Density-Based Clustering

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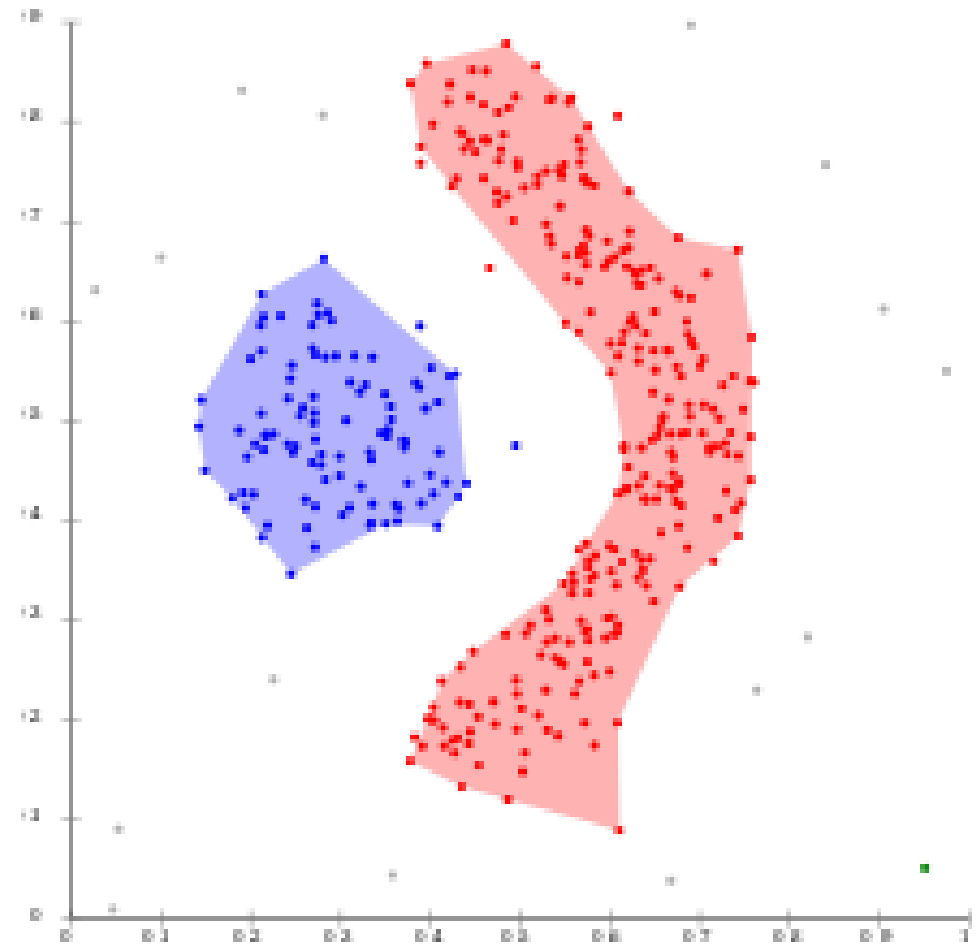
These slides are inspired based on slides from Jing Gao, Chao Zhang and Jiawei Han.

Outline

- Overview
- Basic Concepts
- The DBSCAN Algorithm
- Analysis of DBSCAN

Density-Based Clustering

- Basic Idea
  - Clusters are dense regions in the data space, separated by regions of lower density
  - A cluster is defined as a maximal set of density-connected points
  - Detect arbitrarily shaped clusters



- Method
  - DBSCAN (Density-Based Spatial Clustering of Applications with Noise)

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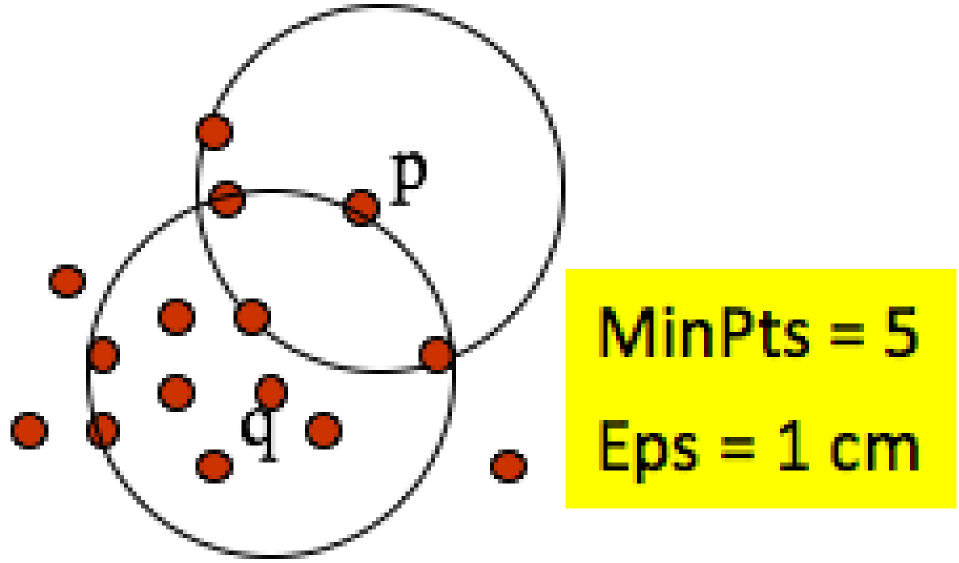
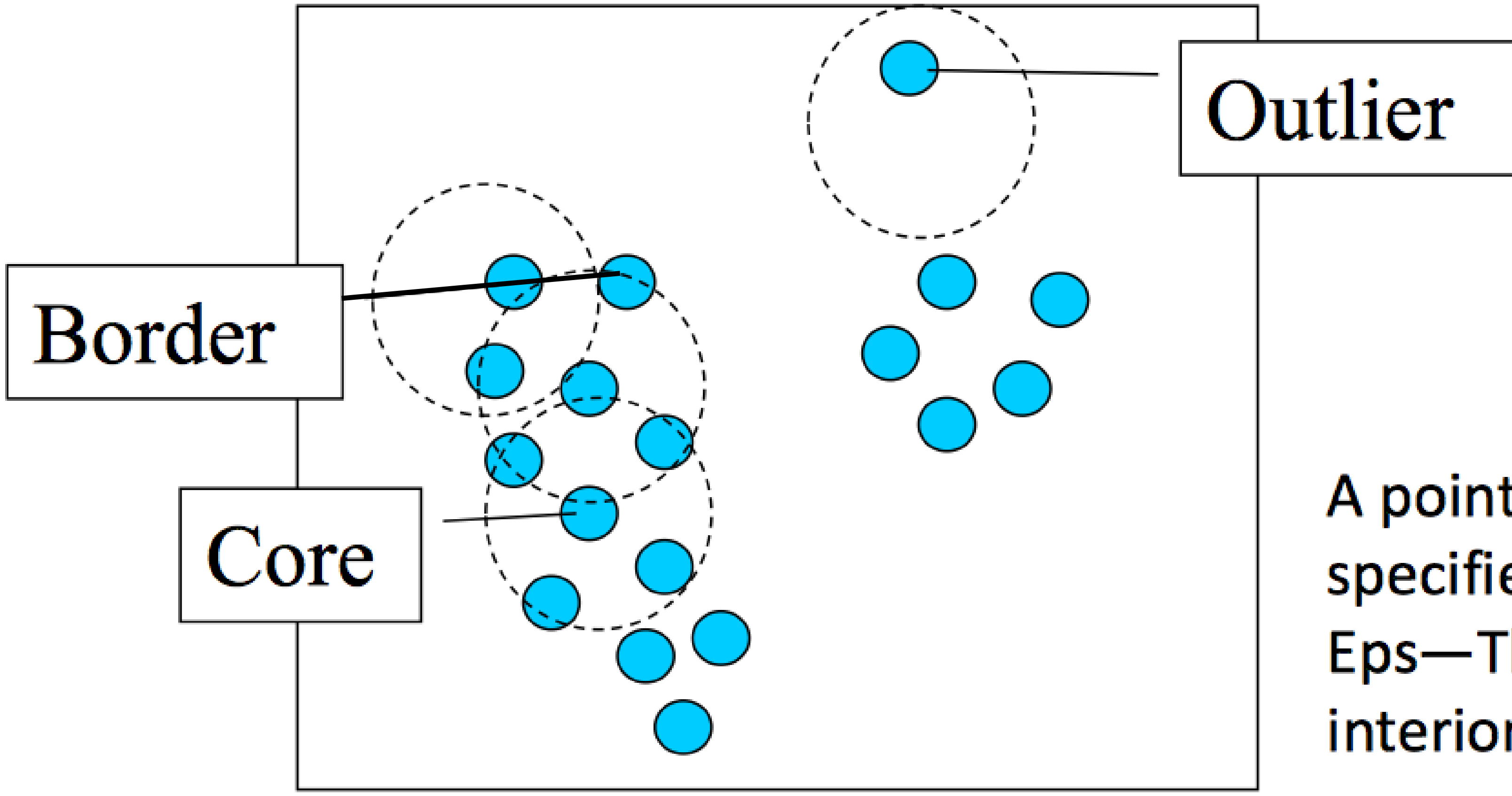
High Density v.s. Low Density

