Lecture 13: 3 March, 2026

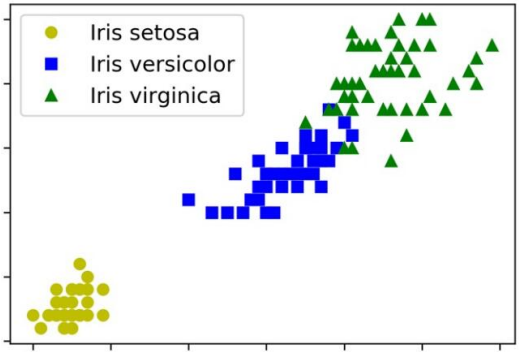
Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
January–April 2026

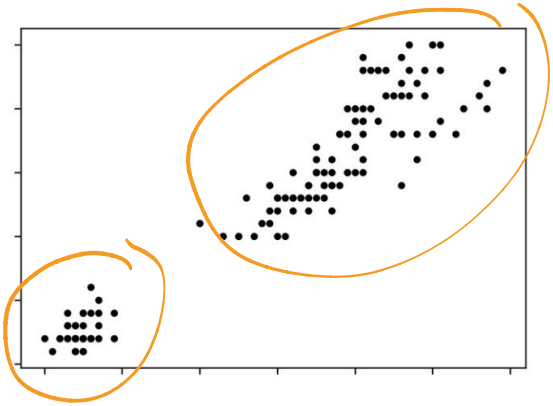
Unsupervised learning

- Supervised learning requires labelled data



Unsupervised learning

- Supervised learning requires labelled data
- Vast majority of data is unlabelled
- What insights can you get with unlabelled data?



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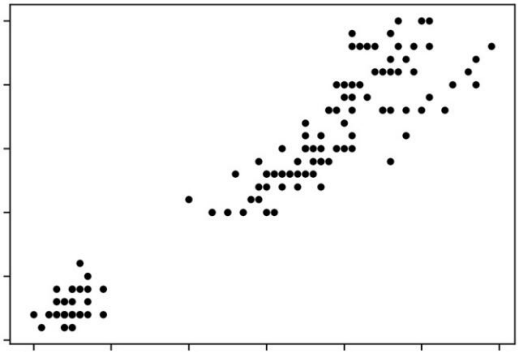

"If intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake . . . "

– Yann LeCun
ACM Turing Award 2018

Applications

- Customer segmentation
  - Marketing campaigns

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- Anomaly detection
  - Outliers

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- Image segmentation
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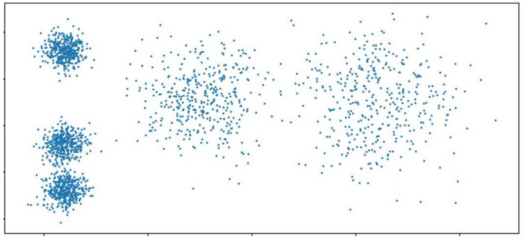
Clustering

- Find natural groups of data



Clustering

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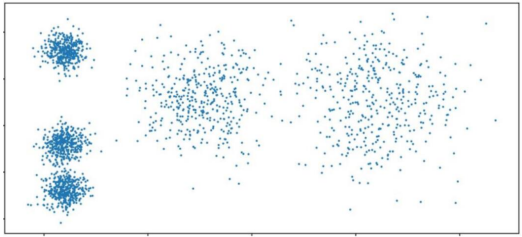
- Define a distance measure



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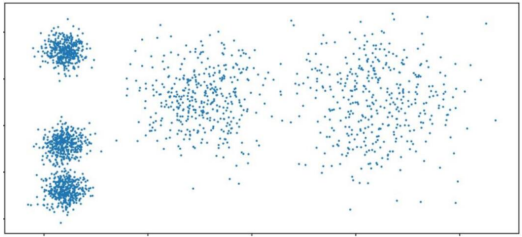
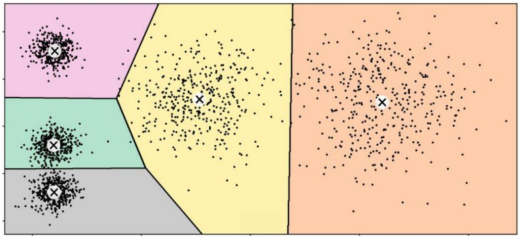
- Group together data that is close together





