Complete link

Single link

0.5 2   5 6   10
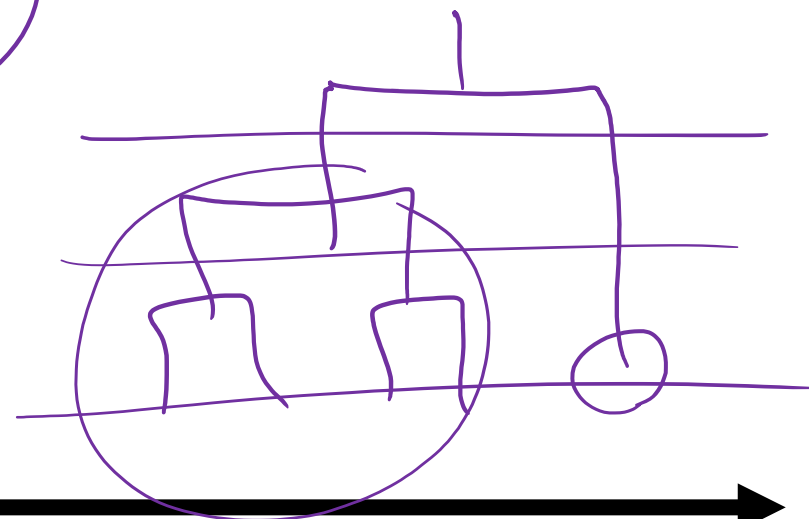
Single link
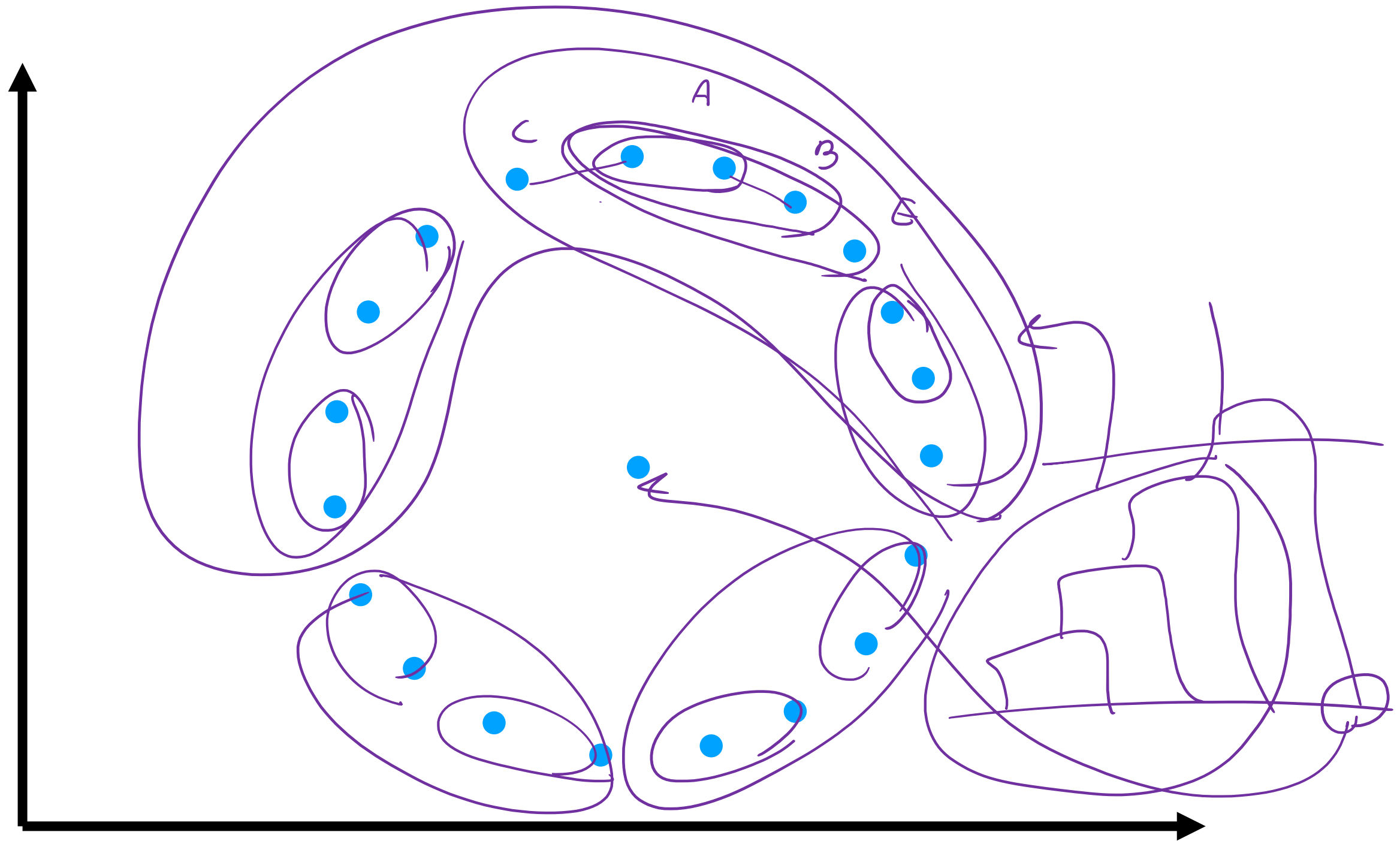
Complete link
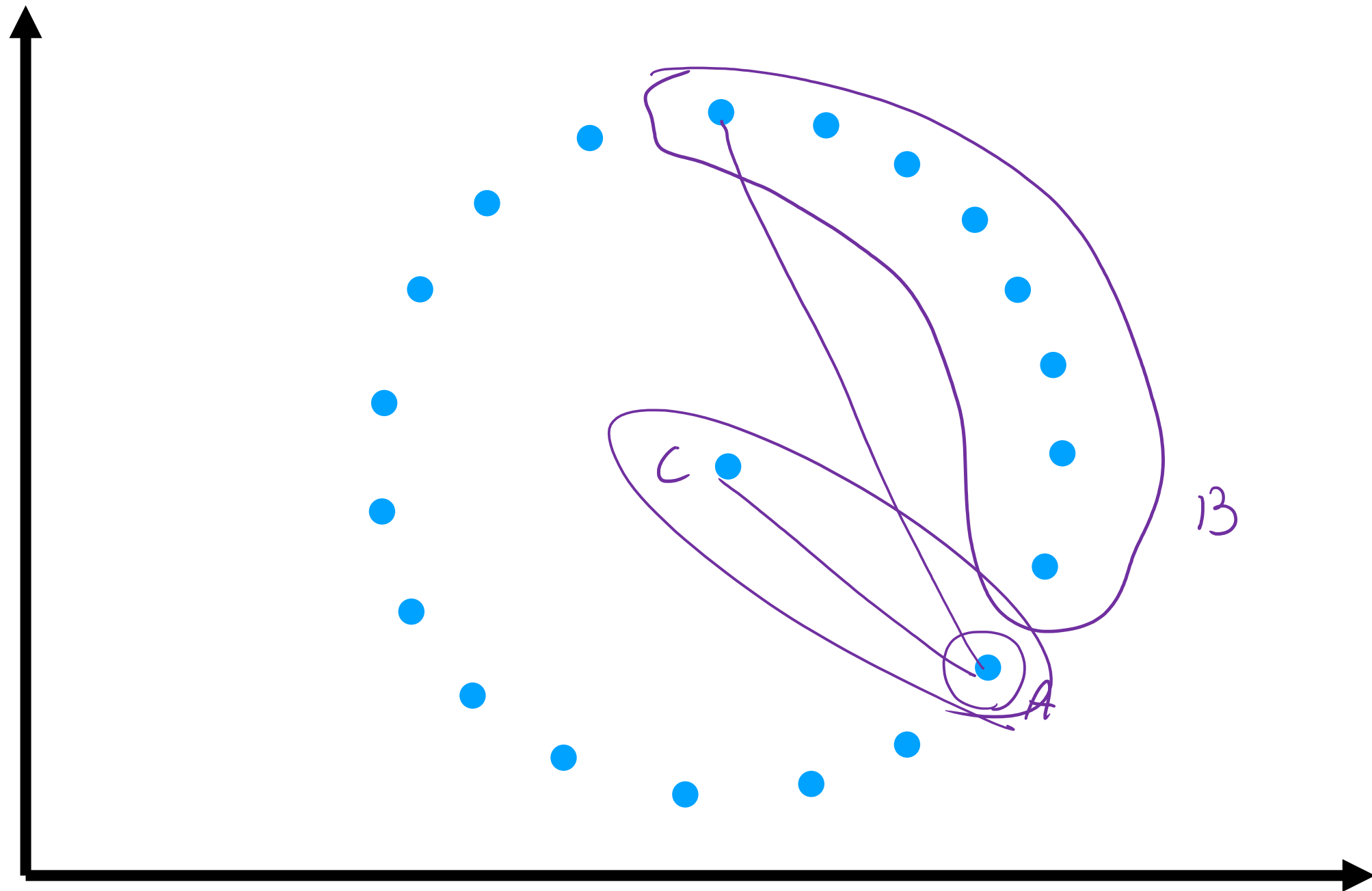
In HC ↝ we don't to know the ≠ clusters in advance