- Two parameters
  - **Eps (ε)**: Maximum radius of the neighborhood
  - **MinPts**: Minimum number of points in the Eps-neighborhood of a point
- High density: ε-Neighborhood of an object contains at least MinPts of objects



Density of ***p*** is low
Density of ***q*** is high

Core Points, Border Points, and Outliers



ε = 1unit, MinPts = 5

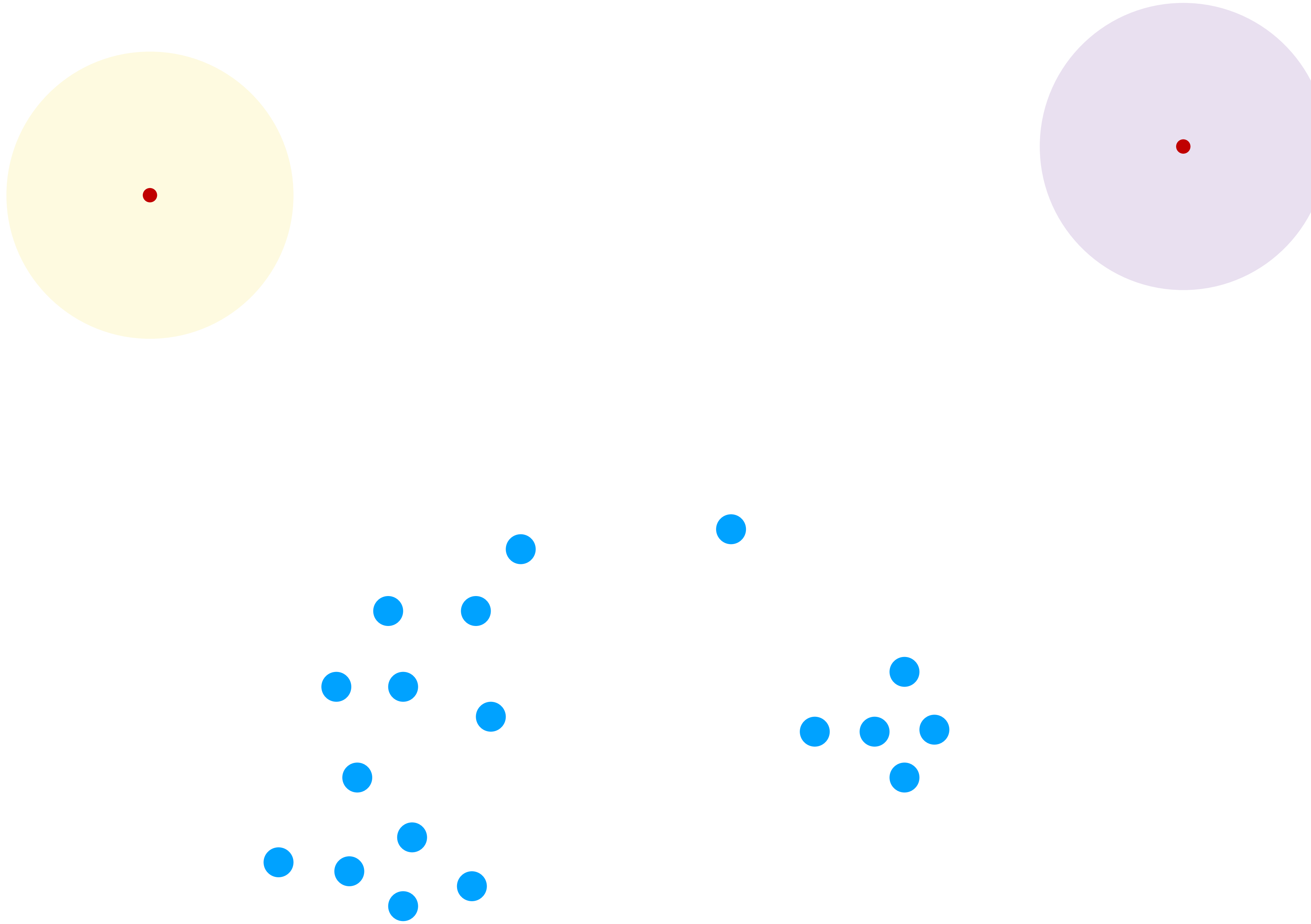
Given ε and *MinPts*, categorize the objects into three exclusive groups.

A point is a core point if it has more than a specified number of points (MinPts) within Eps—These are points that are at the interior of a cluster.

A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.

A noise point is any point that is not a core point nor a border point.

