

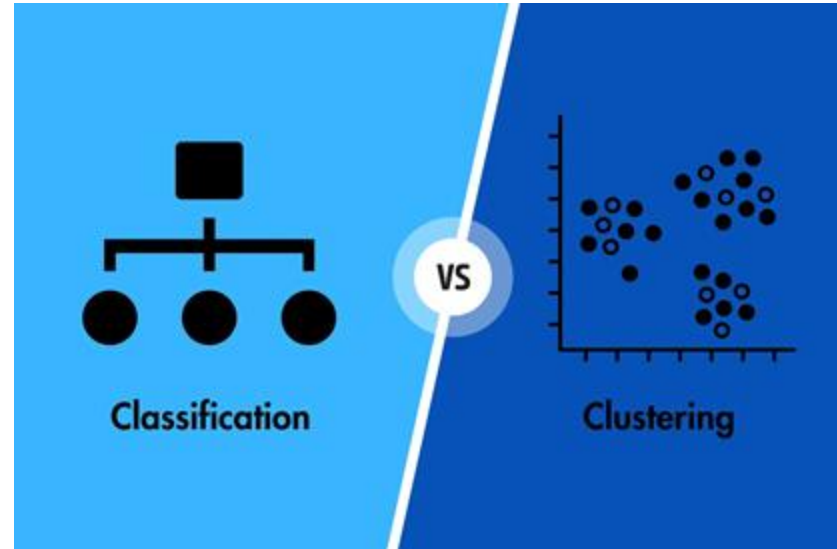
Clustering Methods in Machine Learning

Classification is supervised:

- Discrete, finite, known number of classes with known features
- deterministic rigid models
- stationary models

Clustering is unsupervised:

- Unknown number of classes with unknown features
- High-dim data
- Big Data



Why is clustering useful?

Anomaly and Outlier detection

Identify areas in your data that are not representative or indicate the necessity of changes to the model

Segmentation

Divide your data into segments to use different models for better overall prediction power

Dimensionality Reduction

Overcome the curse of dimensionality by identifying low-variance dimensions/ dimensions that don't contribute to clusters and get rid of them

Algorithms to be covered today

K-means

The fundamental algorithm to all ML

DBSCAN, HDBSCAN, OPTICS

A popular algorithm for data clustering and its less popular more specialised variations

Affinity propagation

A rather exotic algorithm for some special data cases

K-means clustering

Steps to K-means clustering:

- 1) Choose the number of clusters (K) and repetitions (N)
- 2) Select K random points and denote them as initial cluster points
- 3) Assign all other points to the nearest initial cluster points
- 4) Calculate the mean of each cluster and denote each mean as the new initial cluster point
- 5) Recluster until clusters don't change
- 6) Repeat the process N times and choose clustering with lowest sum of variances in each cluster

K-means clustering

K-Means Algorithm

1. Initialize centroid positions ($k = 4$)

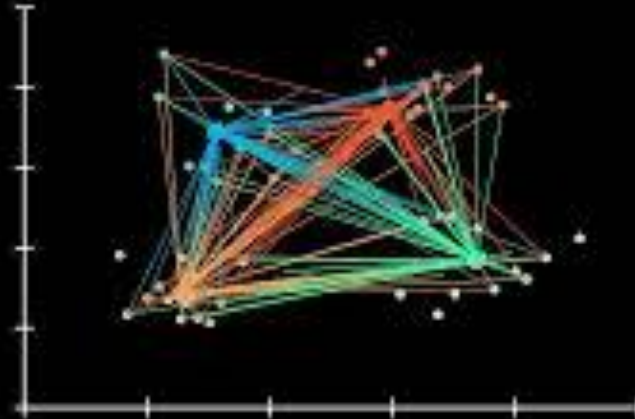
2. Assign labels (μ) to all data (X)

$$\mu_n = \underset{i}{\operatorname{argmin}} \|x_n - c_i\|$$

3. Update centroid positions (C)

$$c_i = \frac{\sum_{n=1}^N x_n A_{nk}}{\sum_{n=1}^N A_{nk}}$$

4. Repeat steps 2 & 3 until convergence



DBSCAN, HDBSCAN, OPTICS

Steps to DBSCAN:

- 1) State radius (eps) and number of neighbours (n)
- 2) Select all points that have n or more neighbours within a euclidean distance of eps and mark them as core points
- 3) Select a random core point and assign it to a new cluster
- 4) Select all core points within the euclidean distance of eps from the previous point and assign them to the same cluster
- 5) Repeat the last step until no core points, then assign all non-core points to the cluster if the euclidean distance to the nearest core point that is a part of that cluster is less or equal eps
- 6) Repeat step 3 until no more core points left
- 7) Mark all non-core points that aren't part of any cluster as separate clusters/ outliers

DBSCAN, HDBSCAN, OPTICS

DBSCAN

Plots clusters according to a preset parameter of the euclidean distance

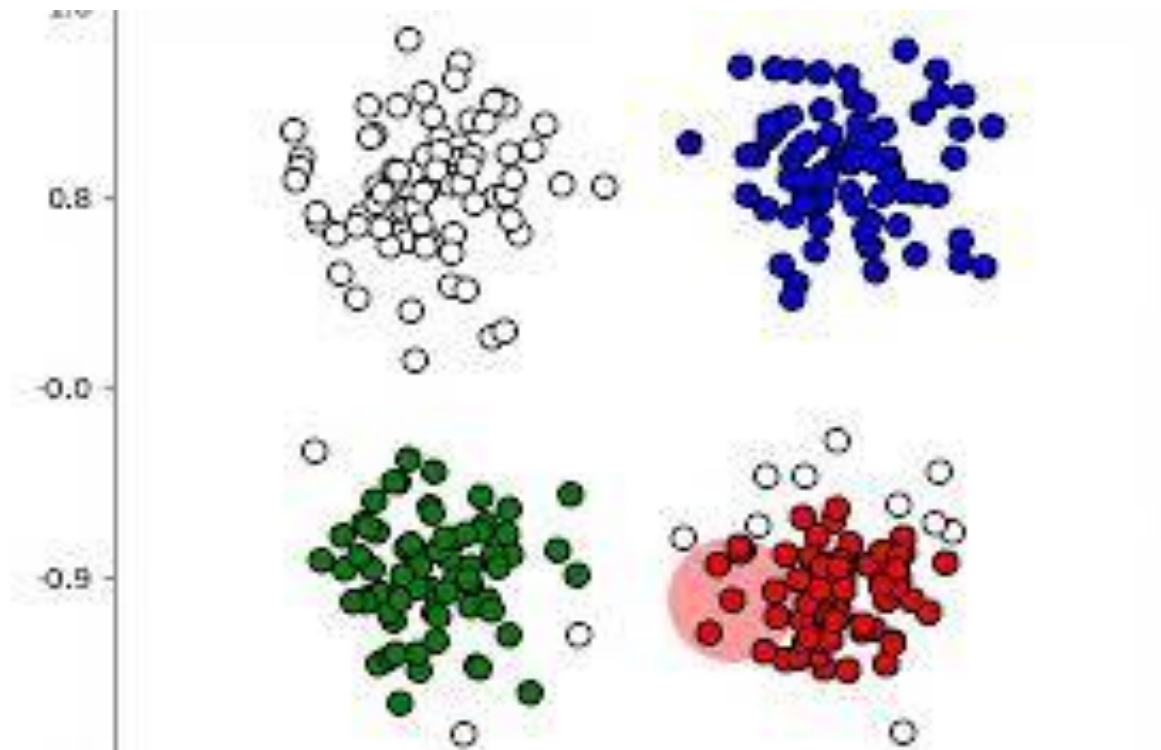
OPTICS

Plots clusters according to a preset change in the density of neighbours

HDBSCAN

Plots clusters according to a best guess for the euclidean distance that arises from using all possible values of it