Georgia Tech

Density-Based Clustering

Mahdi Roozbahani

Georgia Tech

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

when you're a constant
and you see d/dx

My time has come

Outline

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

Course ML-Spring23-7641A
Session ID 470137

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)
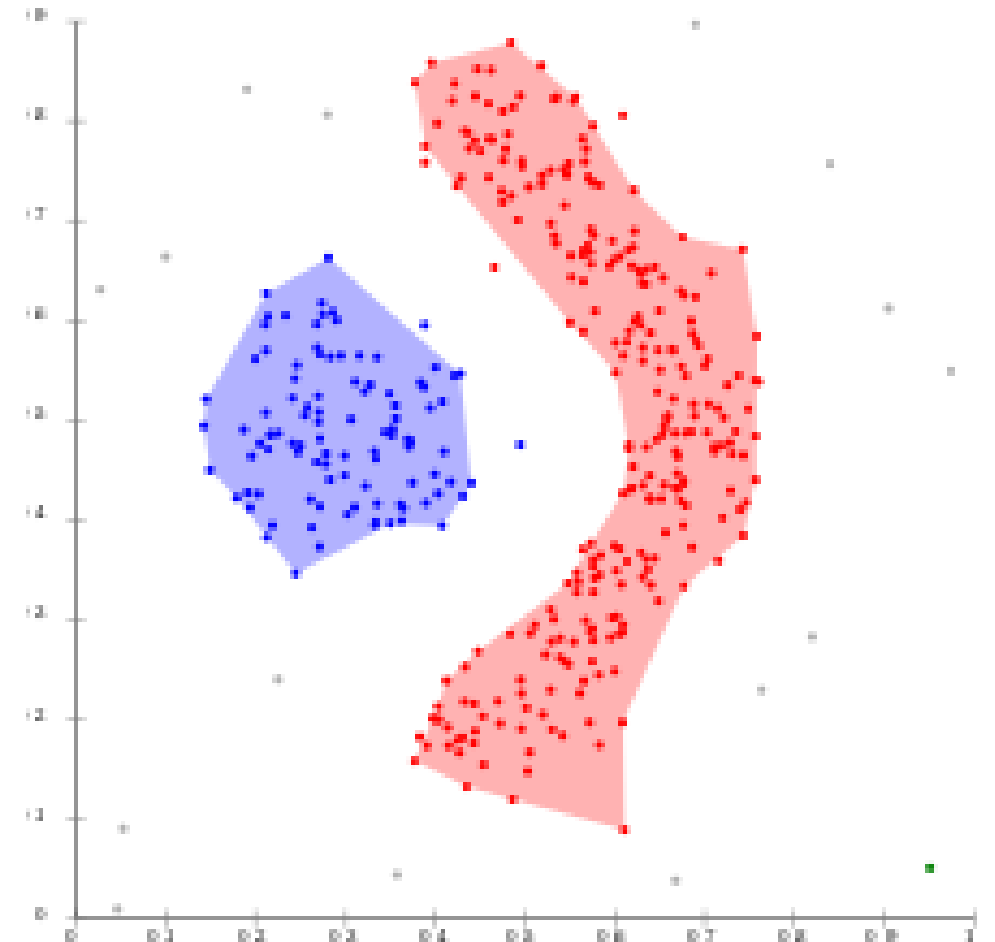
Outline

- Overview

- Basic Concepts ⬅

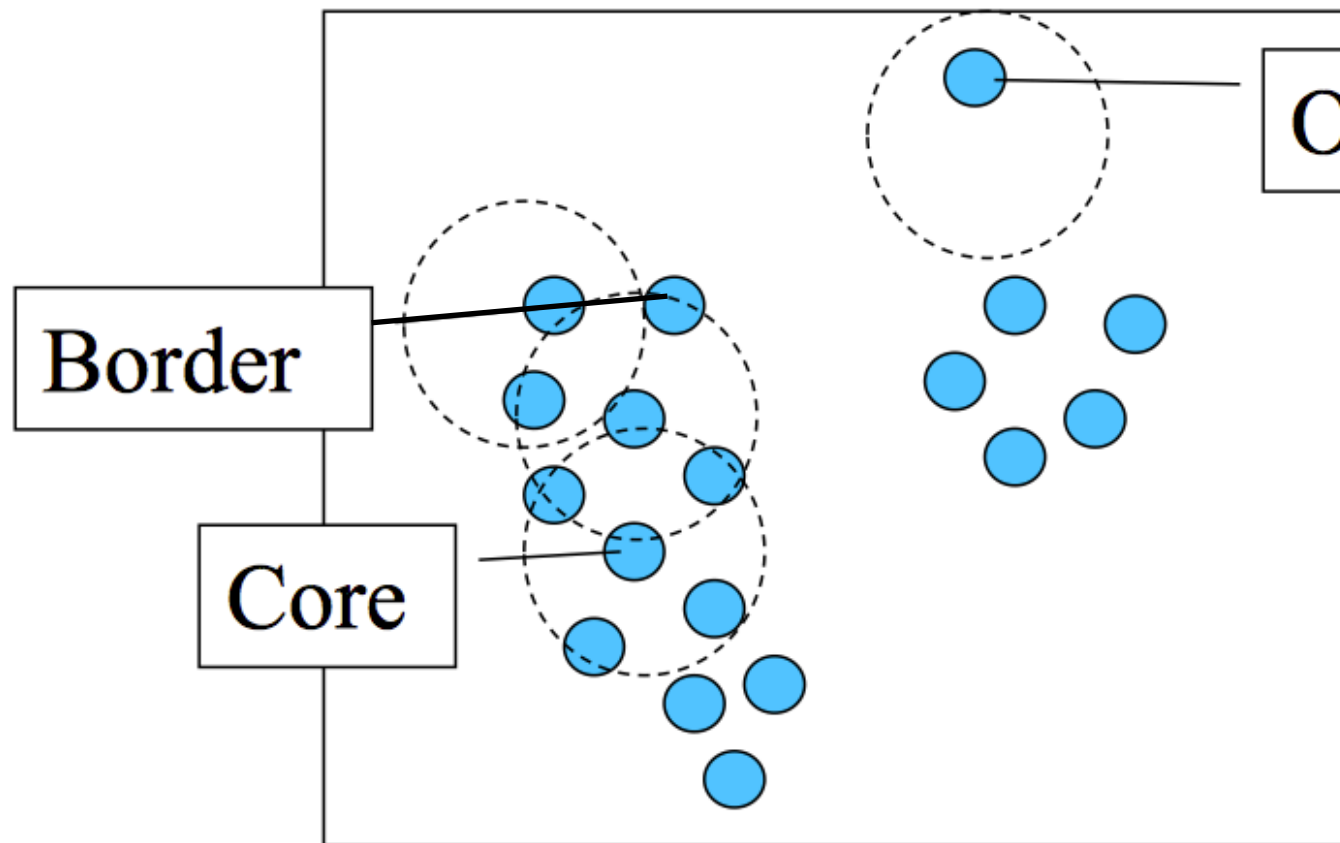- The DBSCAN Algorithm

- Analysis of DBSCAN

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

MinPts = 5

Eps = 1 cm
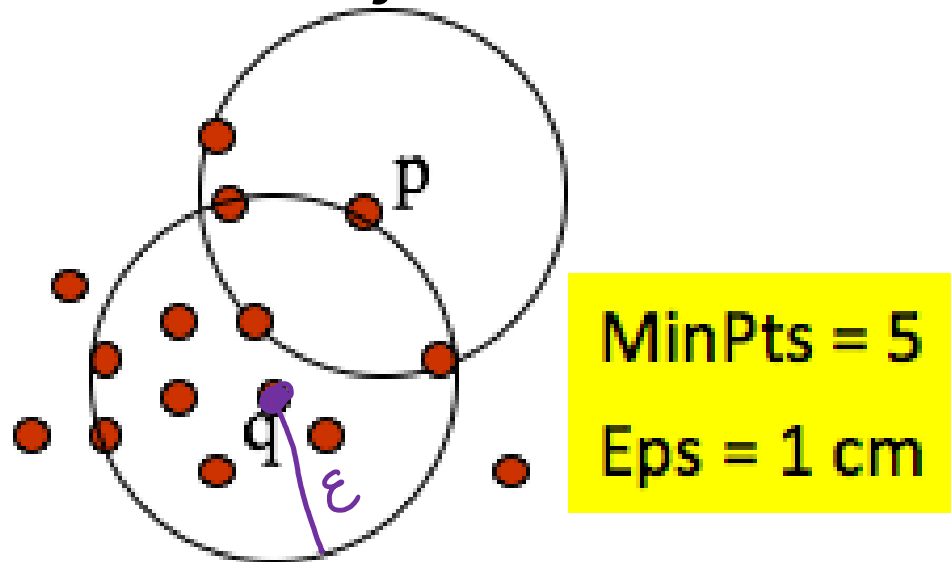
Density of *p* is low
Density of *q* is high