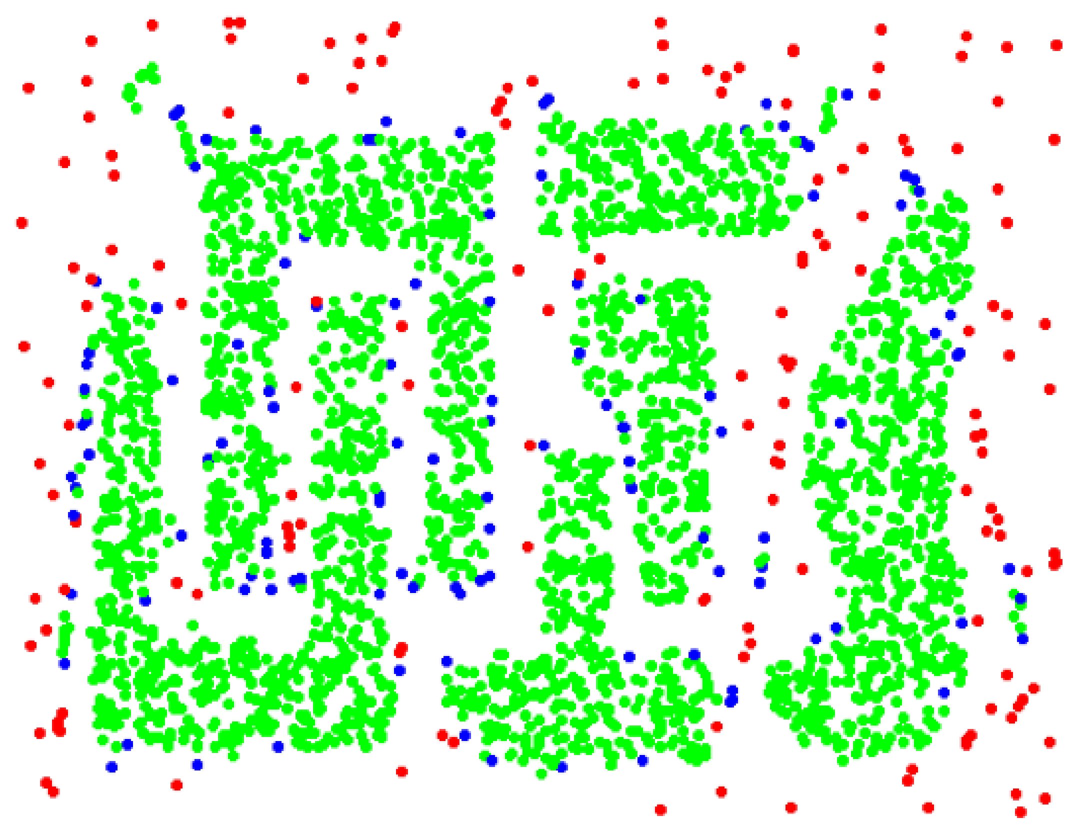
Practice:



ε= 1 unit
MinPts = 5

Examples

Original Points

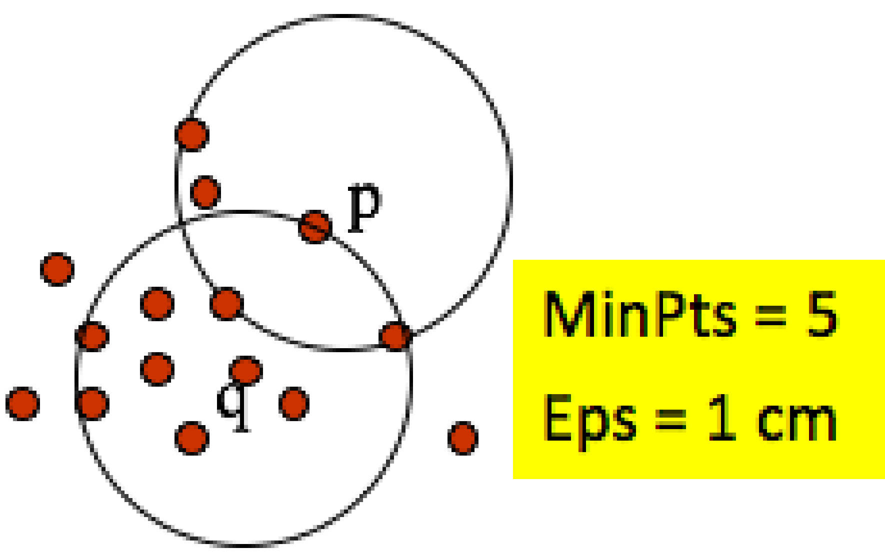


Point types: core, border and outliers

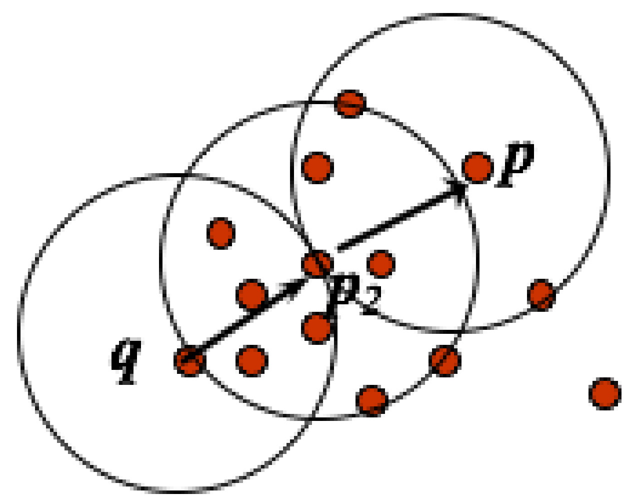
ε = 10, MinPts = 4

Density-based related points

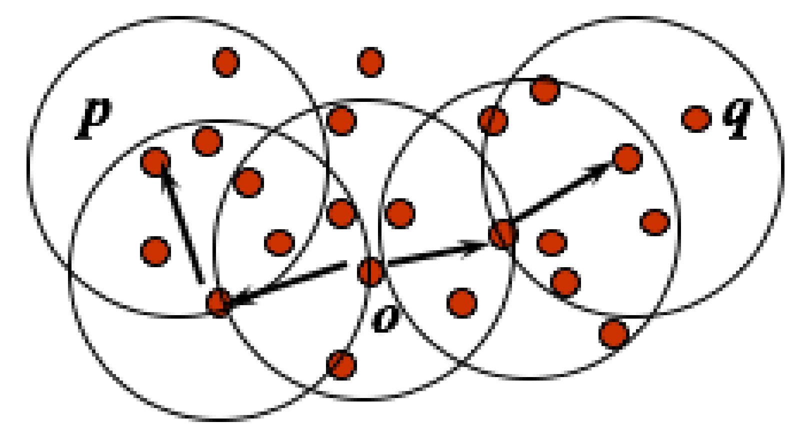
- Direct density reachability:
  - An object p is directly density-reachable from object q if **(1) q is a core object**; and **(2) p is in q's ε-neighborhood**



