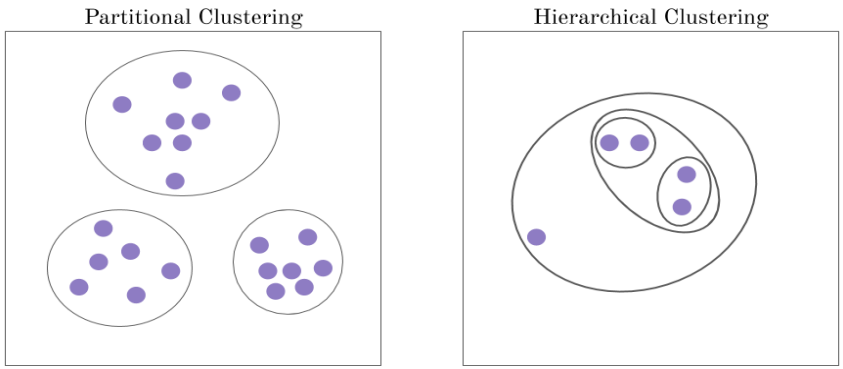
Categories of Clustering

- Hard: Where each point is assigned to exactly one cluster.
- Soft: Where each point can be assigned to several clusters with certain probabilities that add up to 1.
- Partitional: Where all clusters are on the same level.
- Hierarchical Where the clustering is done from fine to coarse by merging points successively to larger and larger clusters (agglomerative hierarchical clustering).



(a) Hard vs Soft Clustering, Source



(b) Partitional vs Hierarchical Clustering, Source

Figure: Different clustering techniques

K-Means

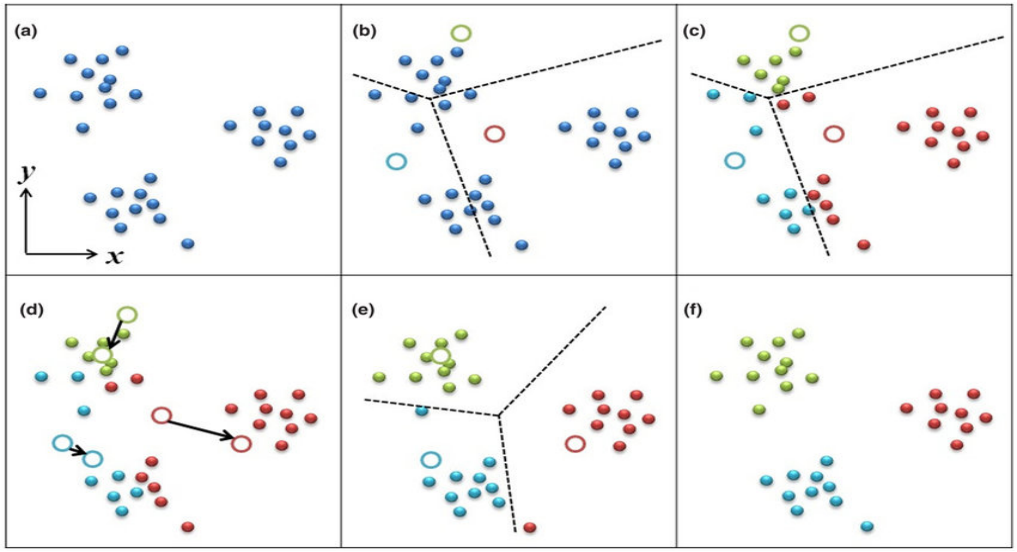


Figure: K-means in practice, Source

- The idea is to represent each cluster $\mathcal{C}_k$ by a center point c_k and assign each data point x_n to one of the clusters $\mathcal{C}_k$.
- The center points and the assignment are then chosen such that the mean squared distance between data points and center points

$$J = \sum_{n=1}^{N} \sum_{n \in \mathcal{C}_k} \|x_n - c_k\|^2$$

is minimized.

K-Means

- If the assignment is fixed, it is easy to show that the optimal choice of the center positions is given by:

$$c_k = \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} x_n$$

- If the center points are fixed, it is obvious that each point should be assigned to the nearest center position.
- The K-means algorithm now consists of applying these two optimizations in turn until convergence.
- The initial center locations?
- Convergence Guaranty?
- Drawbacks:
  - A paramount drawback of this and many other clustering algorithms is that the number of clusters is not determined.
  - The result of the algorithm is not necessarily a global optimum of the error function.
- Solutions
  - Problem 1?
  - Problem 2?

Davies-Bouldin (DB) Index

- To evaluate the quality of a clustering a plethora of validity indices have been proposed, one of which is Davies-Bouldin (DB) index.
- Cluster Dispersion: Which can be interpreted as a generalized standard deviation.

$$\delta_k := \sqrt{\frac{1}{N_k} \sum_{n \in C_k} \|x_n - c_k\|^2}$$

- Cluster Similarity: Is defined such that two clusters are considered similar if they have large dispersion relative to their distance.

$$S_{kl} := \frac{\delta_k + \delta_l}{\|c_k - c_l\|}$$

- A good clustering should be characterized by clusters being as dissimilar as possible.
- Considering aforementioned definitions, an overall validation of the clustering can be done by the DB index:

$$V_{DB} := \frac{1}{k} \sum_{k=1}^{K} \max_{l \neq k} S_{kl}$$

Davies-Bouldin (DB) Index

- The DB index does not systematically depend on K and is therefore suitable to find the best optimal number of clusters.

Figure: DB Index, Source

Thank You!

Any Question?