Core Points, Border Points, and Outliers

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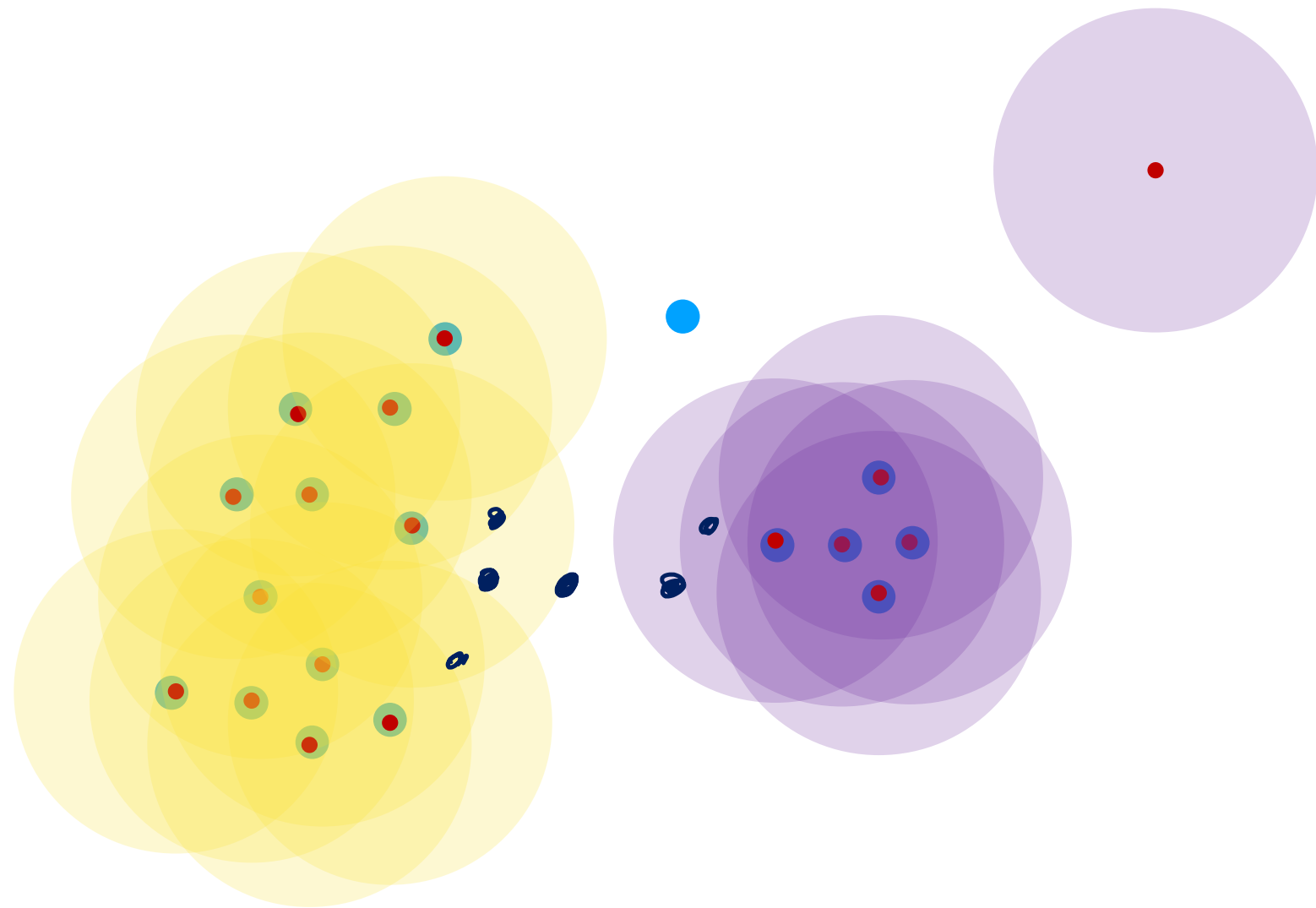
A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.

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

Outlier

Border

Core

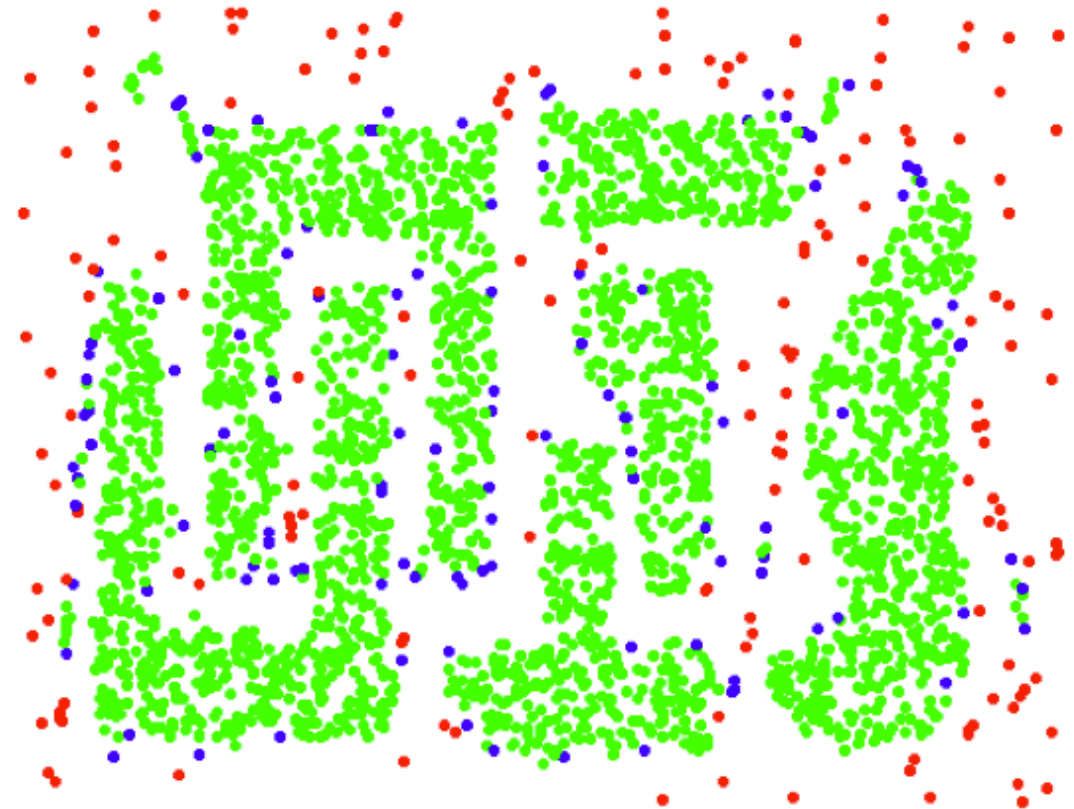$\varepsilon = 1\text{unit}, \text{MinPts} = 5$