Directly Density-Reachable



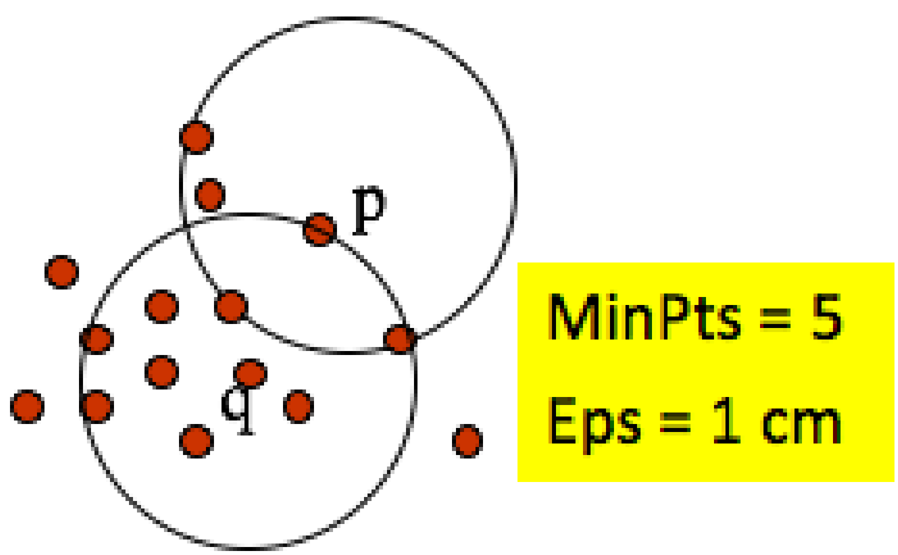
Density-Reachable



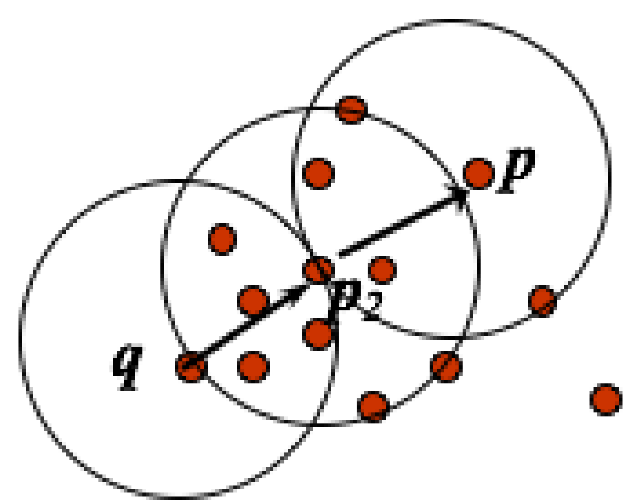
Density-Connected

Density-based related points

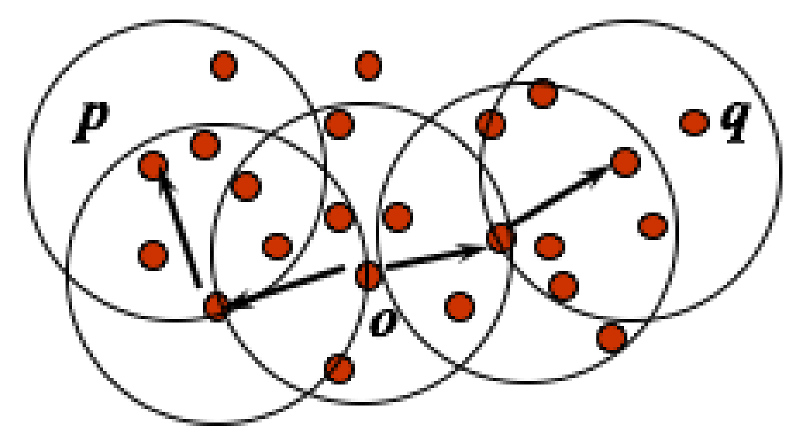
- Density reachability:
  - A point ***p*** is density-reachable from a point ***q*** if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i
  - $p_1 = q \rightarrow p_2 \rightarrow \ldots \rightarrow p_n = q$



Directly Density-Reachable



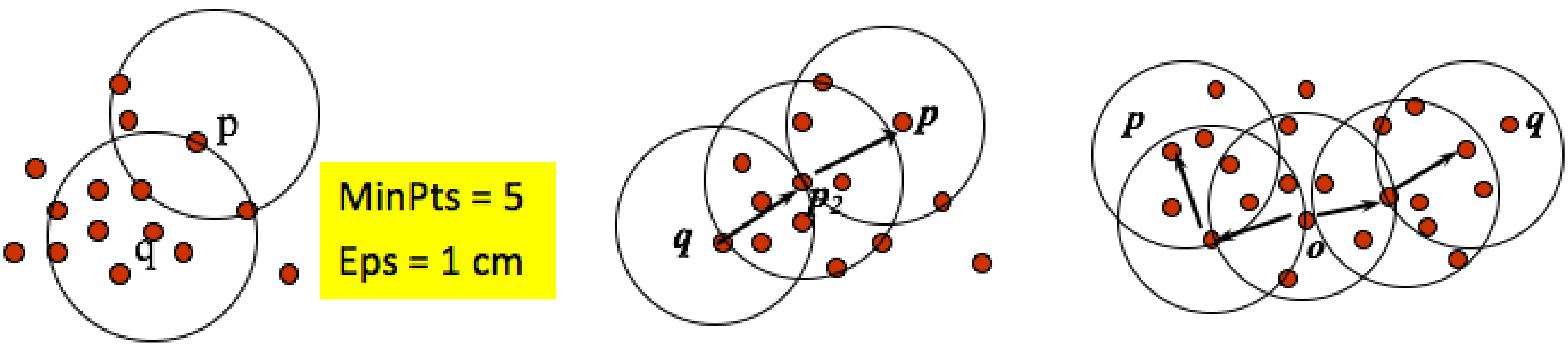
Density-Reachable



Density-Connected

Density-based related points

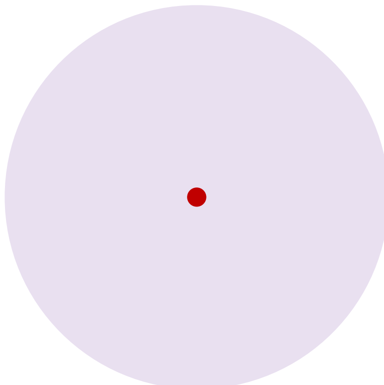
- Density connectivity:
  - A point ***p*** is density-connected to a point ***q*** if there is a point ***o*** such that both ***p*** and ***q*** are density-reachable from ***o***