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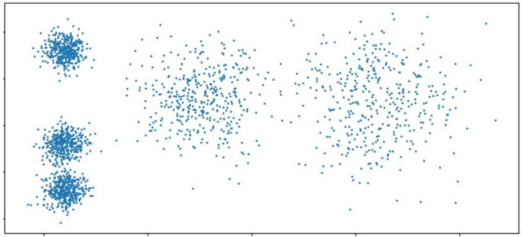
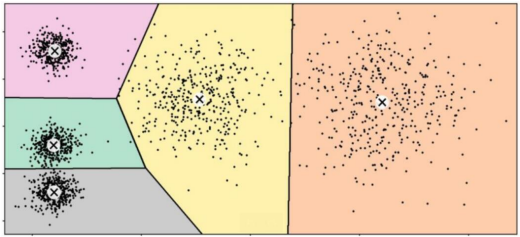
- Top down
  - Partition data into clusters





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- Bottom up
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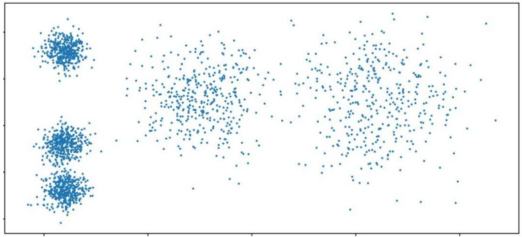
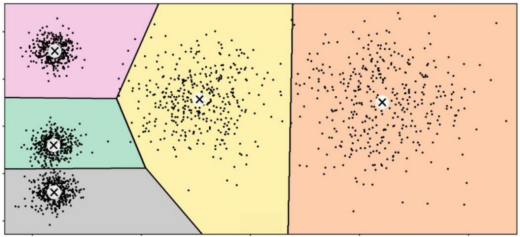
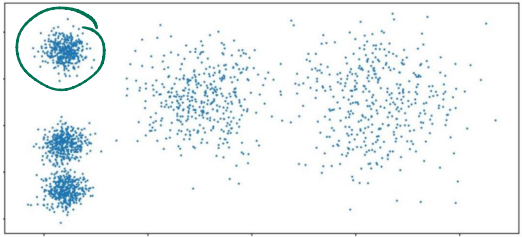


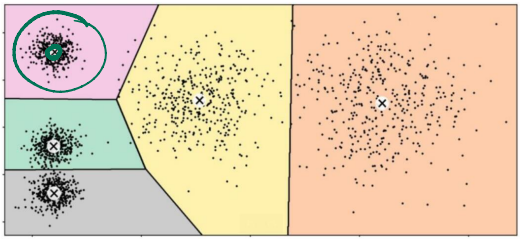


Top down clustering

K Means Clustering

- Data items are points in n dimensions
  - $(x_1, x_2, \ldots, x_n)$





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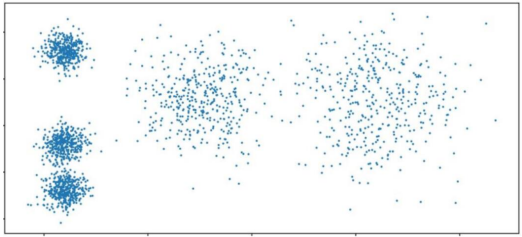

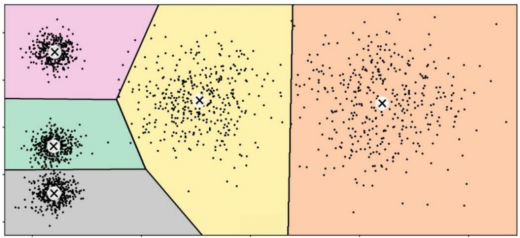

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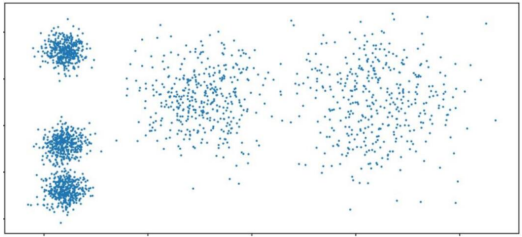
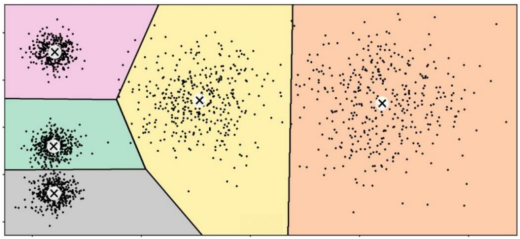
- Each cluster is represented by its geometric centre
  - Centroid, or mean
  - Hence "K means"

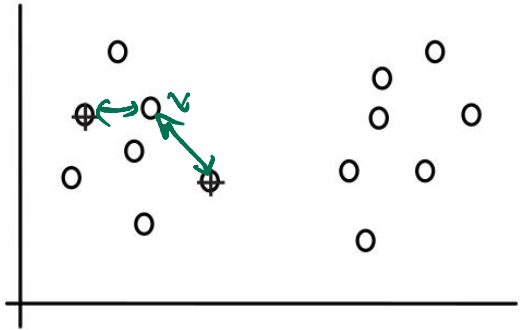




K Means Algorithm

- Choose K points initially as random centroids

K = 2



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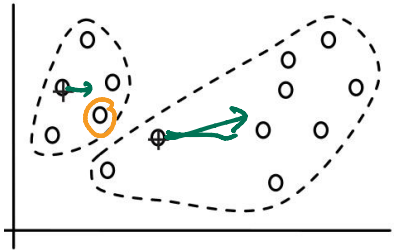

