CS 6170: Computational Topology, Spring 2019
Lecture 12

Topological Data Analysis for Data Scientists

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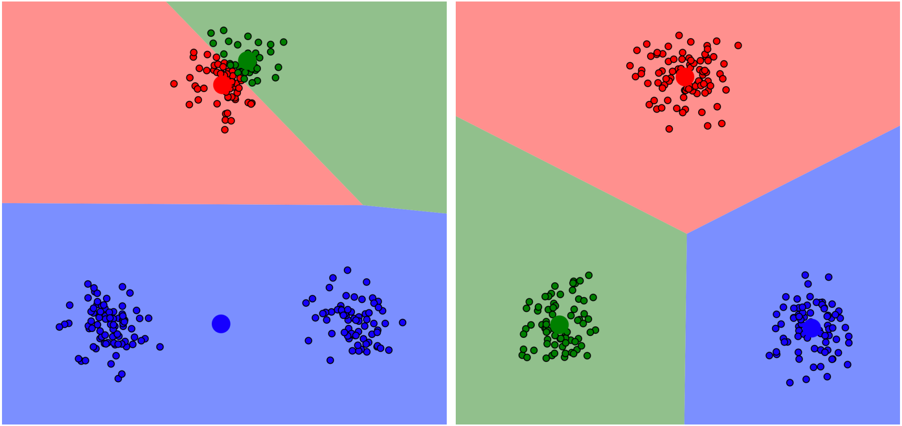
Unsupervised Learning: Clustering

K-Means Clustering

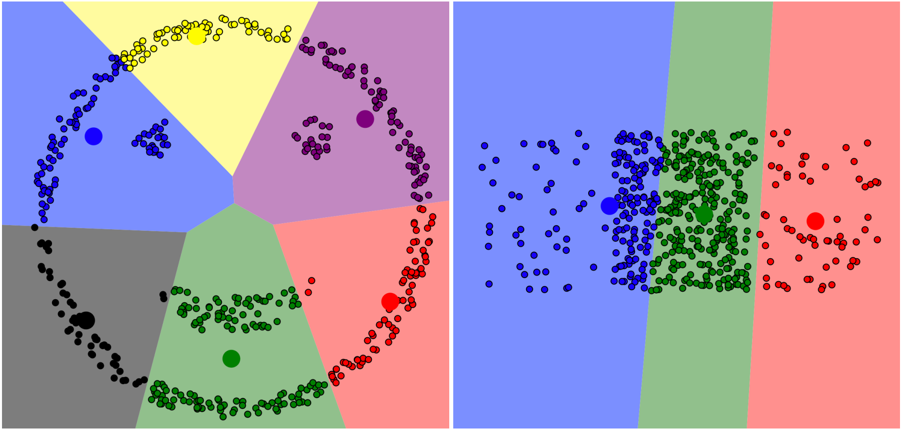
K-means algorithm with different initial *randomly chosen* centroids.



https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

K-Means Clustering

Results of k-means algorithm depends on the initialization step.



https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

K-Means Clustering Algorithm

- Given $X = \{x_1, \cdots, x_n\}$ where $x_i \in \mathbb{R}^d$
- Goal: partition X into k clusters, $S = \{S_1, \cdots, S_k\}$, $k \leq n$
- While: minimizing intracluster variance

$$\arg\min_S \sum_{i=1}^{k} \sum_{x \in S_i} ||x - \mu_i||^2,$$

where $\sum_{x \in S_i} ||x - \mu_i||^2 = |S_i| \mathrm{Var}(S_i)$ and μ_i is mean of points in S_i.

https://en.wikipedia.org/wiki/K-means_clustering

K-Means Clustering Algorithm

1. *Initialization*: Choose a set of initial centroids $c_1^{(1)}, \cdots, c_k^{(1)}$
   - Chose by users, randomly or based on farthest points.
2. *Assignment*: assign each $x \in X$ to its nearest centroid, at step $t \geq 1$:

$$S_i^{(t)} := \{x : ||x - c_i^{(t)}||^2 \leq ||x - c_j^{(t)}||^2\}, \forall j \neq i\}.$$

3. *Update*: Calculate the new centroids of the new clusters,

$$c_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{x \in S_i^{(t)}} x.$$

4. Repeat steps 2 and 3 until it converges: assignments no longer change.
   Algorithm *does not guarantee convergence to the global optimum*.

https://en.wikipedia.org/wiki/K-means_clustering

K-Means++ Clustering Algorithm

- Differ from K-Means by the *Initialization* step.
- High-level idea: spreading out the k initial cluster centroids.
  1. Choose one centroid uniformly at random from X.
  2. For each $x \in X$, compute its distance $d(x)$ to the nearest centroid that has already been chosen.
  3. Choose one new centroid from X at random as a new centroid, using a weighted probability distribution where a point x is chosen with probability proportional to $d(x)^2$.
  4. Repeat Steps 2 and 3 until k centroids have been chosen.
  5. Apply standard k-means clustering.

