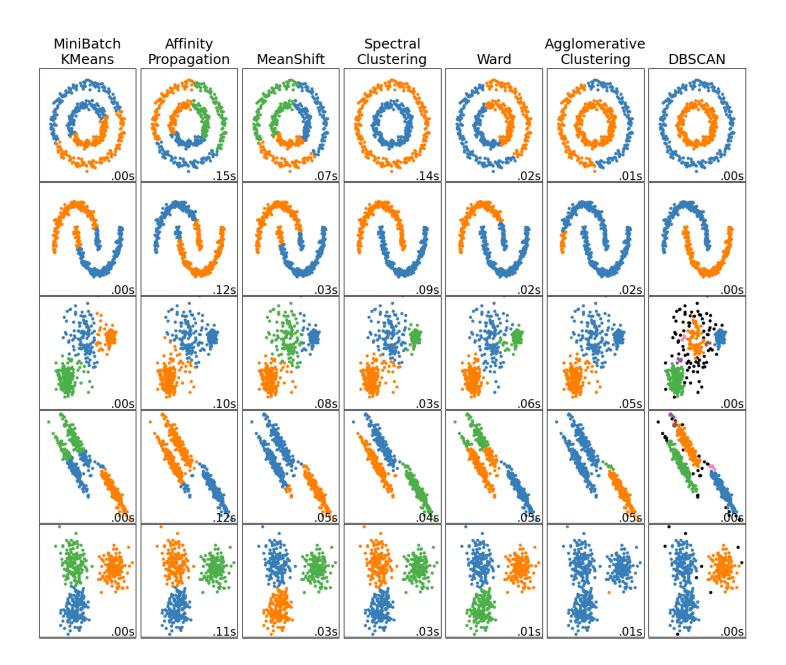
UNSUPERVISED LEARNING PART 3: DENSITY-BASED CLUSTERING



OUTLINE

- Hierarchical Clustering
 - Agglomerative
 - Divisive
- Density Based Clustering
 - DBSCAN

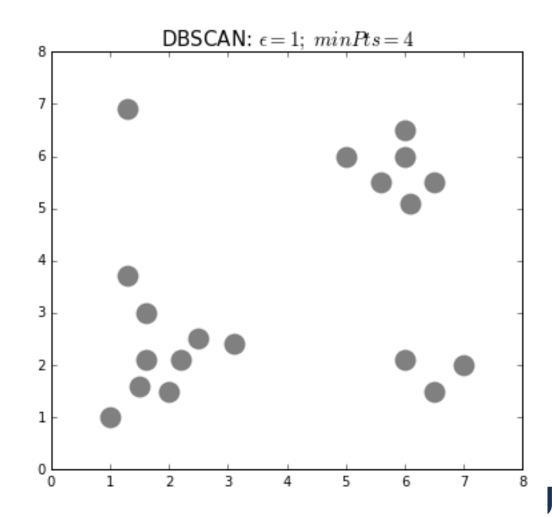
| Clustering Algorithm Type | | Clustering Methodology | Algorithm(s) |
|--|------------------------|---|--|
| | Centroid- based | Cluster points based on proximity to centroid | KMeans KMeans++ KMedoids |
| OF the collection and the production of the prod | Connectivity- based | Cluster points based on proximity between clusters | Hierarchical Clustering (Agglomerative and Divisive) |
| | Density-based | Cluster points based on their density instead of proximity | DBSCAN OPTICS HDBSCAN |
| | Graph-based | Cluster points based on graph distance | Affinitiy Propagation Spectral Clustering |
| | Distribution- based | Cluster points based on their likelihood of belonging to the same distribution. | Gaussian Mixture Models (GMMs) |
| | Compression- based | Transform data to a lower dimensional space and then perform clustering | BIRCH |



DBSCAN (DENSITY-BASED SPATIAL CLUSTERING OF APPS W NOISE)