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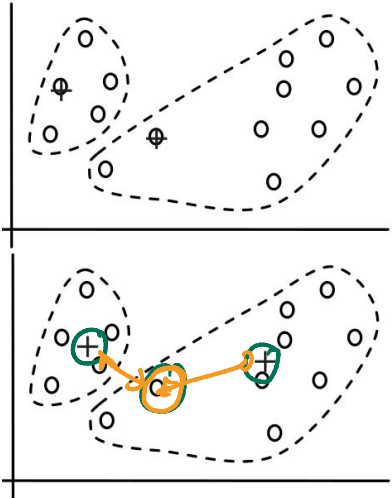

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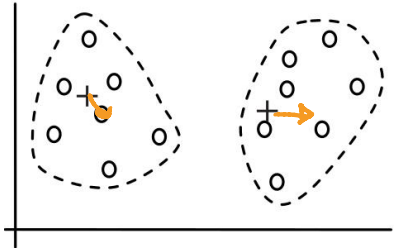

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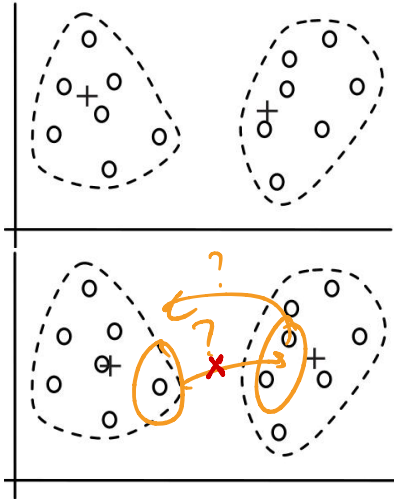

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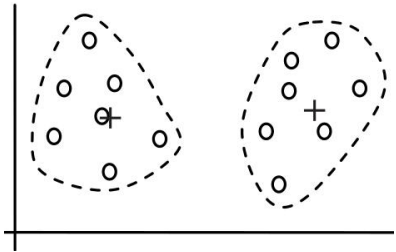

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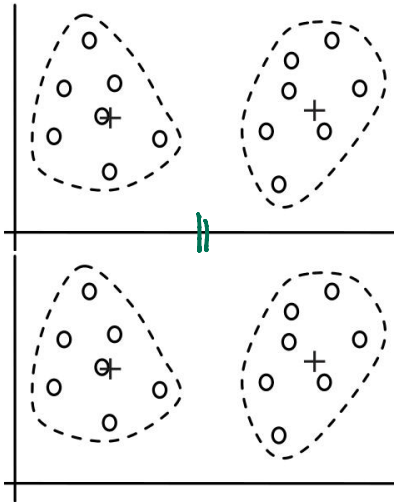

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- Termination
  - Clusters stabilize
  - Sum square distance is below threshold

Evaluating clustering

- How “tight” are the clusters?

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- Mean squared distance from centroids — inertia

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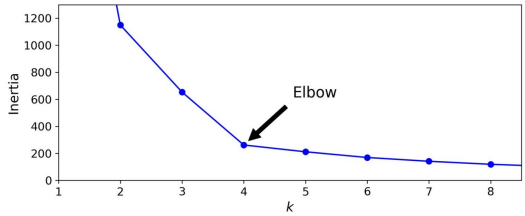

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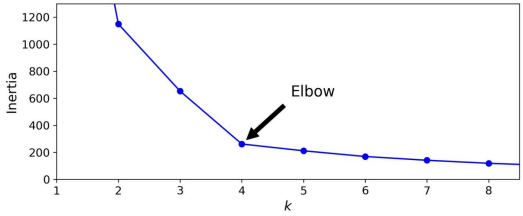

K Means Algorithm

Advantages

- Efficient — each iteration makes a single pass over data
  - Incrementally compute centroid

$$\frac{n * \text{Avg to } n + v_{n+1}}{n+1}$$

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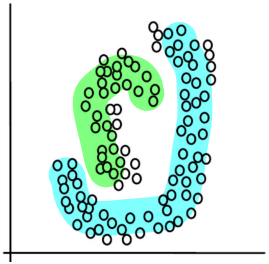