Almost deterministic

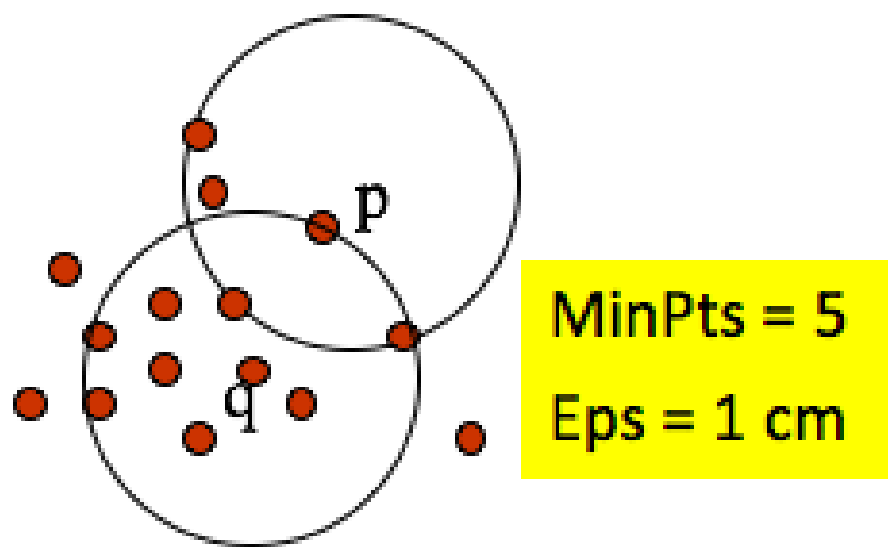ε = 1 unit
MinPts = 5

Examples

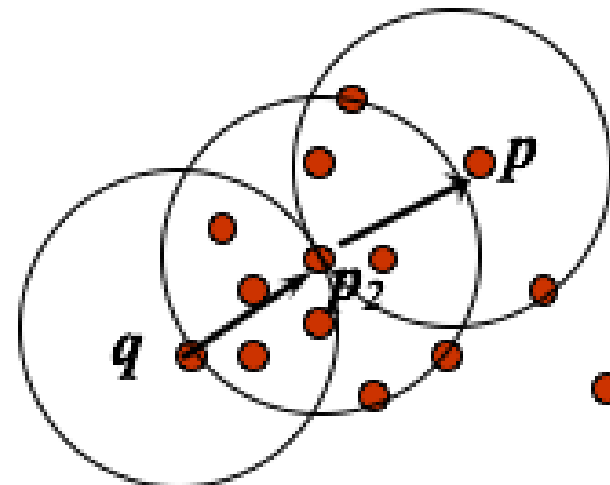**Original Points**

Point types: core, border and outliers
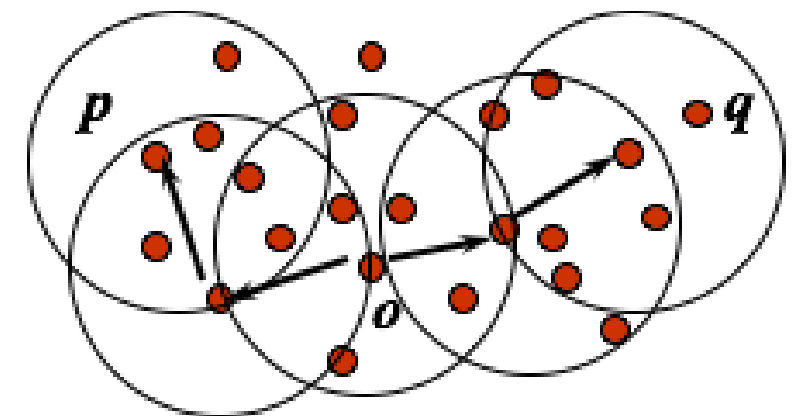
ε = 10, MinPts = 4

Density-based related points

- Direct density reachability:

  o 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**

MinPts = 5

Eps = 1 cm
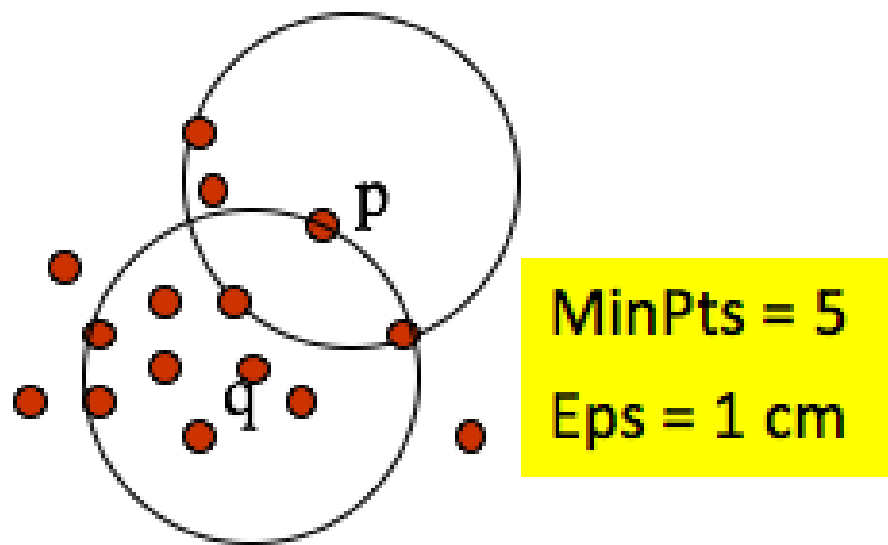
Directly Density-Reachable

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 **p₁, …, pₙ**, **p₁ = q**, **pₙ = p** such that **pᵢ₊₁** is directly density-reachable from **pᵢ**

  ○ $p_1 = q \rightarrow p_2 \rightarrow \ldots \rightarrow p_n = q$

MinPts = 5
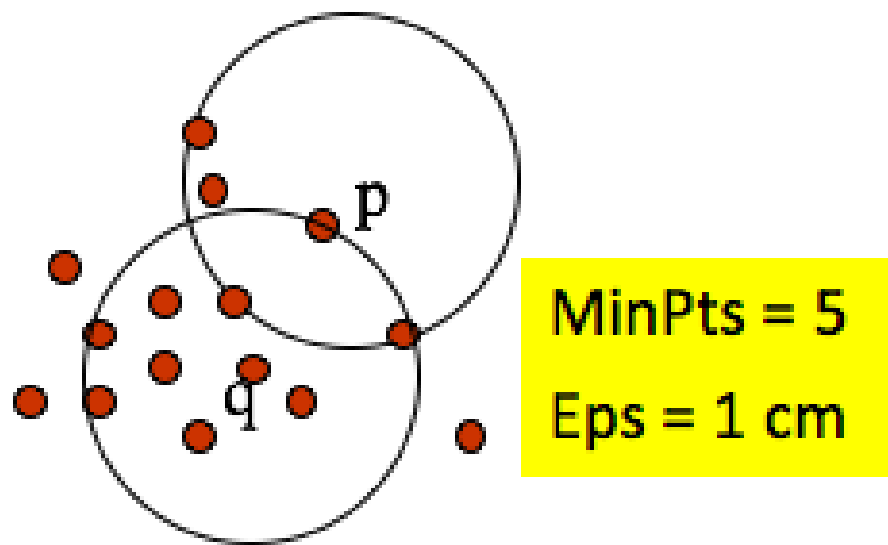
Eps = 1 cm

Directly Density-Reachable
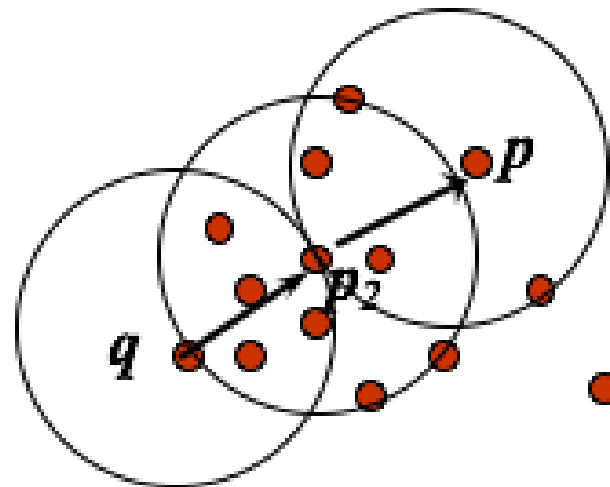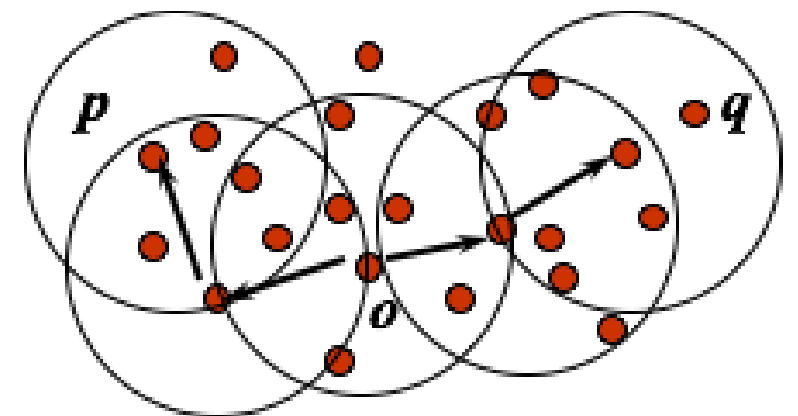
Density-Reachable

Density-Connected

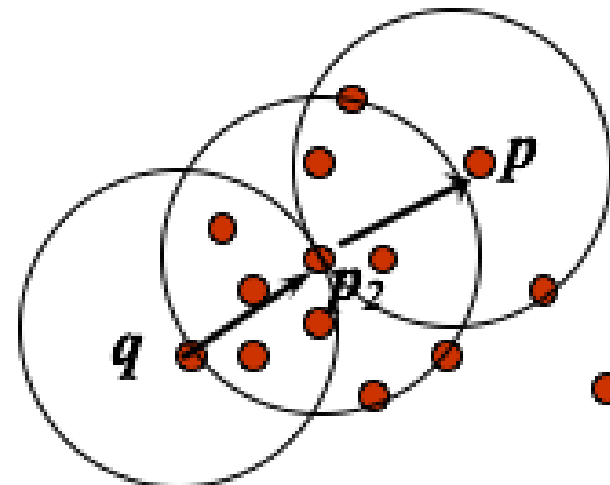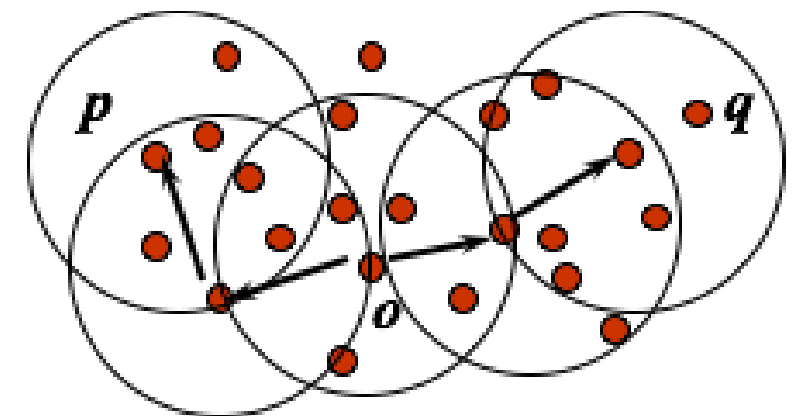# Density-based related points