Directly Density-Reachable

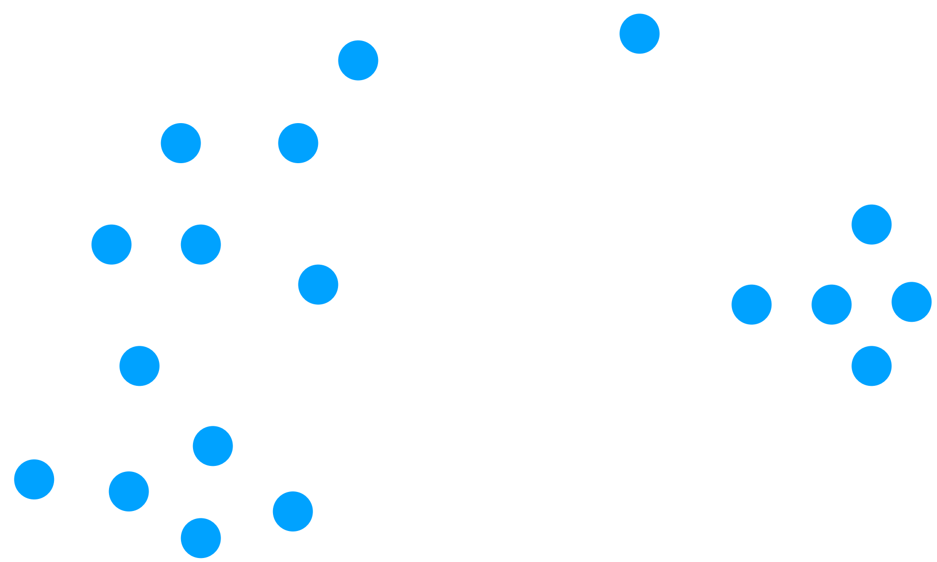
Density-Reachable

Density-Connected



ε= 1 unit

MinPts = 5



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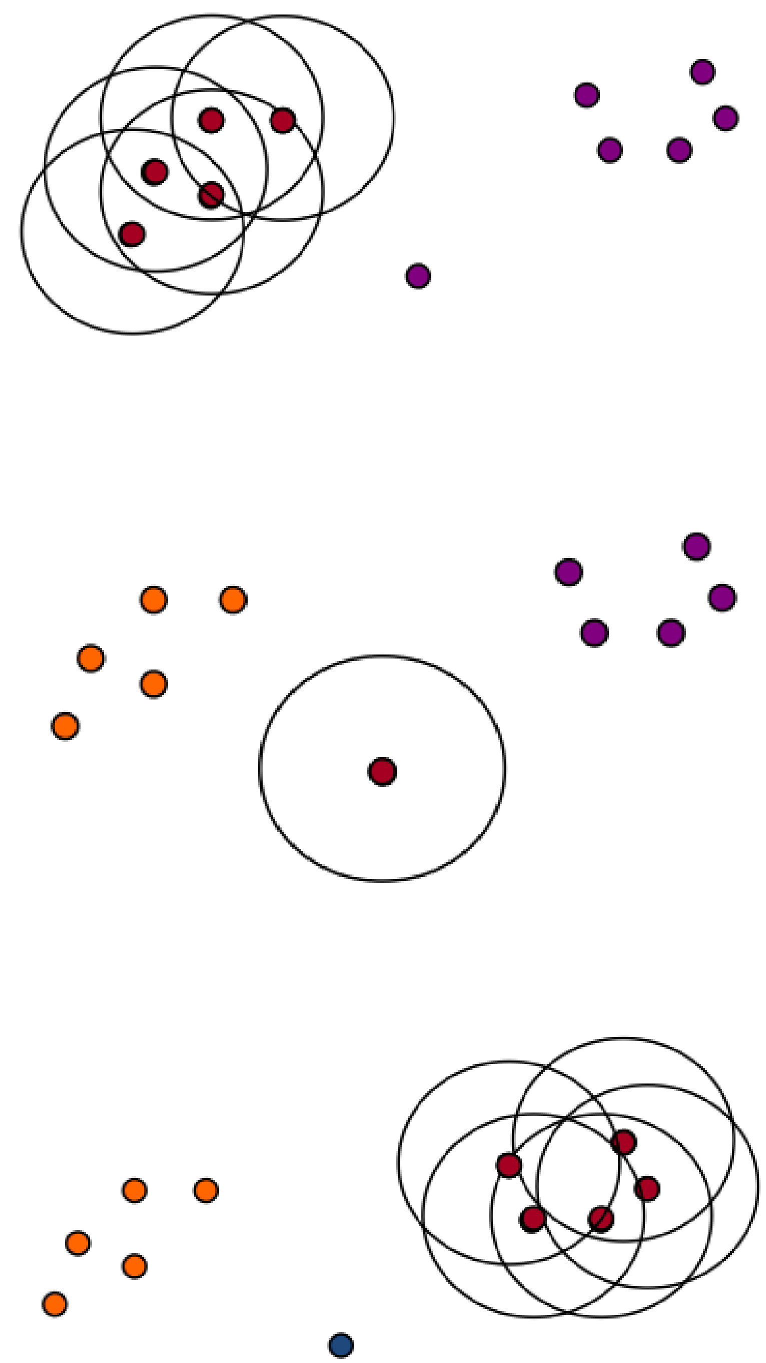
The DBSCAN Algorithm

```
DBSCAN(X, eps, MinPts)
C = 0
for each unvisited point P in dataset X
    mark P as visited
    NeighborPts = regionQuery(P, eps)
    if sizeof(NeighborPts) < MinPts
        mark P as NOISE
    else
        expandCluster(P, NeighborPts, C, eps, MinPts)
        C = next cluster

expandCluster(P, NeighborPts, C, eps, MinPts)
    add P to cluster C
    for each point P' in NeighborPts
        if P' is not visited
            mark P' as visited
            NeighborPts' = regionQuery(P', eps)
            if sizeof(NeighborPts') >= MinPts
                NeighborPts = NeighborPts joined with NeighborPts‘
        if P' is not yet member of any cluster
            add P' to cluster C
```



regionQuery(P, eps) return all points within P's eps-neighborhood (including P)

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

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DBSCAN is Sensitive to Parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