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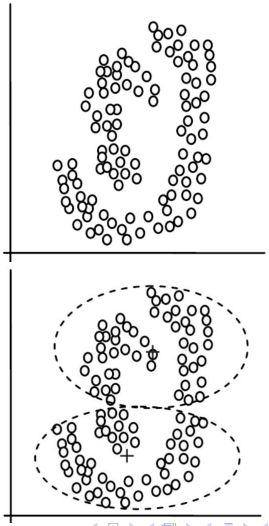

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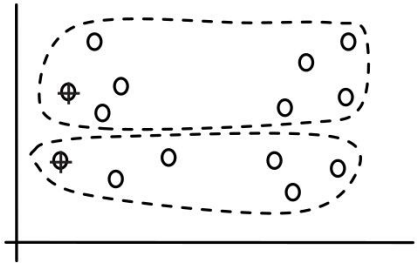

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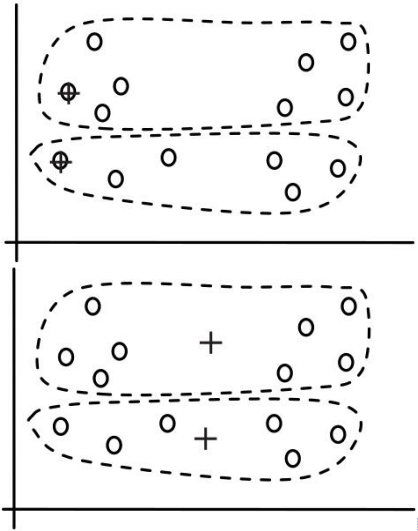
Heuristics to choose initial centroids



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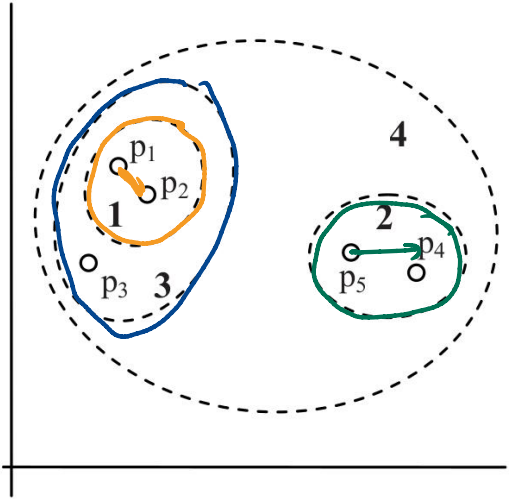

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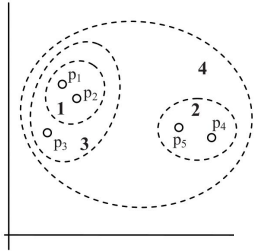
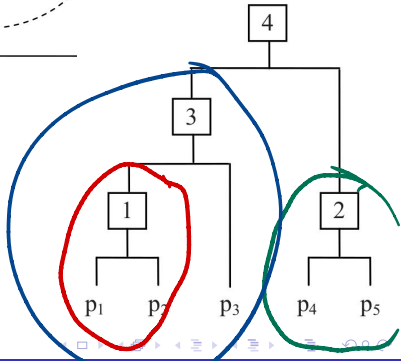
- Choose appropriate level in dendrogram for final clustering





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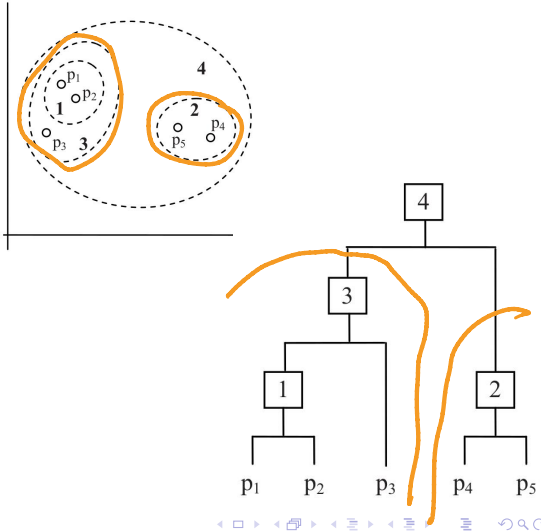

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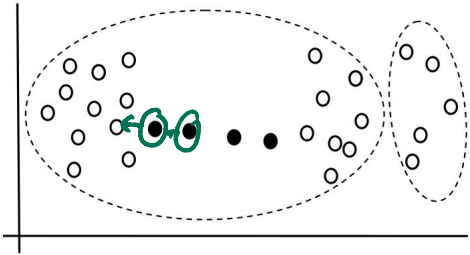