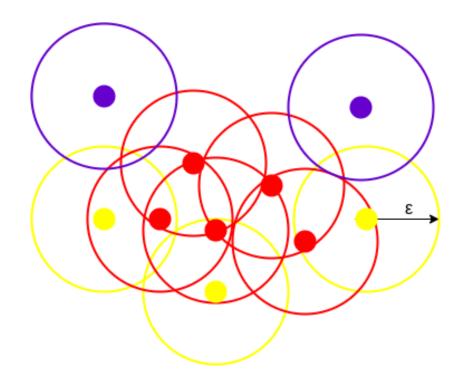
DBSCAN ALGORITHM

- 1. Pick hyperparamters: ε and min. points.
- 2. Pick any unvisited point. Find its neighbors within a specified distance (ε).
- 3. If there are enough neighbors (at least *minPts*), start a new cluster. Otherwise, mark it as noise.
- 4. Add all neighbors to the cluster. Expand the cluster by checking each new point's neighbors and adding them if they qualify.
- 5. Repeat until no more points can be added to the cluster.
- 6. Move to the next unvisited point and repeat the process until all points are either clustered or marked as noise



DENSITY BASED CLUSTERING - DBSCAN

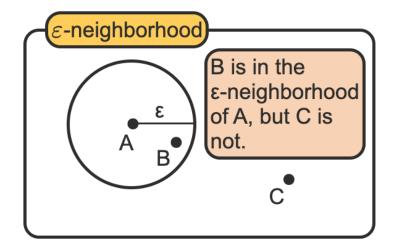
- Density: The number of points within a specified radius (Eps).
- Core Point: Has at least MinPts within Eps (interior of a cluster).
- Border Point: Has fewer than MinPts within Eps but is near a core point.
- Noise Point: Neither a core point nor a border point.

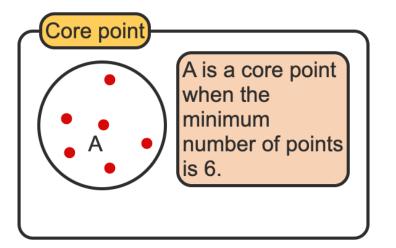


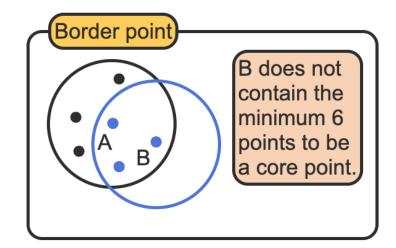
The above figure shows us a cluster created by DBCAN with *minPoints* = 3. Here, we draw a circle of equal radius *epsilon* around every data point.