DBSCAN, HDBSCAN, OPTICS



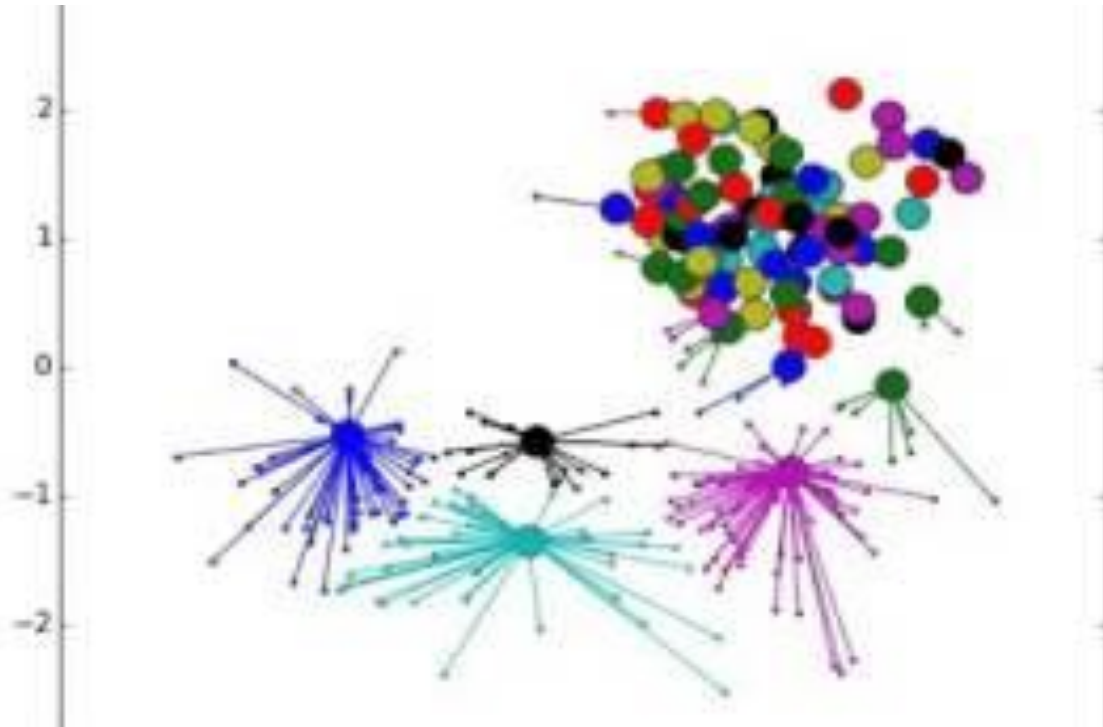
<https://www.youtube.com/watch?v=ldy6xQ5YQ7I>

Affinity propagation

Steps to Affinity propagation:

- 1) Define 2 variables $r(i, k)$ - responsibility and $a(i, k)$ - accumulated evidence for each point, both values are initially zero
- 2) $r(i, k) \leftarrow s(i, k) - \max[a(i, k') + s(i, k') \mid k' \neq k]$ where $s(i, k)$ is the negative of the euclidean distance between i and k
- 3) $a(i, k) \leftarrow \min[0, r(k, k) + \sum r(i', k) \text{ s.t. } i' \notin \{i, k\}]$
- 4) Measure convergence of both $r(i, k)$ and $a(i, k)$ via:
 $r_{t+1}(i, k) = \lambda * r_t(i, k) + (1 - \lambda) * r_{t+1}(i, k)$, λ is user-defined
 $a_{t+1}(i, k) = \lambda * a_t(i, k) + (1 - \lambda) * a_{t+1}(i, k)$, λ is user-defined
- 5) Repeat 2, 3 and 4 until convergence for each element
- 6) Choose points that satisfy $r(k, k) + a(k, k) \geq 0$ as exemplars and assign other points to them based on $\text{argmax}[s(i, k)]$

Affinity propagation



<https://www.youtube.com/watch?v=NaldkmCouLw>



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