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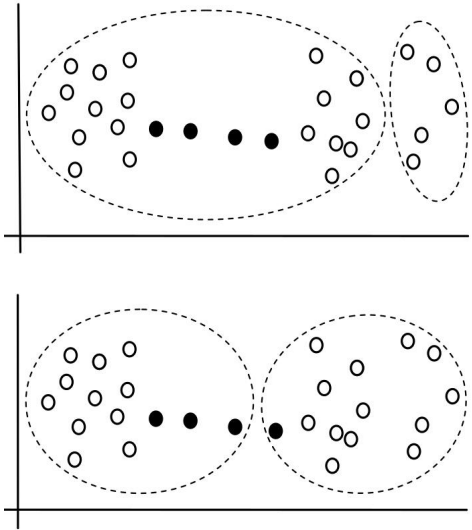
- Complete link: maximum of pairwise distances



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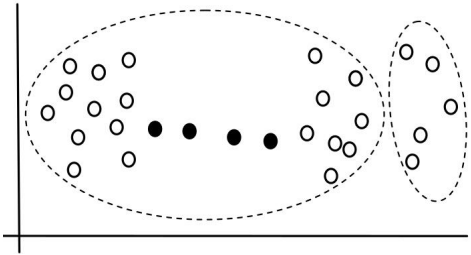
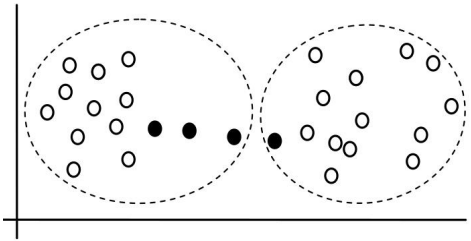
- Average link: mean of pairwise distances





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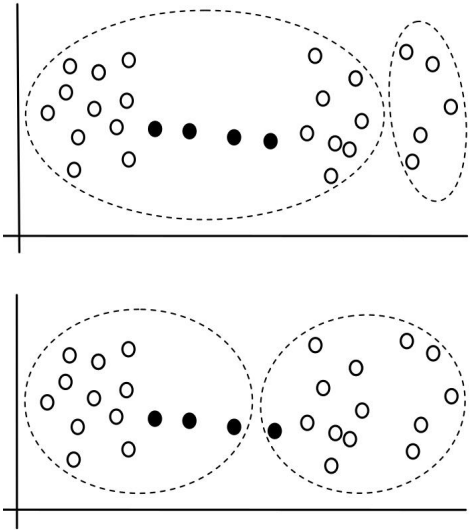
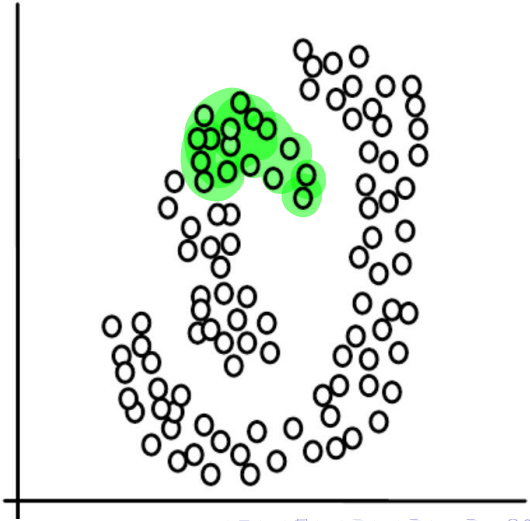
- Complete link: maximum of pairwise distances
- Average link: mean of pairwise distances
- All require $O(n^2)$ computation — expensive



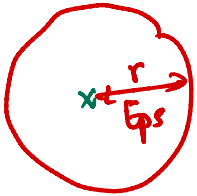
Clustering

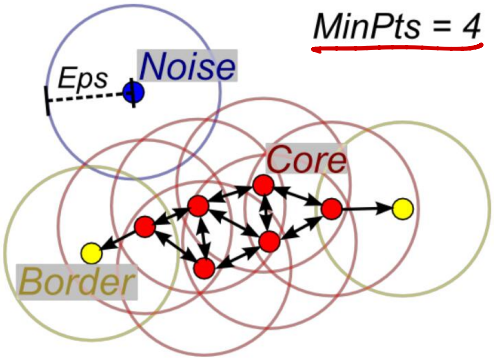
- How to identify odd shaped clusters?
- Cluster — group of points that are "close together"
- Identify "dense" neighbourhoods
- How do we formalize this?



