MLRF Lecture 02

J. Chazalon, LRDE/EPITA, 2020

Clustering

Lecture 02 part 03

Clustering: finding groups in data (1/2)

Many techniques:

Useful for Practice session 2

- Connectivity models: hierarchical clustering, ...
  cluster = set of neighbors
- Centroid models: k-means, ...
  cluster = centroid point
- Distribution model: Gaussian mixtures models est. w. Expectation Maxim., …
  cluster = statistical distribution (center + spread in each direction)
- Density models: DBSCAN, …
  cluster = dense region
- Graph-based models: HCS (Highly Connected Subgraphs) algorithms, …
  cluster = clique in the graph
- ...

Useful for Practice session 4 (eventually)

Clustering: finding groups in data (2/2)

Always the same goal:

- Minimise the differences between elements within the same cluster
- Maximise the differences between elements within different clusters

Number of clusters:

- Many methods require to choose it beforehand
- Several techniques to adjust the number of clusters automatically

Outliers rejection:

- Some techniques do not assign lonely points to any cluster

⇒ Focus on HAC and K-Means today

Hierarchical Agglomerative Clustering (HAC)

Hierarchical Agglomerative Clustering

Algorithm

Initialization:

- Create a cluster from each element

While more than 1 cluster:

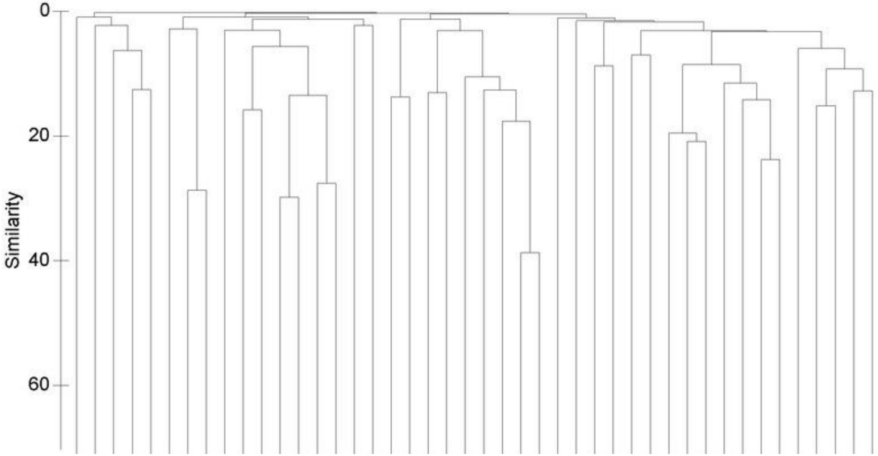
- Merge the two closest clusters

Challenge: distance between clusters

- New center = mean of points
- or distance = maximal distance
- or…

Time complexity: O(n²) for fastest method

Output: Dendrogram



K-Means

K-Mean clustering (again) (1/3)

The K-means algorithm aims to choose centroids that minimise the inertia, or within-cluster sum-of-squares criterion:

$$\sum_{i=0}^{n} \min_{\mu_j \in C}(||x_i - \mu_j||^2)$$

- ie it does not maximizes inter-cluster distance
- ie it puts centers so as to get the best coverage (may not be on a density peak!)

K-Mean clustering (again) (2/3)

Algorithm

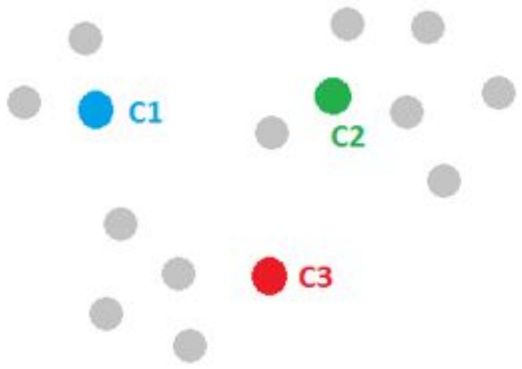
Images: https://healthcare.ai/step-step-k-means-clustering/

K-Mean clustering (again) (2/3)

Algorithm

Initialization:

- (randomly) select cluster centers



Images: https://healthcare.ai/step-step-k-means-clustering/

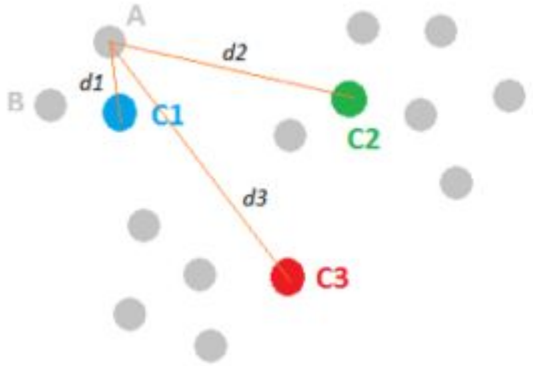
K-Mean clustering (again) (2/3)

Algorithm

Initialization:

- (randomly) select cluster centers

- Calculate distance points ⇔ centers



Images: https://healthcare.ai/step-step-k-means-clustering/

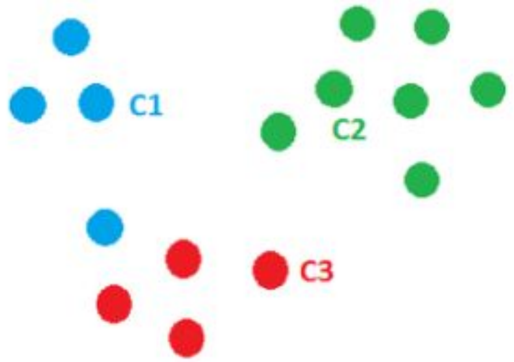
K-Mean clustering (again) (2/3)

Algorithm

Initialization:

- (randomly) select cluster centers

- Calculate distance points ⇔ centers
- Assign each point to closest center



Images: https://healthcare.ai/step-step-k-means-clustering/

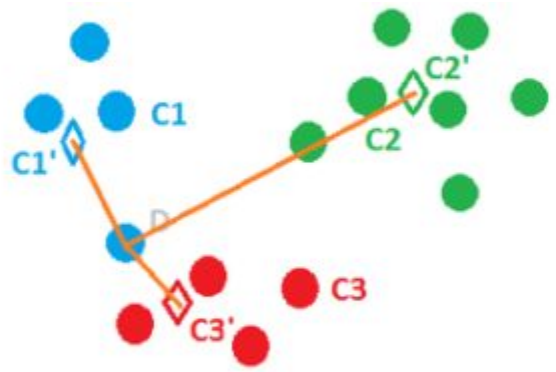
K-Mean clustering (again) (2/3)

Algorithm

Initialization:

- (randomly) select cluster centers

- Calculate distance points ⇔ centers
- Assign each point to closest center
- <u>Update cluster centers: avg of points</u>



Images: https://healthcare.ai/step-step-k-means-clustering/

K-Mean clustering (again) (2/3)

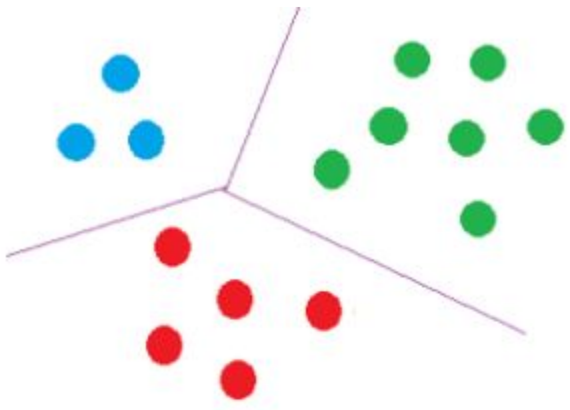
Algorithm

Initialization:

- (randomly) select cluster centers

Loop until converged:

- Calculate distance points ⇔ centers
- Assign each point to closest center
- Update cluster centers: avg of points



Result: centroid centers

- local maximas
- tessellation / Voronoi set over the dataset

Images: https://healthcare.ai/step-step-k-means-clustering/

K-Mean clustering (again) (3/3)

The previous algorithm is called **“Batch K-Means”**, or simply “**K-Means”**, because it considers the **whole the dataset at each iteration**.

Batch K-Means is not only **sensible to outliers** and **initialization**, it is also **very slow** to compute on large datasets. (I got OOM errors with the *Twin it!* poster!!)

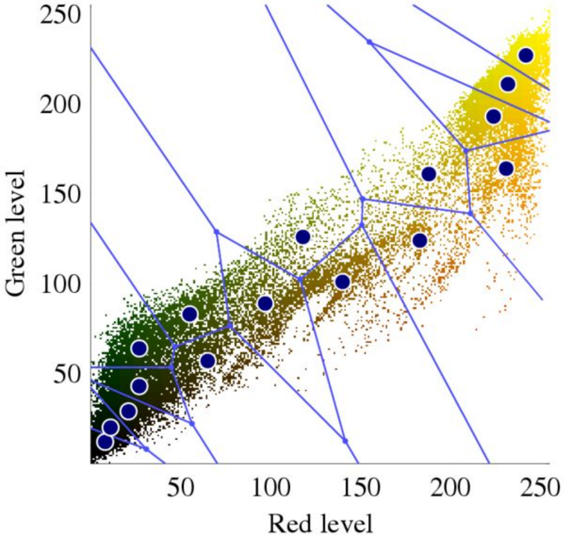
It is possible to avoid this speed / memory issue by **randomly sampling the dataset at each step.**

- Results are only slightly worse
- Speed and memory requirements make it usable on bigger datasets
- This approach is call **“Online K-Means”** or **“MiniBatch K-Means”**

Application: Color quantization

K=16

Original RG image
(no blue channel)



Color quantization showing original colors, target colors and boundaries (Voronoi cells here)

Color-indexed image
(no dithering)

Left/middle images by: Dcoetzee

Many clustering techniques to play with!

https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html