- 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**
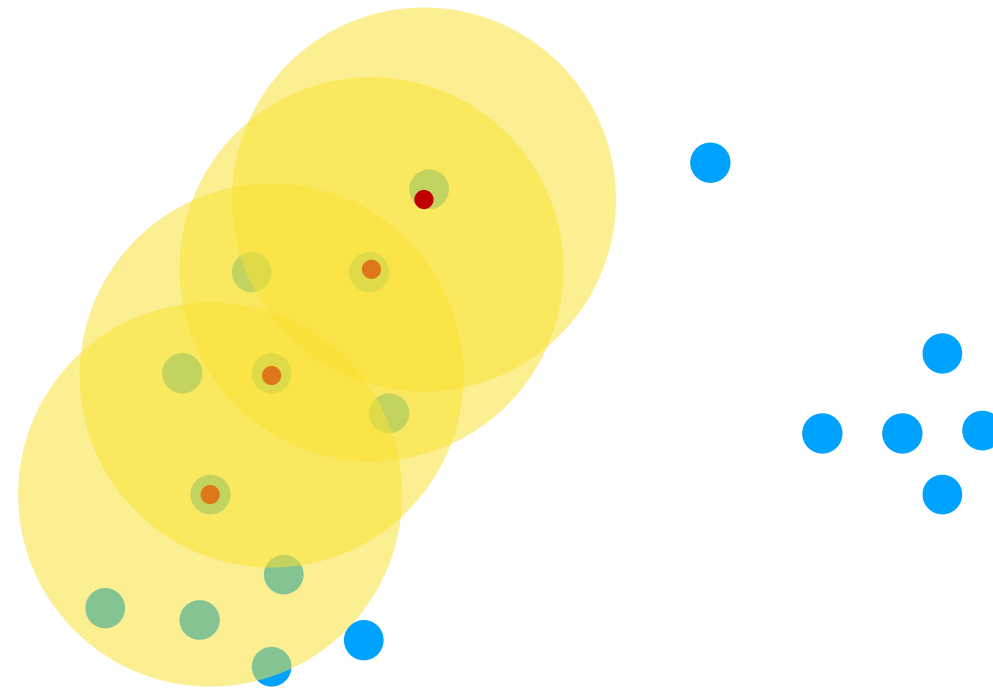