Density based clustering

- Construct a small ball around each point, radius *Eps*
- Identify a threshold for neighbours within ball, *MinPts*





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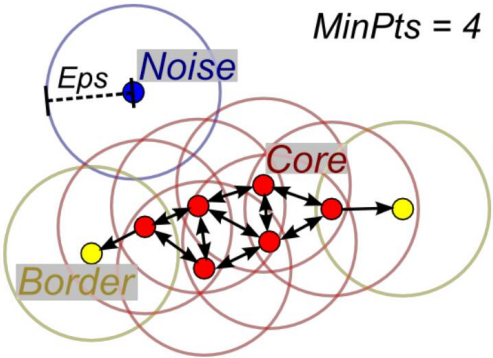
- Core point — has at least *MinPts* neighbours inside *Eps* ball



Density based clustering

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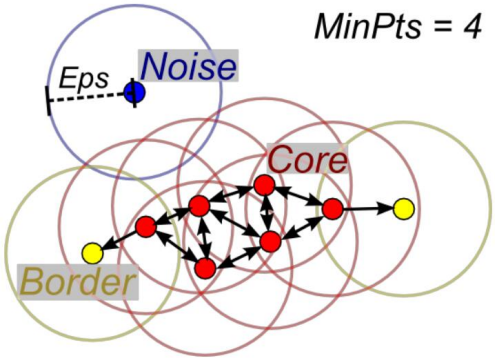
- Connect each core point to all its neighbours → Directed edge



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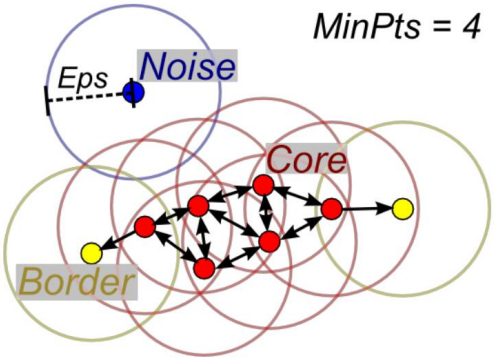

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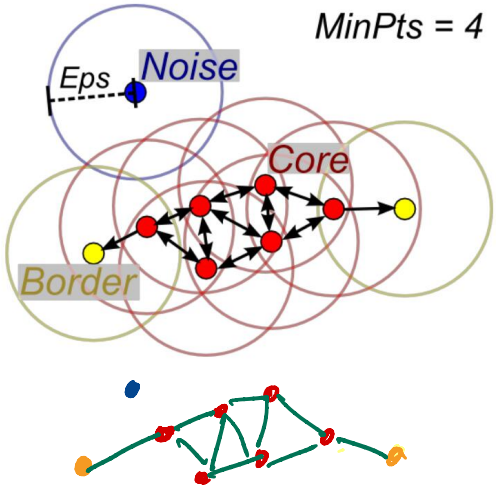
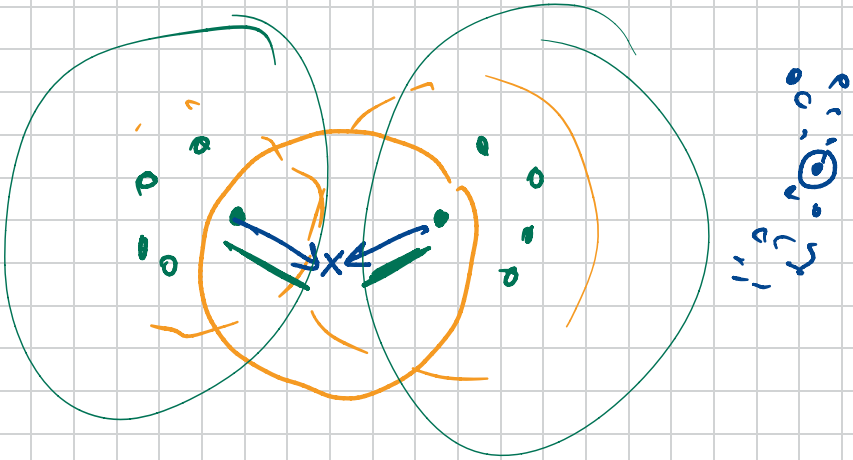
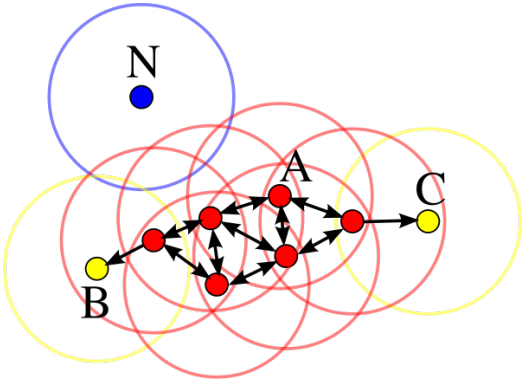
- Noise — isolated, disconnected points





Density based clustering

- Formally, edges from core points to neighbours define a directed graph
- Border points are part of this graph, but cannot add edges to extend the graph
- Discard the edge directions
- Connected components are clusters