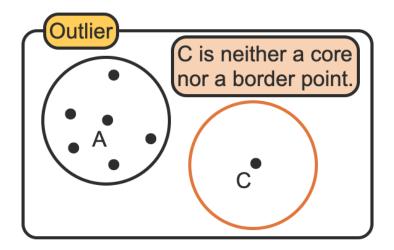


DBSCAN DEFINITIONS



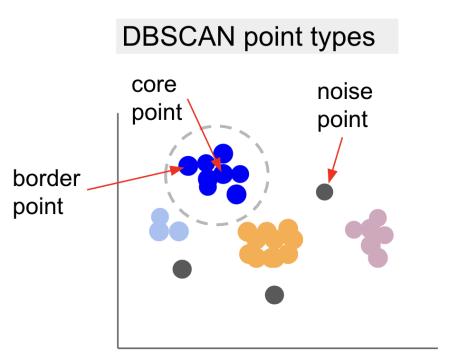




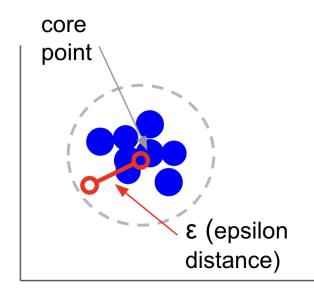




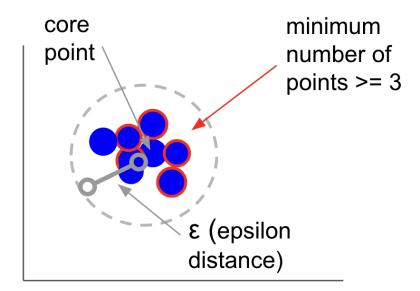
DBSCAN: CORE, BORDER, AND NOISE POINTS





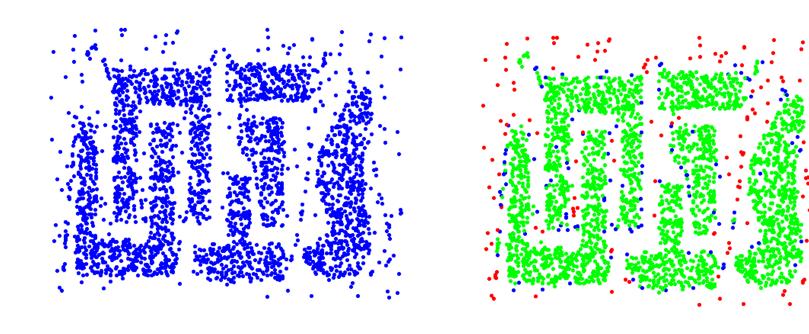


DBSCAN min. points





DBSCAN: CORE, BORDER AND NOISE POINTS

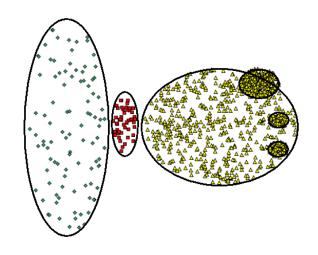


Original Points

Point types: core, border and noise

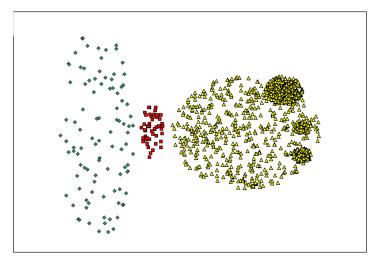


WHEN DBSCAN DOES NOT WORK WELL

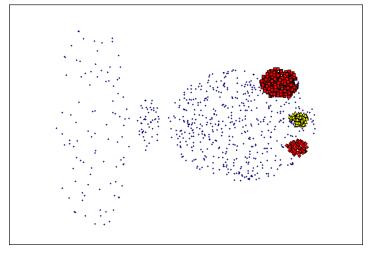


Original Points

- Varying densities
- High-dimensional data



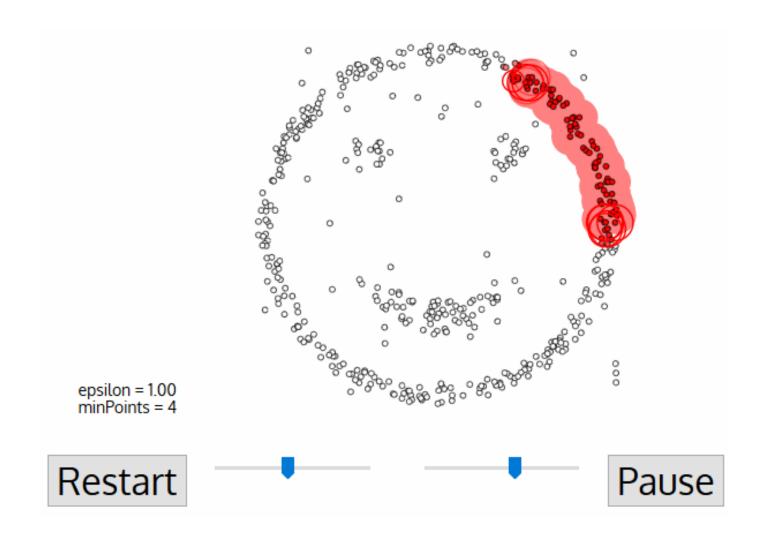
(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)



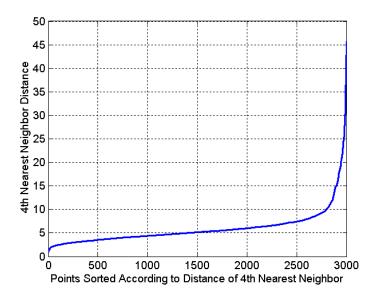
DBSCAN VISUALIZED (https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/)