MinPts = 5

Eps = 1 cm

Directly Density-
Reachable

Density-
Reachable

Density-
Connected

ε= 1 unit
MinPts = 5

Outline

- Overview

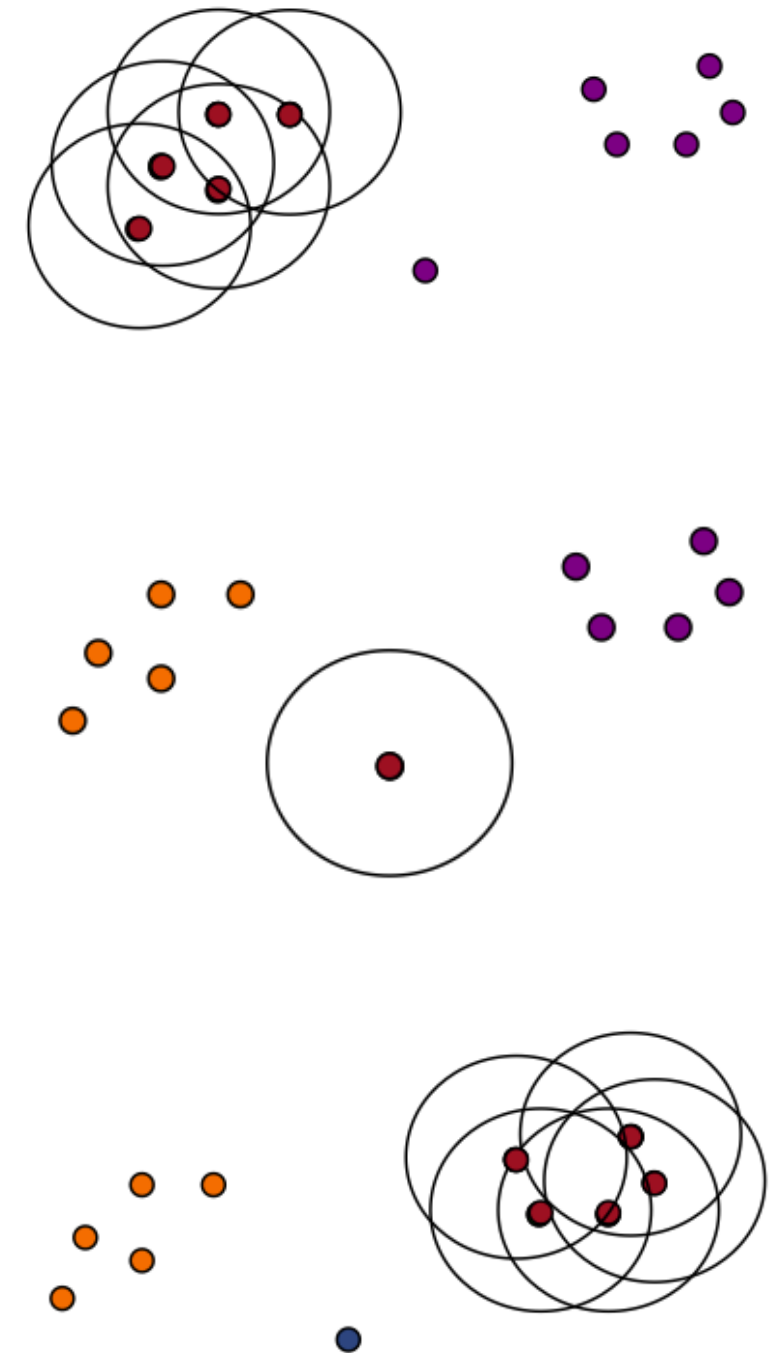- Basic Concepts

- The DBSCAN Algorithm ⬅

- Analysis of DBSCAN

Dataset

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

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/

Outline

- Overview

- Basic Concepts

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- Analysis of DBSCAN ⬅

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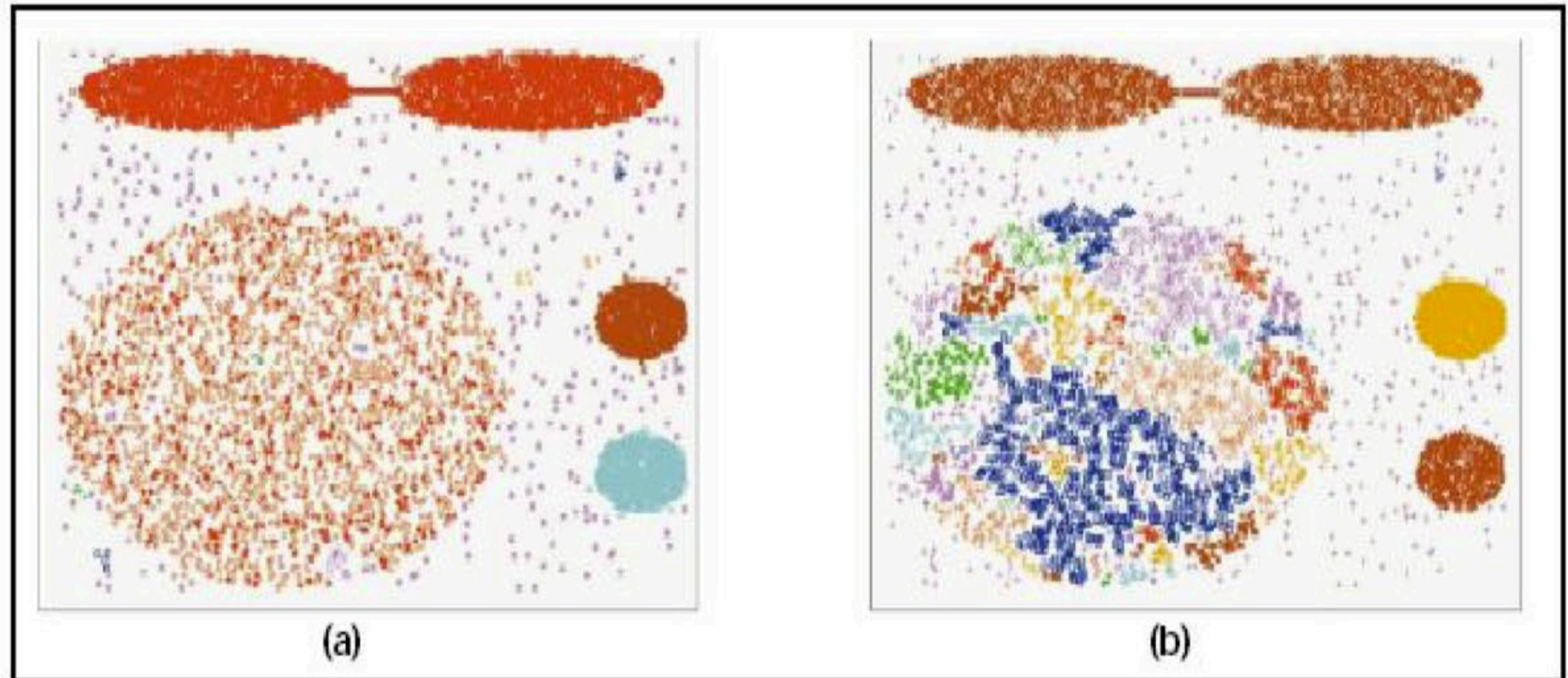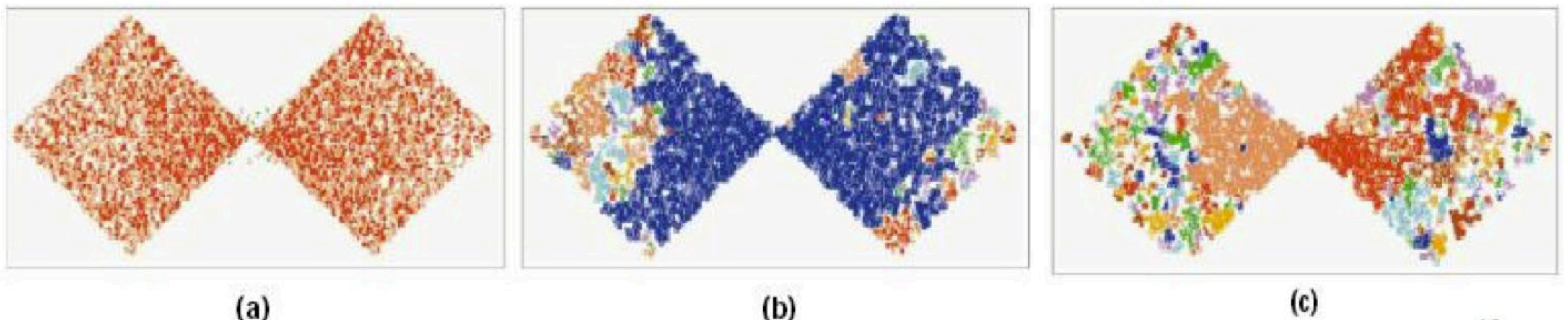
Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.

(a)　(b)

(a)　(b)　(c)

ε
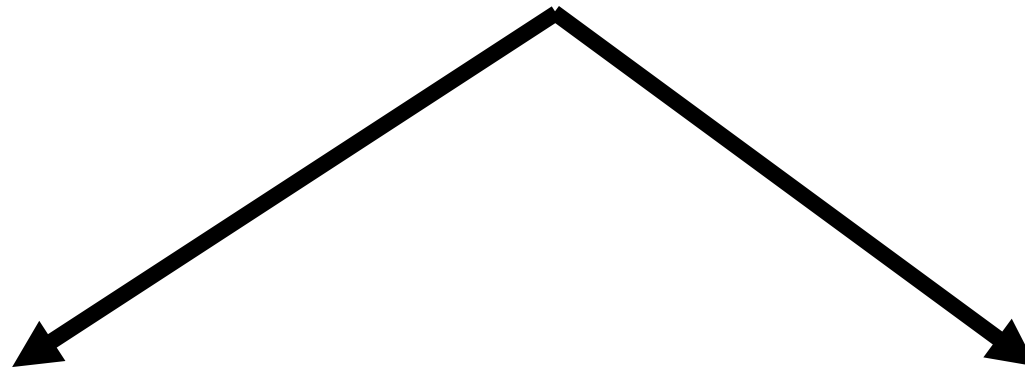
High value (what will happen?)

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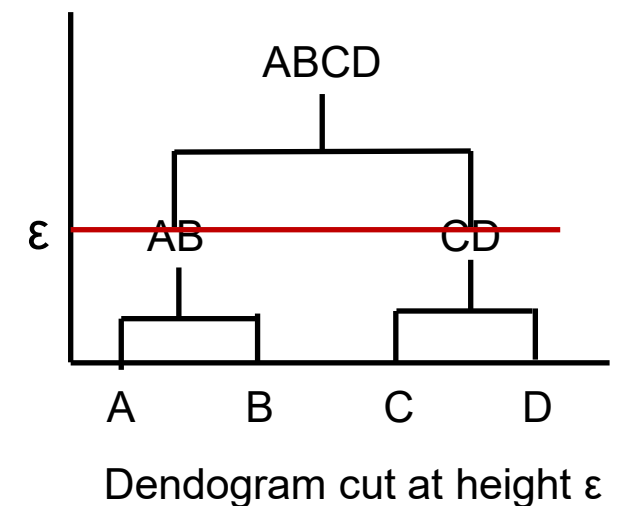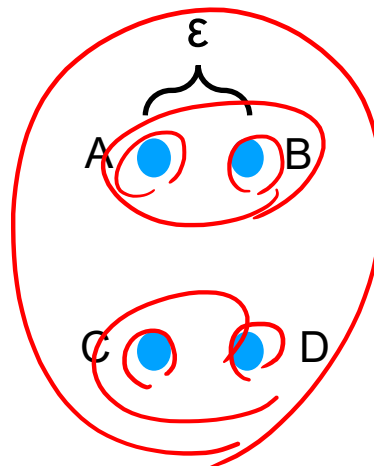
Don't forget, in DBSCAN, a core point is counted as the number of neighboring points

MinPts = 2?

Dendogram cut at height ε

So, MinPts should be at least 3

Rule of thumb, MinPts >= D+1;   ← Dimension
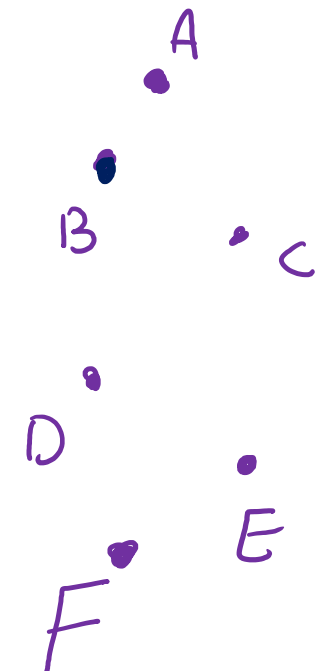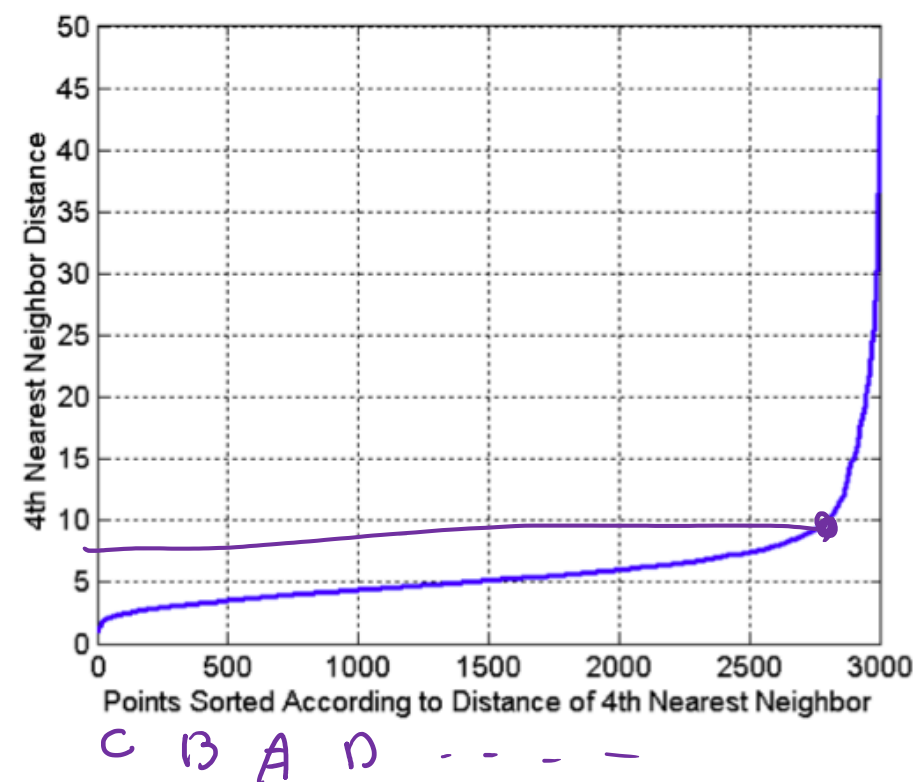For noisy data => MinPts = 2*D (yield more significant clusters)

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 kth nearest neighbor at farther distance
- So, plot sorted distance of every point to its kth nearest neighbor