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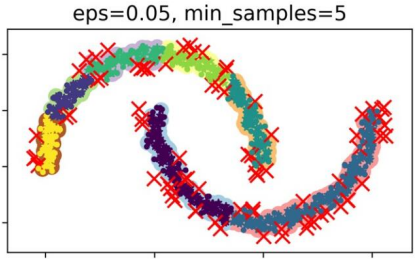
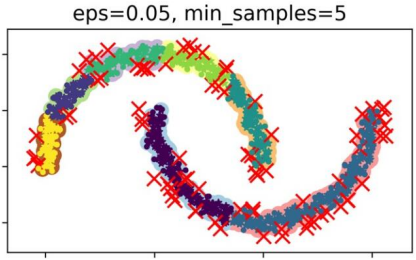
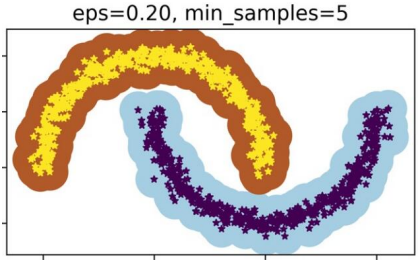


Dbscan

- Implementation of density based clustering available in Python and R
- Smaller value of *Eps* subdivides into small clusters
- Larger *Eps* groups larger clusters





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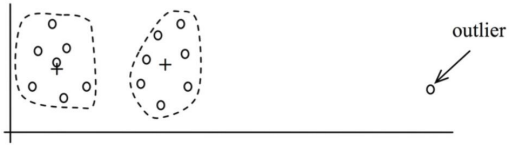

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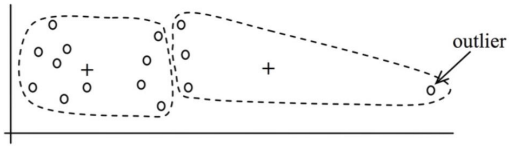

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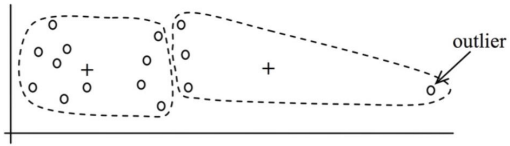

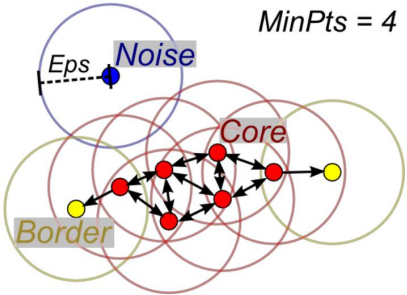

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- Density based clustering — not connected to any core point
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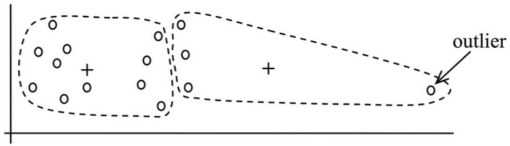
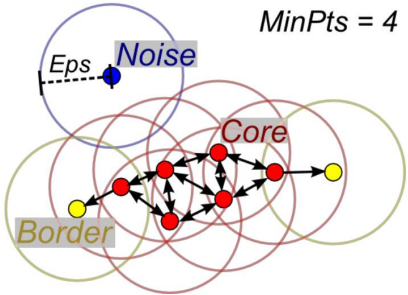
- How to identify outliers before clustering?





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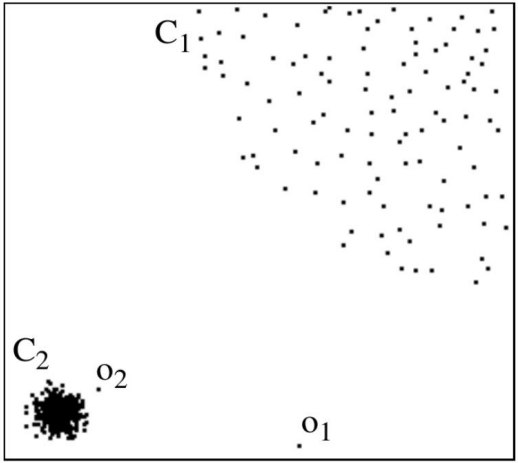

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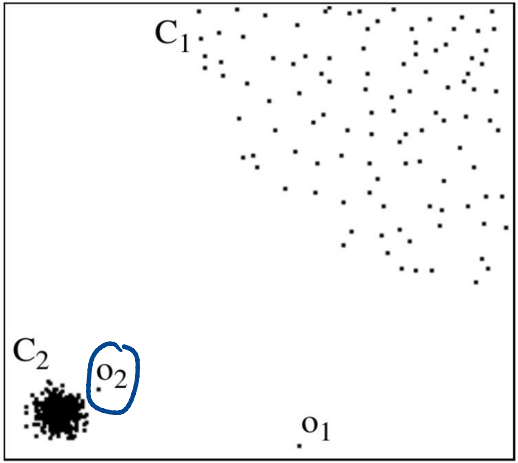