DBSCAN: DETERMINING EPS AND MINPTS

- Choosing Epsilon (ε): Use the K-distance graph; the "elbow" point indicates the optimal value.
- Nearest Neighbor Concept: In a cluster, the k-th nearest neighbors are at similar distances.
- **Noise Points**: Their k-th nearest neighbor is farther away.
- **Finding ε**: Plot the sorted distances to the k-th nearest neighbor.
- Choosing minPoints: Set it at least one greater than the dataset's dimensions: minPoints ≥ Dimensions + 1





DBSCAN ADVANTAGES AND DISADVANTAGES

Advantages:

- If we look at its advantages, it is very good at picking up dense areas in data and points that are far from others. This means that the data doesn't have to have a specific shape and can be surrounded by other points if they are also densely connected.
- It has two hyperparameters, minimum points and ε, but there is no need to specify the number of clusters, as in K-Means.
- It can be used with large databases since it was designed for high-dimensional data.

Disadvantages:

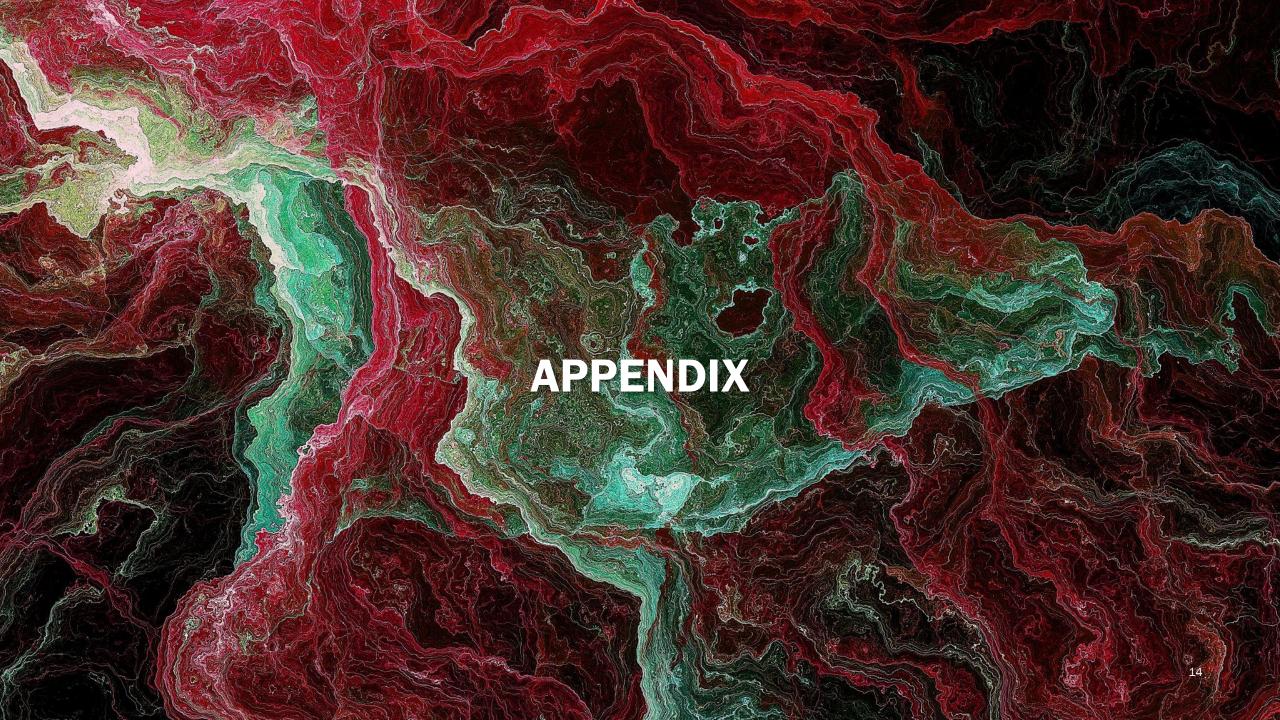
- Can't address different densities in the same cluster
- It is also dependent on the distance metric and scaling of the points.
- O(nlog(n)) time complexity

DBSCAN Extensions

- Other algorithms, such as Hierarchical DBSCAN (HDBSCAN) and Ordering points to identify the clustering structure (OPTICS), are considered extensions of DBSCAN.
- HDBSCAN and OPTICS can usually perform better when there are clusters of varying densities in the data and are less sensitive to the choice or initial min points and ε parameters.