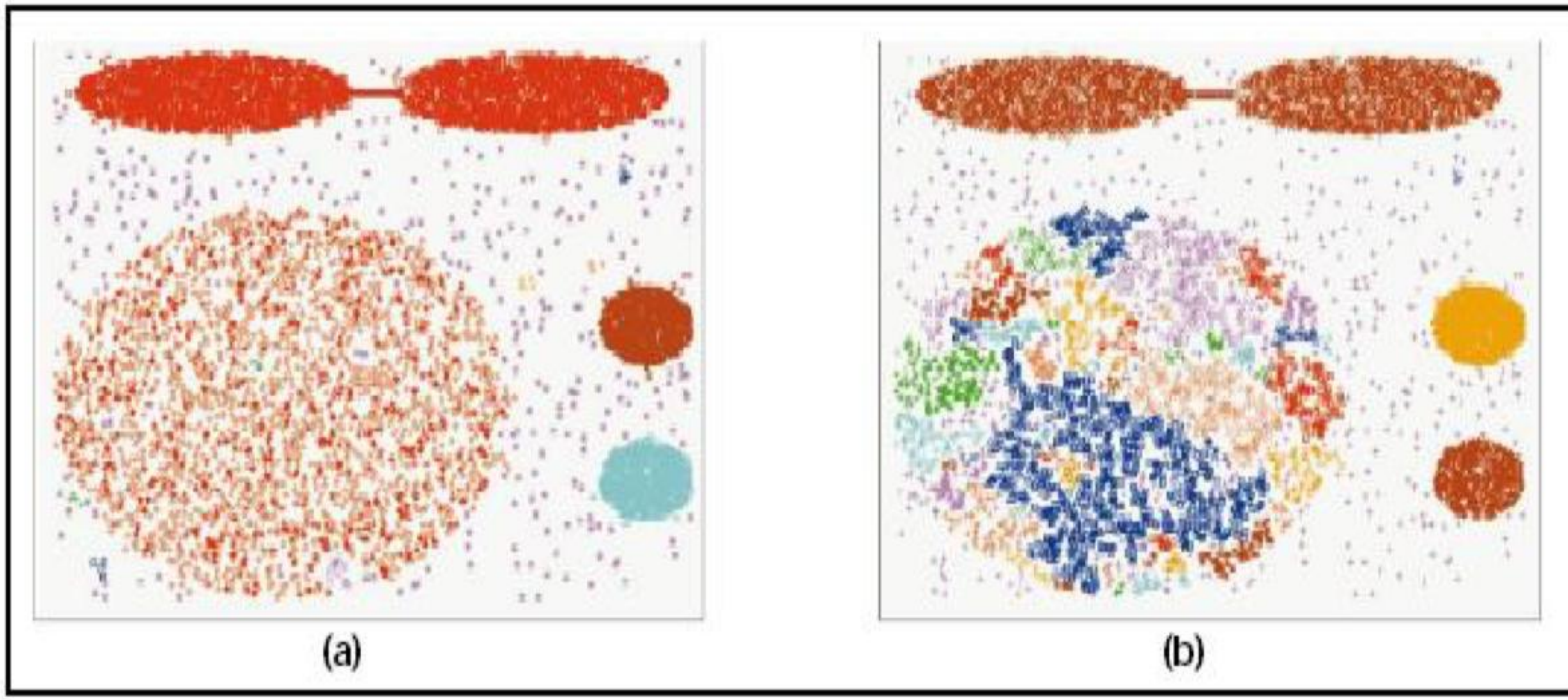


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.

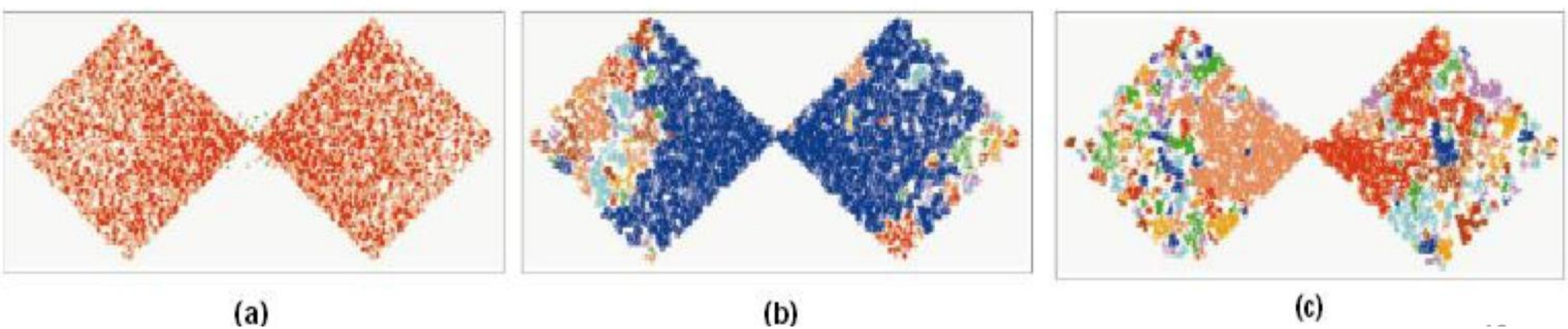


Image Credit: George Karypis.

ε

High value (what will happen?)

Clusters will merge and the majority of data points will be in the same cluster

Low value (what will happen?)

A large part of data won’t be clustered and considered as outliers. Because, they won’t satisfy the number of pints to create a dense region

Do we need to define the number of clusters in DBSCAN?

Nope

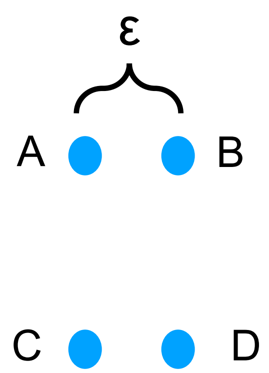
Minimum number of Points (**MinPts**)

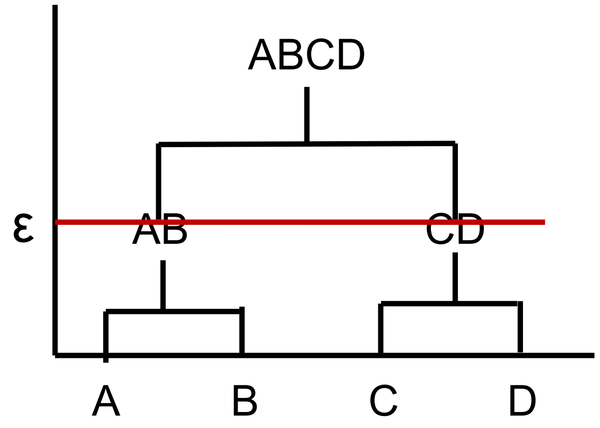
MinPts = 1?

Every point will be a cluster on its own, Why?

Don't forget, in DBSCAN, a core point is counted as the number of neighboring points

MinPts = 2?





Dendogram cut at height ε

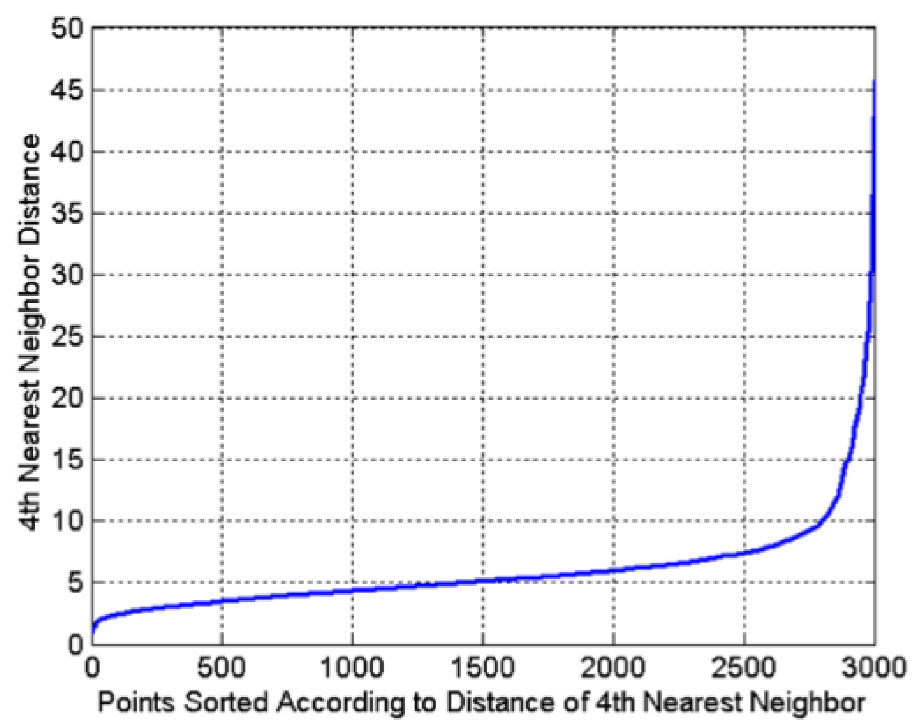
So, MinPts should be at least 3

Rule of thumb, MinPts >= D+1;