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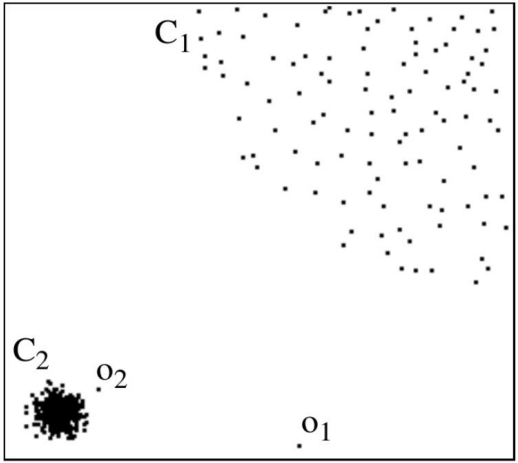
- A distance metric to eliminate o_2 could make all of C_1 outliers
- C_1 has 400 points, C_2 has 100 points
- Larger distance would make all of C_2 outliers with respect to C_1



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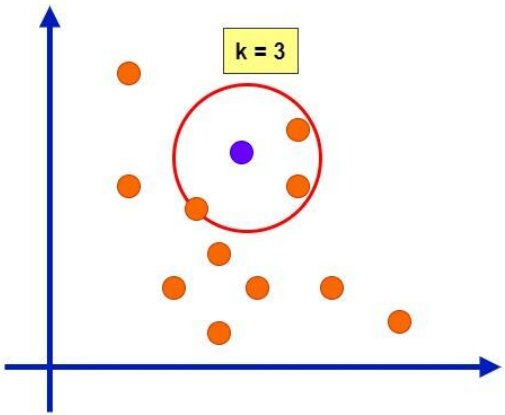

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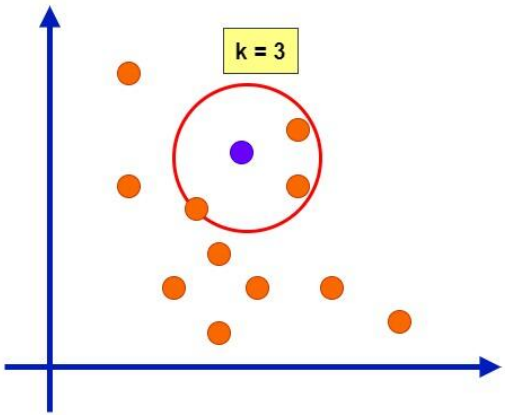

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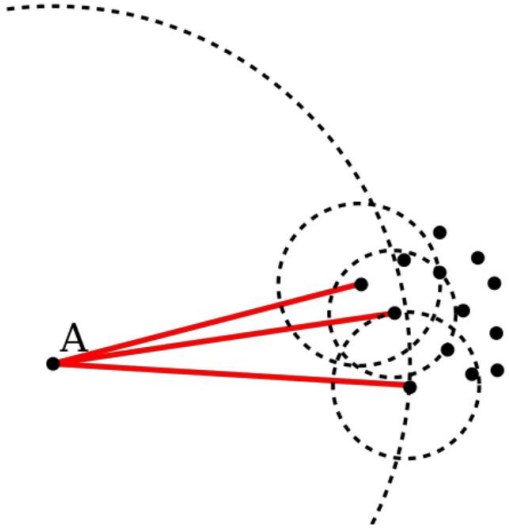
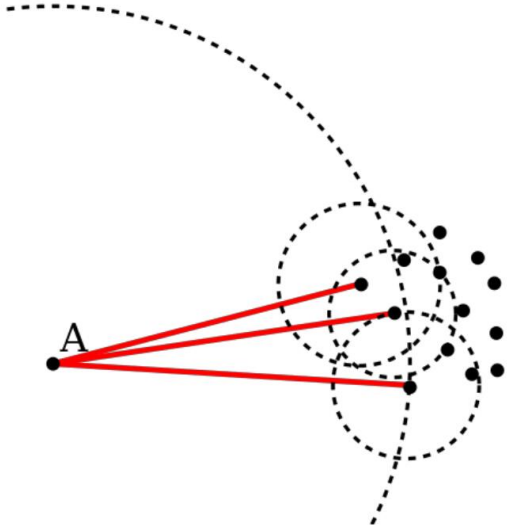
- Compare *radius(p)* with radius of its neighbours
- *A* is an outlier because its radius is much more than that of its neighbours



Outliers and density

- Local outlier factor $LOF(p)$

$$\frac{\text{Mean radius of } MinPts\text{-neighbours}(p)}{radius(p)}$$

- The smaller this ratio, the more likely that p is an outlier
- Comparison is local to neighbourhood, so this can deal with different densities across range of data