SUMMARY OF SELECTED CLUSTERING ALGORITHMS IN SCIKIT-LEARN

| Method name | Parameters | Scalability | Usecase | Geometry (metric used) |
|------------------------------|---|---|--|---|
| <u>K-Means</u> | number of clusters | Very large n_samples, medium n_clusters with MiniBatch code | General-purpose, even cluster size, flat geometry, not too many clusters, inductive | Distances between points |
| Affinity propagation | damping, sample preference | Not scalable with n_samples | Many clusters, uneven cluster size, non-flat geometry, inductive | Graph distance (e.g., nearest- neighbor graph) |
| Mean-shift | bandwidth | Not scalable with n_samples | Many clusters, uneven cluster size, non-flat geometry, inductive | Distances between points |
| Spectral clustering | number of clusters | Medium n_samples, small n_clusters | Few clusters, even cluster size, non-flat geometry, transductive | Graph distance (e.g., nearest- neighbor graph) |
| Ward hierarchical clustering | number of clusters or distance threshold | Large n_samples and n_clusters | Many clusters, possibly connectivity constraints, transductive | Distances between points |
| Agglomerative clustering | number of clusters or distance threshold, linkage type, distance | Large n_samples and n_clusters | Many clusters, possibly connectivity constraints, non-Euclidean distances, transductive | Any pairwise distance |
| <u>DBSCAN</u> | neighborhood size | Very large n_samples, medium n_clusters | Non-flat geometry, uneven cluster sizes, outlier removal, transductive | Distances between nearest points |
| <u>HDBSCAN</u> | minimum cluster membership, minimum point neighbors | large n_samples, medium n_clusters | Non-flat geometry, uneven cluster sizes, outlier removal, transductive, hierarchical, variable cluster density | Distances between nearest points |
| Gaussian mixtures | many | Not scalable | Flat geometry, good for density estimation, inductive | Mahalanobis distances to centers |
| <u>BIRCH</u> | branching factor, threshold, optional global clusterer. | Large n_clusters and n_samples | Large dataset, outlier removal, data reduction, inductive | Euclidean distance between points 15 |

DISTANCE MEASURES

Minkowski Distance (http://en.wikipedia.org/wiki/Minkowski_distance)

For

$$\mathbf{x} = (x_1 \ x_2 \cdots x_n)$$
 and $\mathbf{y} = (y_1 \ y_2 \cdots y_n)$

$$d(\mathbf{x}, \mathbf{y}) = \left(|x_1 - y_1|^p + |x_2 - y_2|^p + \dots + |x_n - y_n|^p \right)^{\frac{1}{p}}, \quad p > 0$$

• p = 1: Manhattan (city block) distance

$$d(\mathbf{x}, \mathbf{y}) = |x_1 - y_1| + |x_2 - y_2| \dots + |x_n - y_n|$$

• p = 2: Euclidean distance

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{|x_1 - y_1|^2 + |x_2 - y_2|^2 + \dots + |x_n - y_n|^2}$$

- Do not confuse p with n, i.e., all these distances are defined based on all numbers of features (dimensions).
- A generic measure: use appropriate p in different applications



REFERENCES

- https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68
- https://www.geeksforgeeks.org/ml-k-medoids-clustering-with-example/
- https://www.analyticsvidhya.com/blog/2021/06/kmodes-clustering-algorithm-for-categorical-data/#h-what-iskmodes
- https://towardsdatascience.com/the-k-prototype-as-clustering-algorithm-for-mixed-data-type-categorical-and-numerical-fe7c50538ebb
- http://scikit-learn.org/stable/modules/clustering.html
- https://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.15.4028&rep=rep1&type=pdf
- https://github.com/nicodv/kmodes/blob/master/kmodes/kprototypes.py
- https://dashee87.github.io/data%20science/general/Clustering-with-Scikit-with-GIFs/
- https://www.geeksforgeeks.org/difference-between-agglomerative-clustering-and-divisive-clustering/
- https://stackabuse.com/dbscan-with-scikit-learn-in-python/

