

Datascience fundamentals

Fernando Lovera Lecture: DBSCAN





INDEX

- 1 Intuition of DBSCAN
- 2 DBSCAN vs. K-Means Clustering
- 3 DBSCAN Hyperparameters Theory
- 4 DBSCAN Hyperparameters Coding
- 5 Outlier Project Exercise
- 6 Project Solutions



 DBSCAN - Density-based spatial clustering of applications with noise is a powerful technique which can be used for clustering and outlier detection.



Let's get started!



Theory and Intuition



- DBSCAN stands for <u>D</u>ensity-<u>b</u>ased <u>s</u>patial
 <u>c</u>lustering of <u>a</u>pplications with <u>n</u>oise.
- Let's review a brief history of the algorithm and then explore an intuition based approach to understanding how it works.



- 1972: Robert F. Ling published a closely related algorithm in "The Theory and Construction of k-Clusters" with an expected run time of O(n³).
- This means that as n number of points grows, the run time of the algorithm grows cubically!



- 1996: Martin Ester, Hans-Peter Kriegel, Jörg Sander and Xiaowei Xu proposed the modern version of DBSCAN with a runtime of O(n²).
- 2014: DBSCAN was awarded the test of time award at the leading data mining conference, SIGKDD.



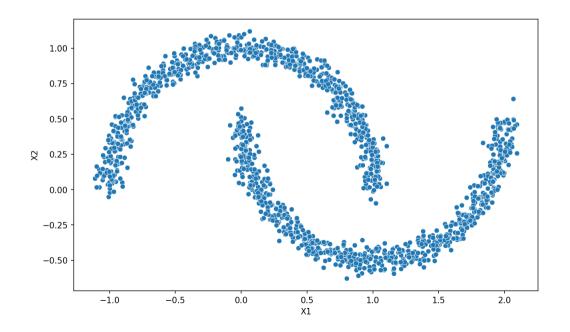
- Questions to consider:
 - O How does DBSCAN work?
 - O Advantages and disadvantages of DBSCAN?
 - O How does it deal with outliers and noise?



- DBSCAN Key Ideas
 - DBSCAN focuses on using **density** of points as its main factor for assigning cluster labels.
 - O This creates the ability to find cluster segmentations that other algorithms have difficulty with.

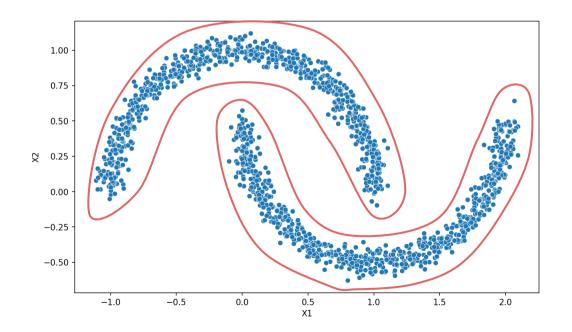


Consider the following data set:



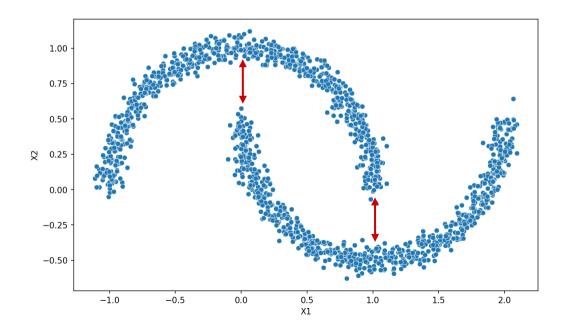


Cleary two "moon" shaped clusters:



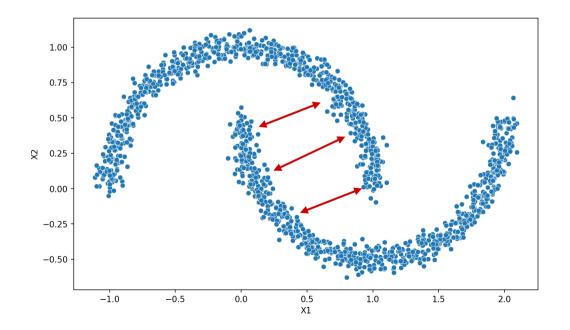


• But distance based clustering has issues:



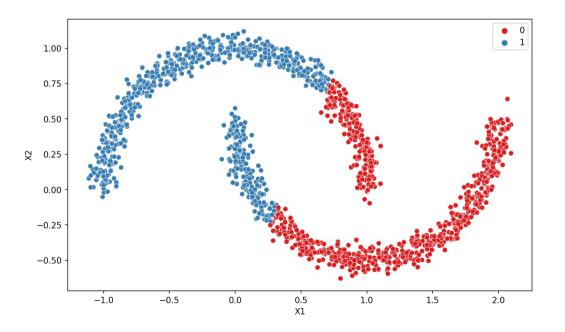


• But distance based clustering has issues:



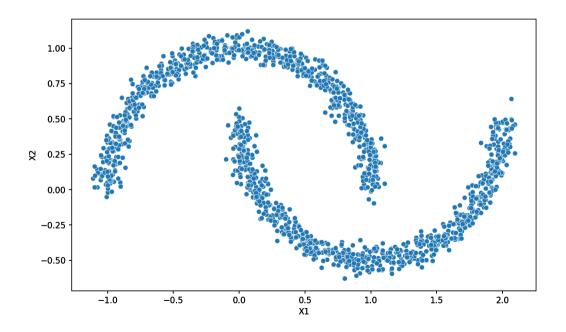


Results of K-Means:



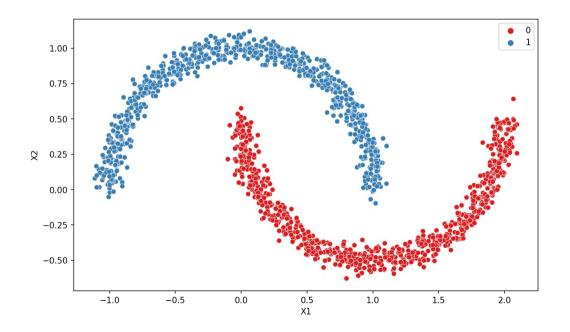


Results of DBSCAN:





Results of DBSCAN:





- DBSCAN iterates through points and uses two key hyperparameters (epsilon and minimum number of points) to assign cluster labels.
- Unlike K-Means, it focuses on density as the main factor for cluster assignment of points.



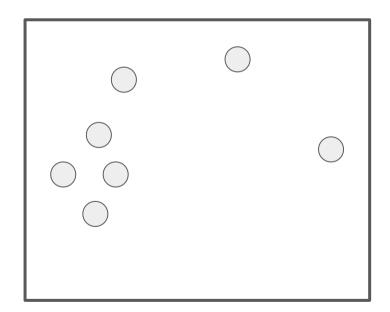
- DBSCAN Key Hyperparameters:
 - O Epsilon:
 - Distance extended from a point.
 - O Minimum Number of Points:
 - Minimum number of points in an epsilon distance.



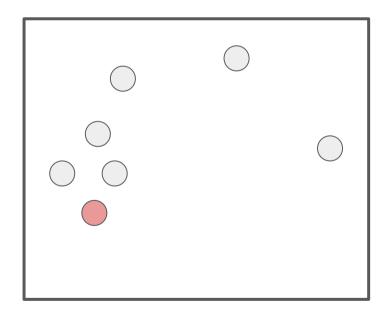
- DBSCAN Point Types:
 - O Core
 - Border
 - Outlier



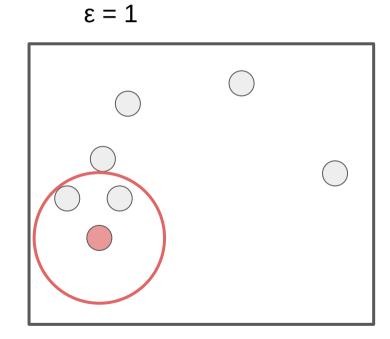
- DBSCAN Point Types:
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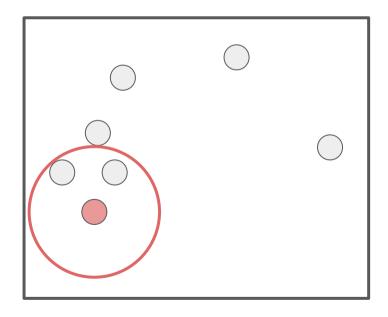