For noisy data => MinPts = 2*D (yield more significant clusters)

How about Eps? (Elbow effect)

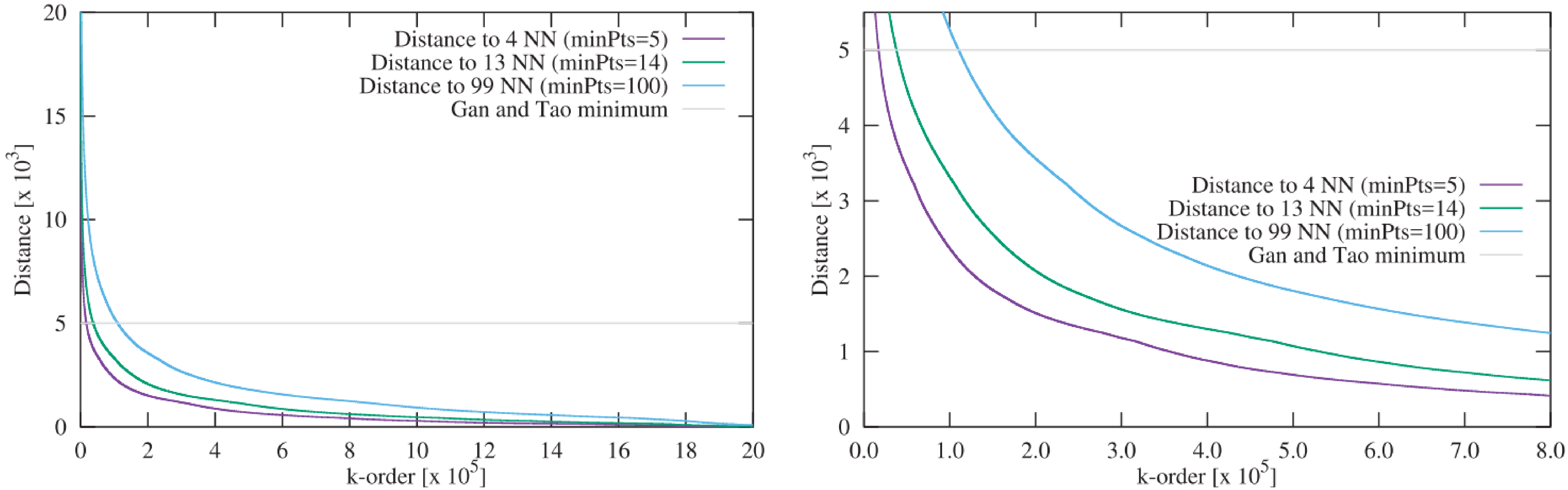
- Idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor



Here we have 3000 points and x-axis shows just a point index.

Point indices are sorted in ascending order based on their 4^{th} nearest neighbor distance

Elbow effect another example



(a) *k*-distance plots

(b) *k*-distance plots (magnified region)

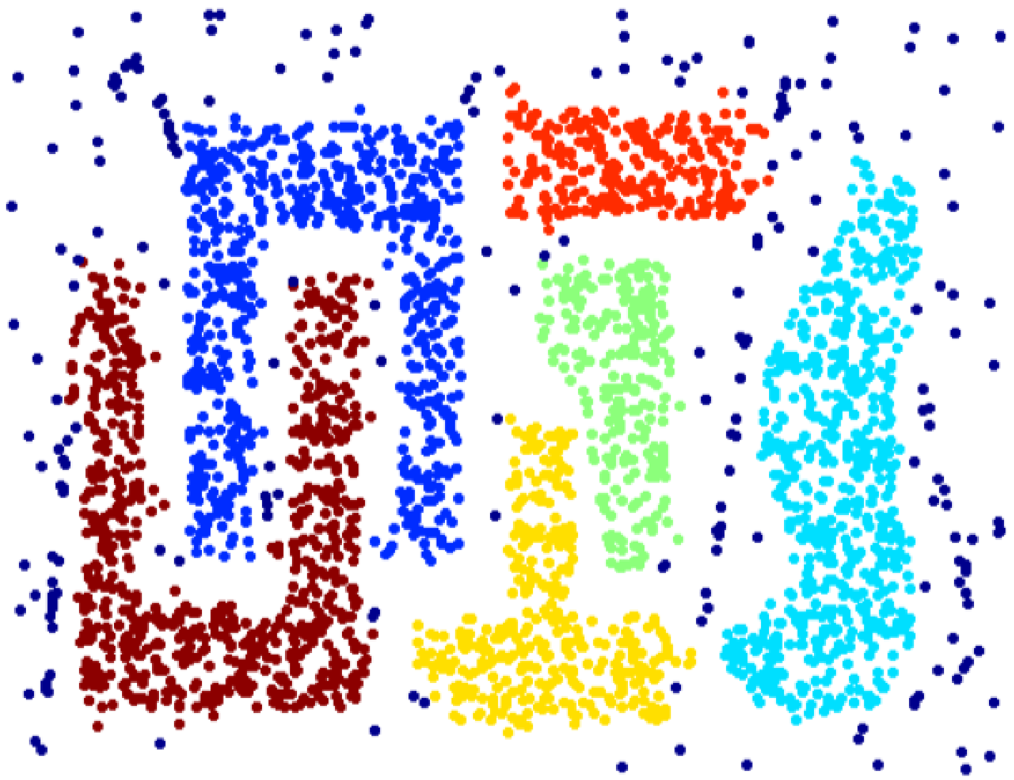
minPts often does not have a significant impact on the clustering results