4th

A → 30   → C ↝ 18

B → 25   B ↝ 25

C → 18   A → 30

D → 35   D → 35

;

C B A D - - - - -

A
B   C
D
E
F

Here we have 3000 points and x-axis shows just a point index.
Point indices are sorted in ascending order based on their 4th nearest neighbor distance

24

Elbow effect another example
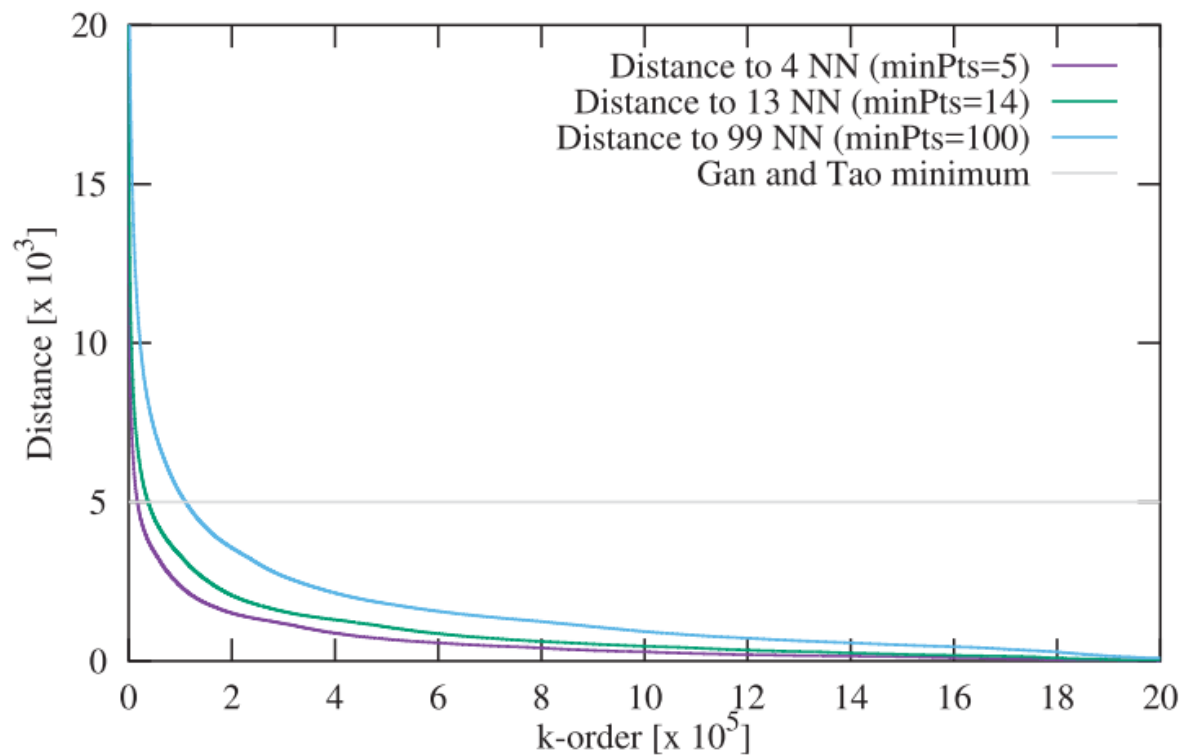
(a) *k*-distance plots
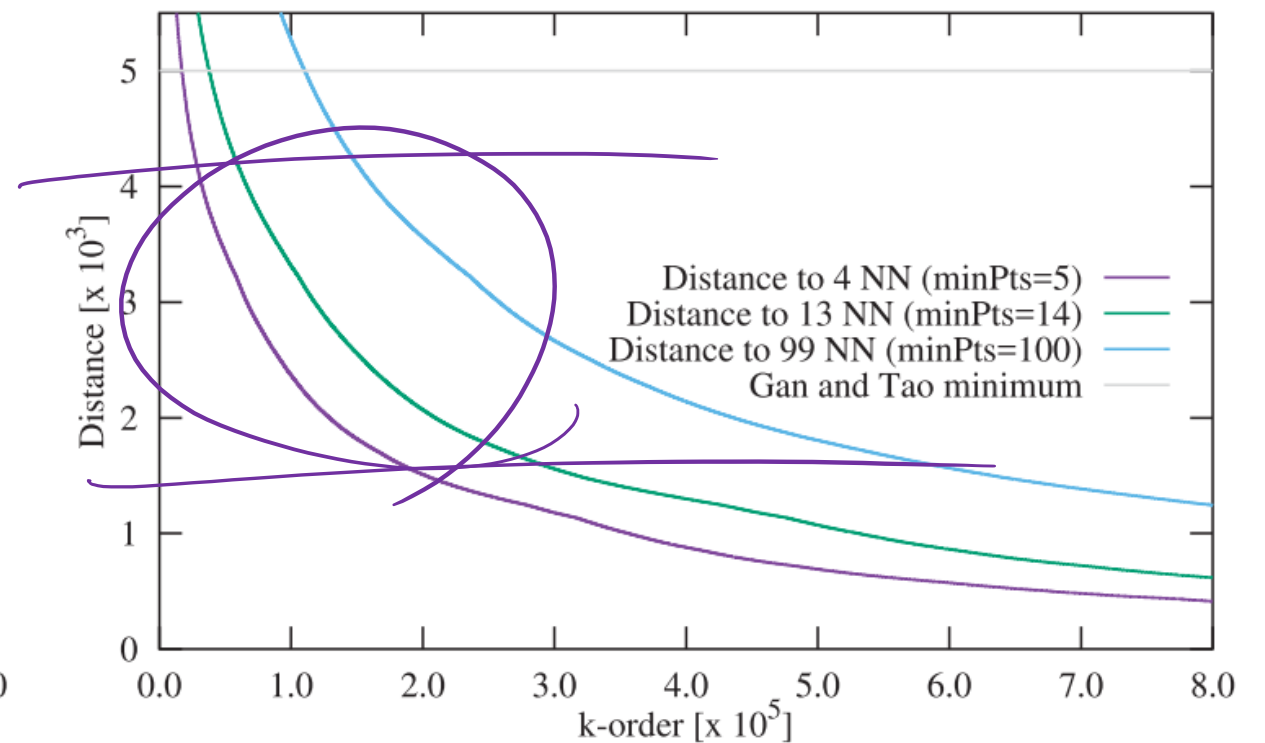
(b) *k*-distance plots (magnified region)

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
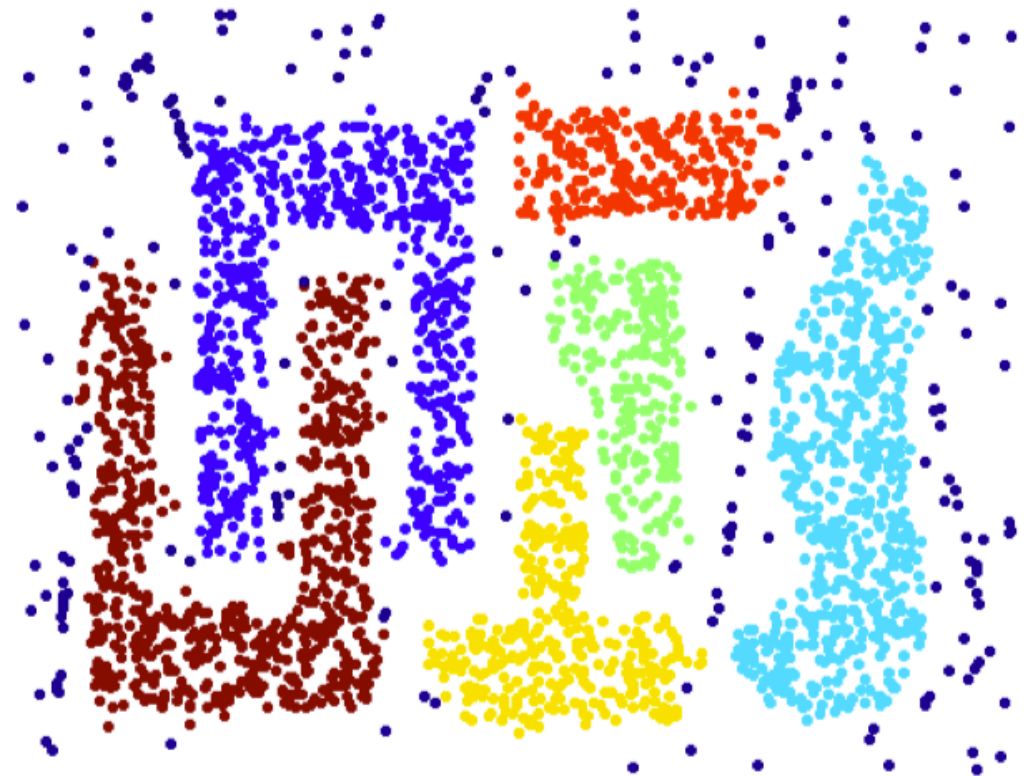
Clusters