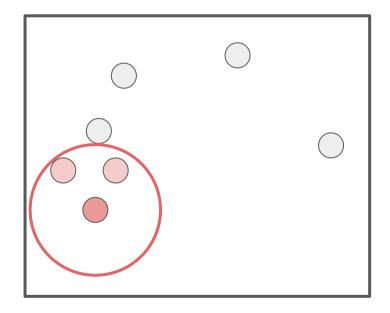


 $\varepsilon = 1$ and Min Points = 2





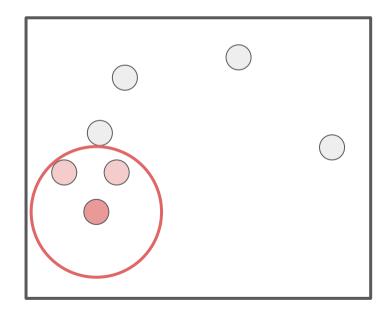
 $\varepsilon = 1$ and Min Points = 2





- DBSCAN Point Types:O Core:
 - Point with min. points in epsilon range.

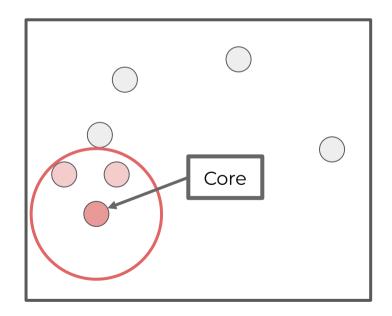
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- DBSCAN Point Types:O Core:
 - Point with min. points in epsilon range.

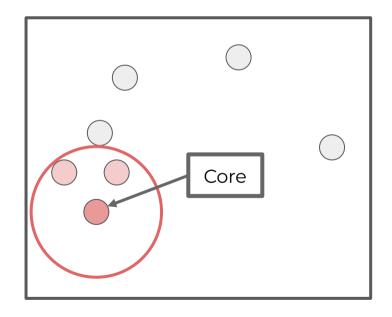
 $\varepsilon = 1$ and Min Points = 2





- DBSCAN Point Types:O Core:
 - Point with min. points in epsilon range (including itself).

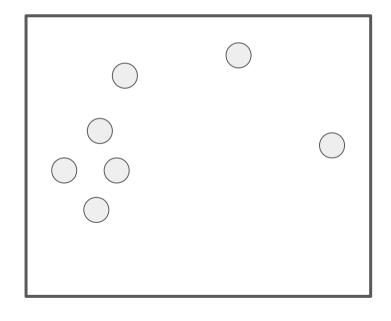
 $\varepsilon = 1$ and Min Points = 3





- DBSCAN Point Types:O Border:
 - In epsilon range of core point, but does not contain min. number of points.

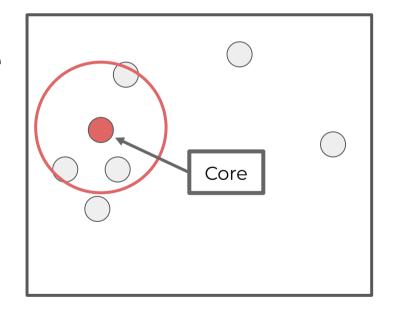






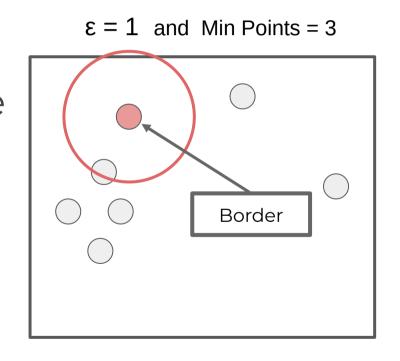
- DBSCAN Point Types:O Border:
 - In epsilon range of core point, but does not contain min. number of points.

$$\varepsilon = 1$$
 and Min Points = 3



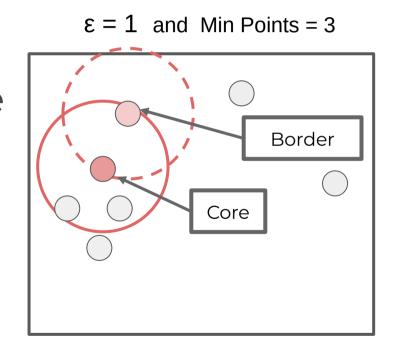


- DBSCAN Point Types:O Border:
 - In epsilon range of core point, but does not contain min. number of points.