`https://en.wikipedia.org/wiki/K-means%2B%2B`

DBSCAN Algorithm

- Density-based spatial clustering of applications with noise (DBSCAN)
- Martin Ester, Hans-Peter Kriegel, Jörg Sander and Xiaowei Xu,1996
- KDD 2014: the test of time award
- Density-based clustering algorithm
- High-level: groups together points that are closely packed together (points with many nearby neighbors), marking as outliers points that lie alone in low-density regions (whose nearest neighbors are too far away).
- High-level idea: spreading out the k initial cluster centroids.

`https://en.wikipedia.org/wiki/DBSCAN`

DBSCAN: Preliminary

- X: points to be clustered.
- ϵ: the radius of a neighborhood.
- $minPts$: threshold.
- Core points, (density-)reachable points and outliers:
  - A point p is a *core point* if at least $minPts$ points are within distance ϵ of it (including p).
  - A point q is directly *reachable* from p if point q is within distance ϵ from the core point p. Points are only said to be directly reachable from core points.
  - A point q is reachable from p if there is a path $p_1, \cdots, p_n$ with $p_1 = p$ and $p_n = q$, where each p_{i+1} is directly reachable from p_i. Note that this implies that all points on the path must be core points, with the possible exception of q.
  - All points not reachable from any other point are *outliers* or noise points.

`https://en.wikipedia.org/wiki/DBSCAN`

DBSCAN: High-level Overview

- If p is a core point, then it forms a cluster together with all points (core or non-core) that are reachable from it.
- Each cluster contains at least one core point; non-core points can be part of a cluster, but they form its "edge", since they cannot be used to reach more points.

`https://en.wikipedia.org/wiki/DBSCAN`

DBSCAN: Pseudocode

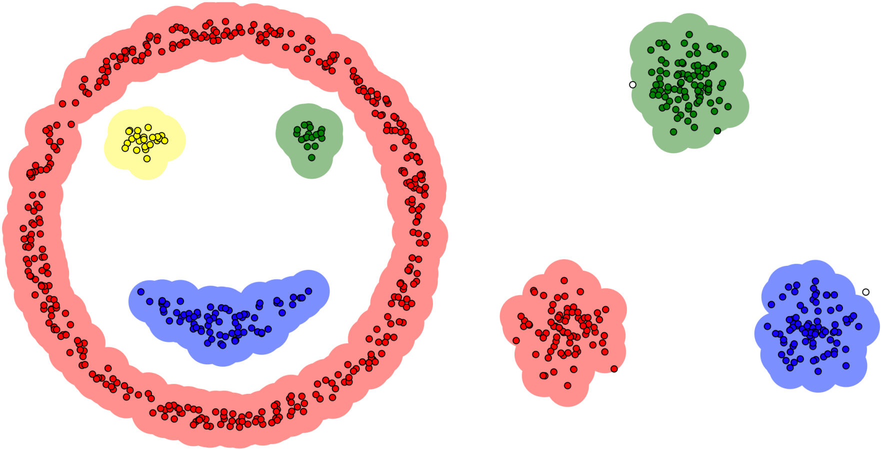
```
DBSCAN(D, epsilon, min_points):
    C = 0
    for each unvisited point P in dataset
        mark P as visited
        sphere_points = regionQuery(P, epsilon)
        if sizeof(sphere_points) < min_points
            ignore P
        else
            C = next cluster
            expandCluster(P, sphere_points, C, epsilon, min_points)

expandCluster(P, sphere_points, C, epsilon, min_points):
    add P to cluster C
    for each point P’ in sphere_points
        if P’ is not visited
            mark P’ as visited
            sphere_points’ = regionQuery(P’, epsilon)
            if sizeof(sphere_points’) >= min_points
                sphere_points = sphere_points joined with sphere_points’
            if P’ is not yet member of any cluster
                add P’ to cluster C

regionQuery(P, epsilon):
    return all points within the n-dimensional sphere centered at P with radius epsilon (including P)
```

https://algorithmicthoughts.wordpress.com/2013/05/29/machine-learning-dbscan/

DBSCAN Algorithm



https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

Unsupervised Learning: Clustering: Mapper

High-Dimensional Data Analysis

WhiteBoard

Singh et al. (2007)

References I

Singh, G., Mémoli, F., and Carlsson, G. (2007). Topological methods for the analysis of high dimensional data sets and 3D object recognition. In *Eurographics Symposium on Point-Based Graphics*.