When DBSCAN Does NOT Work Well

- Cannot handle varying densities

- Sensitive to parameters—hard to determine the best setting of parameters
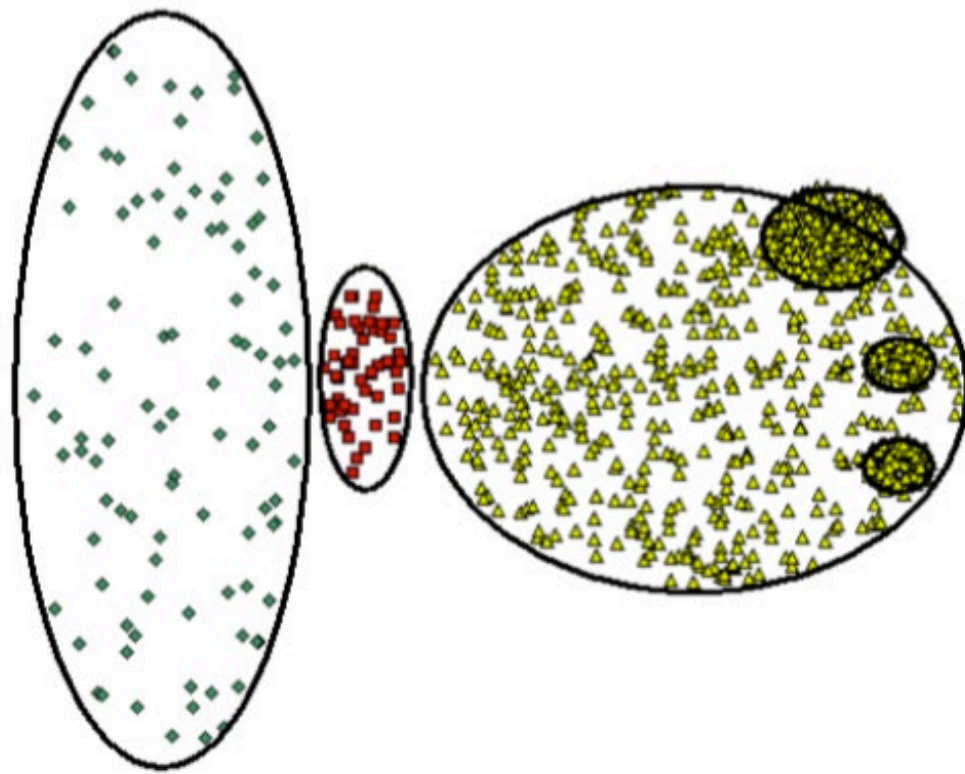
Original Points
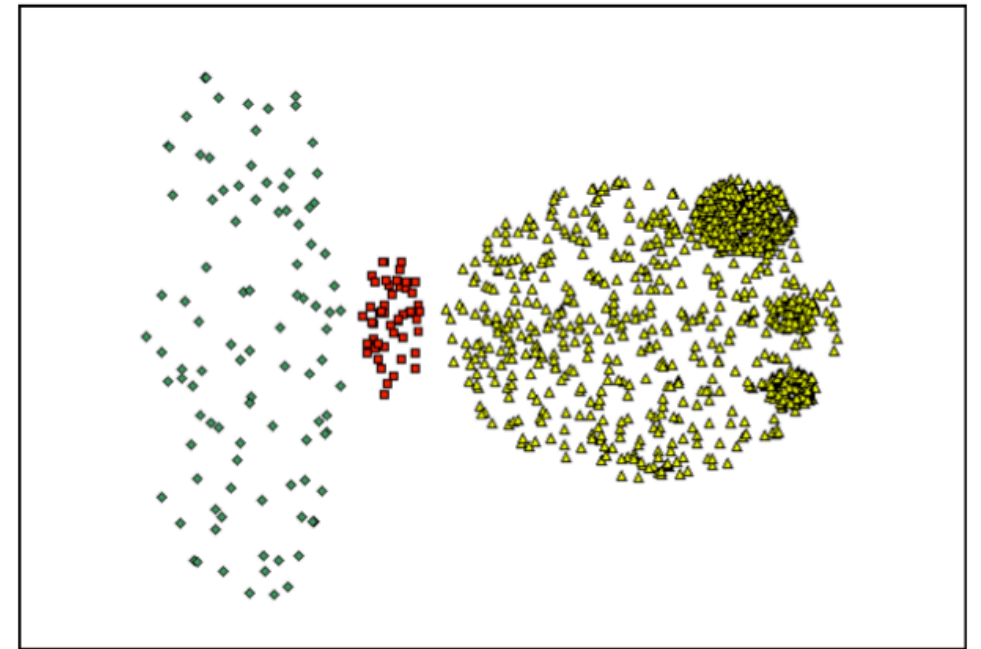
(MinPts=4, Eps=9.92).

(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

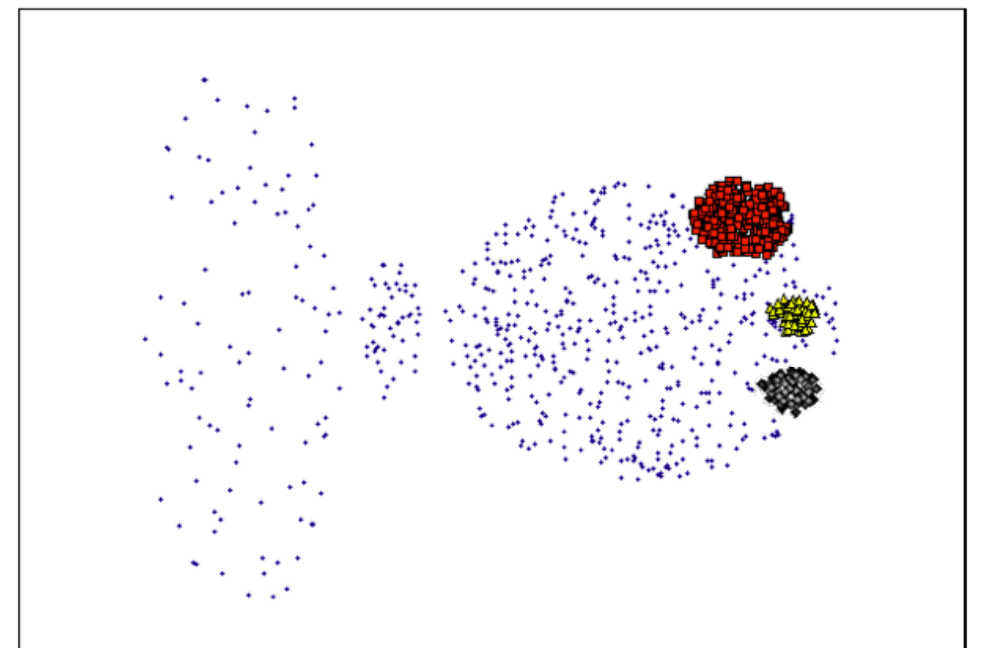# Clustering Evaluation

- 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

$$\mu_i = \frac{1}{n_i} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$$
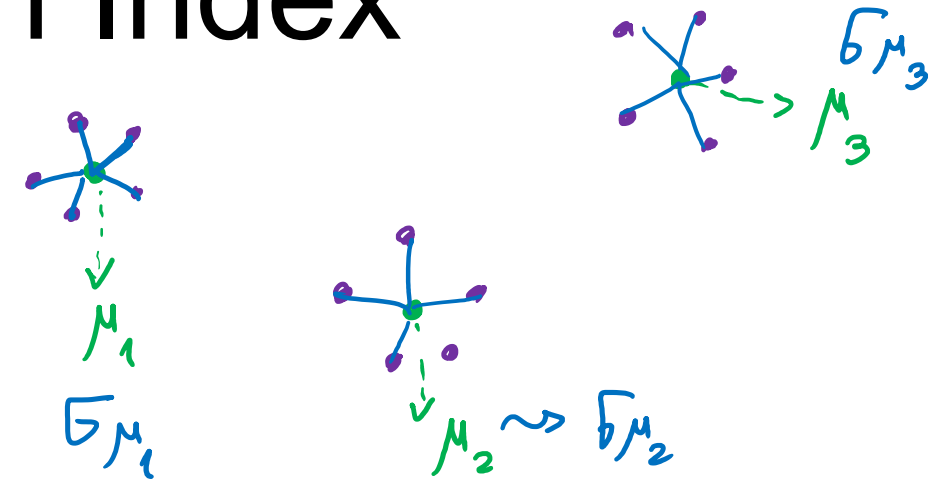
Let σ_{μ_i} denote the dispersion or spread of the points around the cluster mean

distance

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

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

$$DB_{12} = \frac{\sigma_{\mu_1} + \sigma_{\mu_2}}{\delta(\mu_1, \mu_2)}$$

Calculate the DB of i cluster from other clusters

$$DB_{ij} = \frac{\sigma_{\mu_i} + \sigma_{\mu_j}}{\delta(\mu_i, \mu_j)}$$

$$D_1 = \max \{DB_{12}, DB_{13}\}$$

$$D_i = \max_{i \neq j} DB_{ij}$$

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