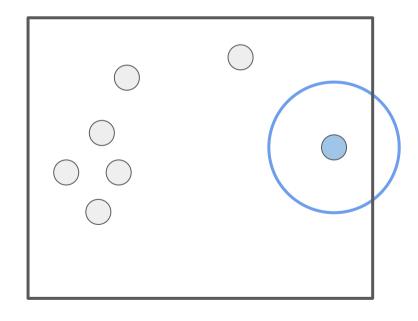
- DBSCAN Point Types:O Border:
 - In epsilon range of core point, but does not contain min. number of points.





- DBSCAN Point Types:Outlier:
 - Can not be "reached" by points in a cluster assignment.

 $\varepsilon = 1$ and Min Points = 3





 We will discuss neighborhoods, epsilon, and minimum number of points in further detail later on, but let's review the actual process of DBSCAN for assigning clusters.



- DBSCAN Procedure:
 - O Pick a random point not yet assigned.
 - O Determine the point type.
 - Once a **core** point has been found, add all directly reachable points to the same cluster as core.
 - O Repeat until all points have been assigned to a cluster or as an outlier.



Let's explore a useful visualization of the procedure!



Coding Example on Data Sets



Let's explore how DBSCAN compares to K-Means clustering on some unique data sets to get an intuitive understanding of the density based approach of DBSCAN versus a distance based clustering approach of K-Means.



Key Hyperparameters



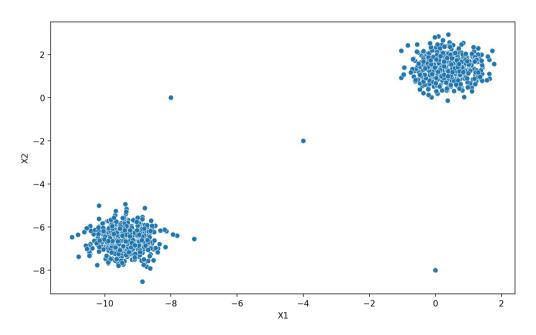
- As we've seen already, there are two key hyperparameters to consider for DBSCAN:
 O Epsilon:
 - Distance extended from a point to search for Min. Number of Points.
 - O Min. Number of Points:
 - Min. Number of Points within Epsilon distance to be a core point.



- Adjusting these hyperparameters have two main outcomes:
 - O Changing number of clusters.
 - O Changing what is an outlier point.

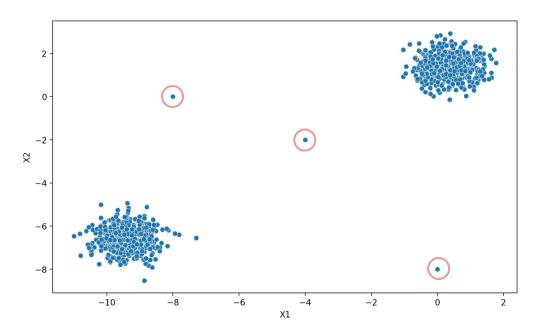


Example Data Set:



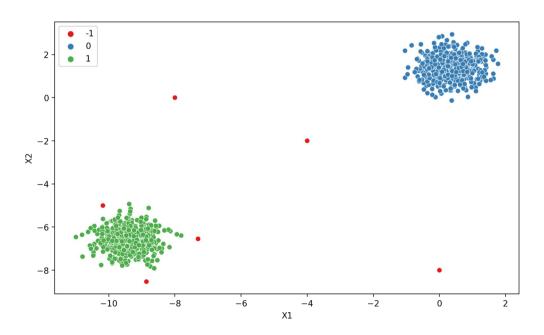


Example Data Set:



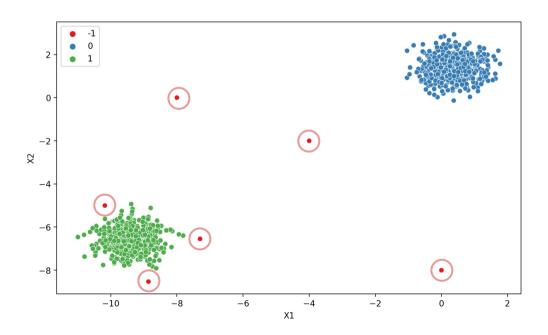


DBSCAN Results:



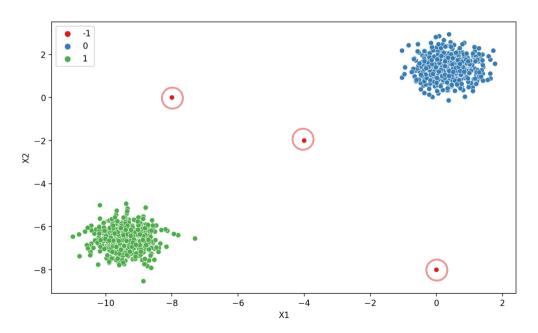


DBSCAN Results:





DBSCAN Results:





- Epsilon Intuition:
 - O Increasing epsilon allows more points to be **core** points which also results in more **border** points and less outlier points.
 - O Imagine a huge epsilon, all points would be within the neighborhood and classified as the same cluster!



- Epsilon Intuition:
 - O Decreasing epsilon causes more points not to be in range of each other, creating more unique clusters.
 - O Imagine a tiny epsilon, the range would not extend far out enough to come into contact with any other points!



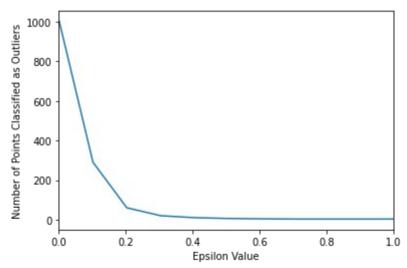
- Methods for finding an epsilon value:
 - O Run multiple DBSCAN models varying epsilon and measure:
 - Number of Clusters
 - Number of Outliers
 - Percentage of Outliers



- Methods for finding an epsilon value:
 - O Extremely dependent on the particular data set and domain space.
 - Requires user to have some expectation or intuition about number of clusters and relative percentage of outliers.



 Plot "elbow/knee" diagram comparing epsilon values:





- Minimum Number of Samples/Points:
 - O Number of samples in a neighborhood for a point to be considered as a **core** point (including the point itself).



- Min. Number of Samples Intuition:
 - O Increasing to a larger number of samples needed to be considered a core point, causes more points to be considered unique outliers.



- Min. Number of Samples Intuition:
 - O Imagine if min. number of samples was close to total number of points available, then very likely all points would become outliers.



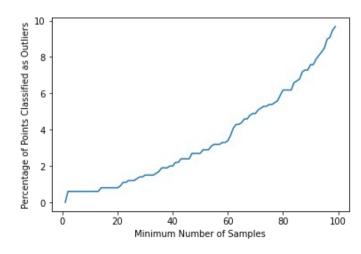
- Choosing Min. Number of Samples:
 - Test multiple potential values and chart against number of outliers labeled.



Choosing Min. Number of Samples:

 Test multiple potential values and chart against number of outliers

labeled.

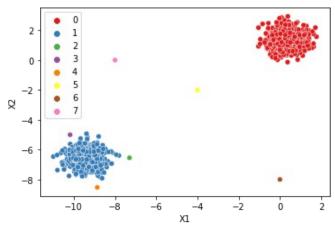




- Min. Number of Samples Note:
 - O Useful to increase to create potential new small clusters, instead of complete outliers.



- Min. Number of Samples Note:
 - O Useful to increase to create potential new small clusters, instead of complete outliers.





 Let's continue by exploring hyperparameters with code and data examples!



Hyperparameter Search



Project Exercise Overview



Project Exercise Solutions