Erich Schuber et al

When DBSCAN Works Well

- Robust to noise
- Can detect arbitrarily-shaped clusters

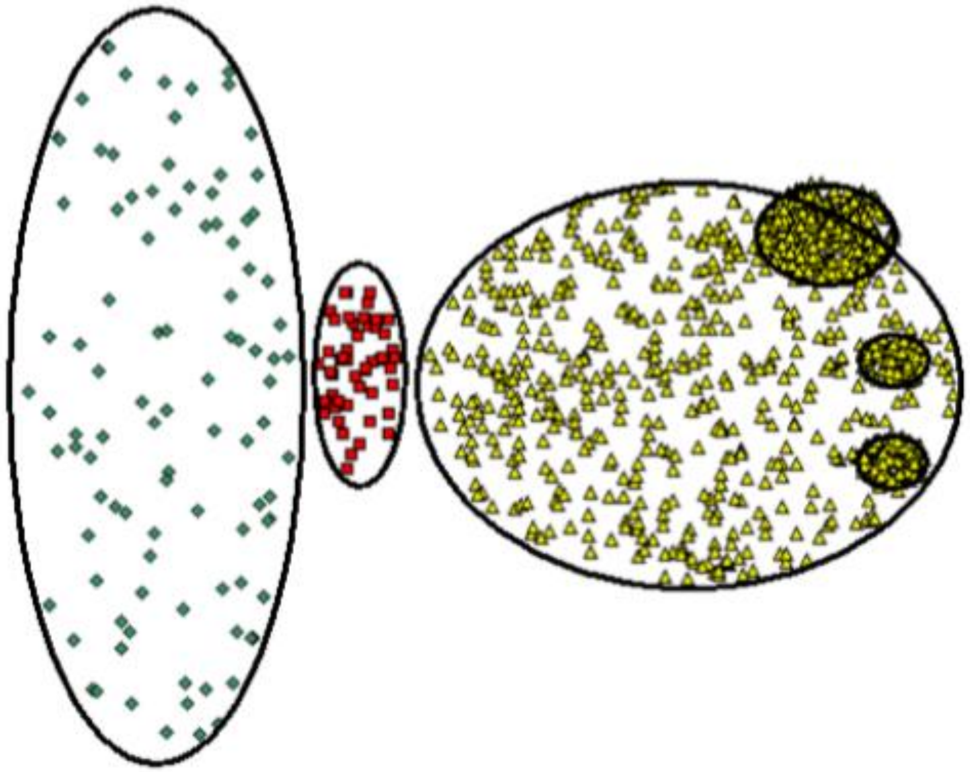
Original Points



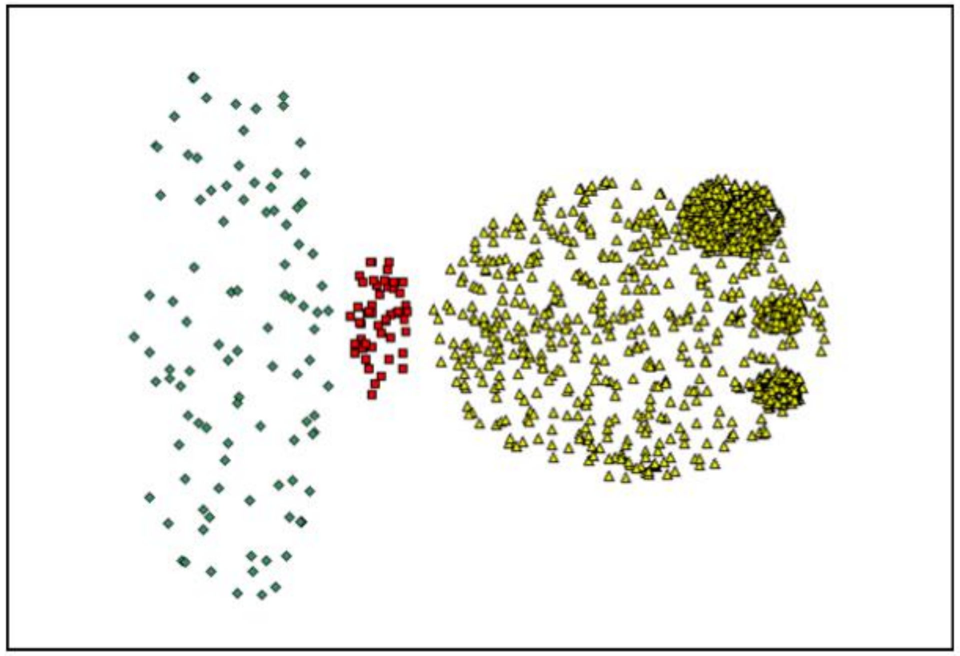
Clusters

When DBSCAN Does NOT Work Well

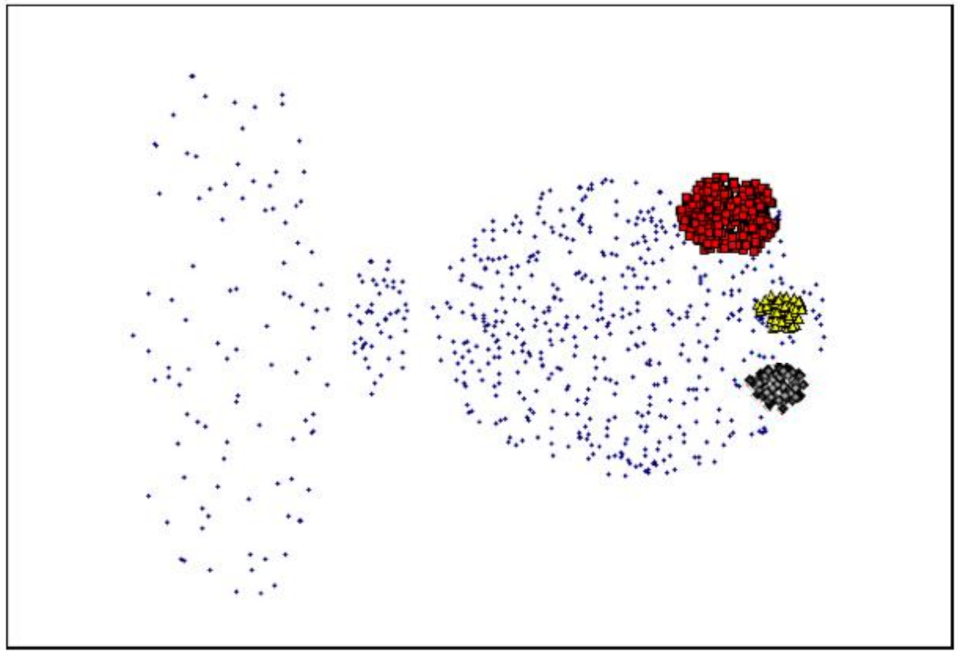
- Cannot handle varying densities
- Sensitive to parameters—hard to determine the best setting of parameters



Original Points



(MinPts=4, Eps=9.92).



(MinPts=4, Eps=9.75)

Take-Home Messages

- The basic idea of density-based clustering
- The two important parameters and the definitions of neighborhood and density in DBSCAN
- Core, border and outlier points
- DBSCAN algorithm
- DBSCAN's pros and cons

Clustering Evaluation

- Internal measures for clustering evaluation
  - Elbow method
  - Silhouette Coefficient
  - Graph-based measures (Beta-CV and Normalized cut)
  - Davies-Bouldin Index

We want intra-cluster datapoints to be as close as possible to each other and inter-clusters to be as far as possible from each other

The Davies-Bouldin Index

Let μ_i denote the cluster mean

$$\mu_i = \frac{1}{n_i} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$$

Let σ_{μ_i} denote the dispersion or spread of the points around the cluster mean

$$\sigma_{\mu_i} = \sqrt{\frac{\sum_{\mathbf{x}_j \in C_i} \delta(\mathbf{x}_j, \mu_i)^2}{n_i}} = \sqrt{var(C_i)}$$

The Davies–Bouldin measure for a pair of clusters C_i and C_j is defined as the ratio

Calculate the DB of i cluster from other clusters

$$DB_{ij} = \frac{\sigma_{\mu_i} + \sigma_{\mu_j}}{\delta(\mu_i, \mu_j)} \qquad D_i = \max_{i \neq j} DB_{ij}$$

DB_{ij} measures how compact the clusters are compared to the distance between the cluster means. The Davies–Bouldin index is then defined as

$$DB = \frac{1}{k} \sum_{i=1}^{k} D_i$$

a lower value means that the clustering is better