Lecture 13: 7 March, 2022

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Data Mining and Machine Learning
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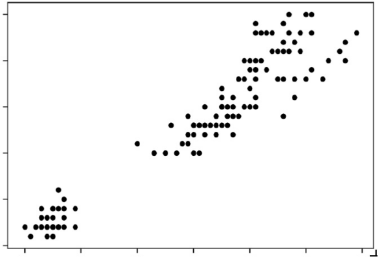
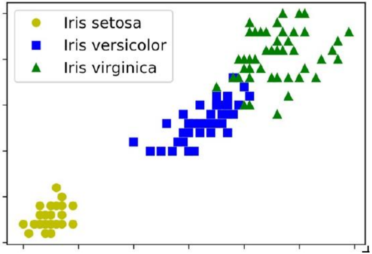
Unsupervised learning

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





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

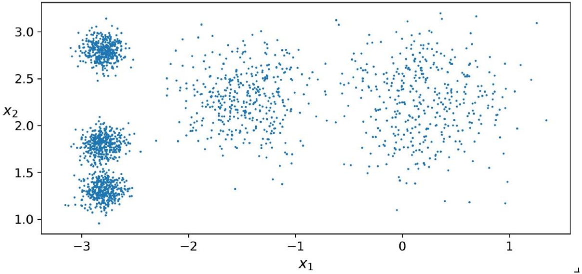
- Yann LeCun
ACM Turing Award 2018

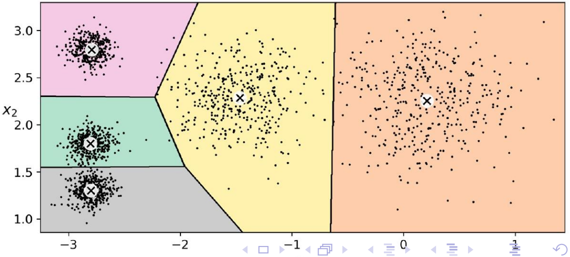
Applications

- Customer segmentation
    - Marketing campaigns
- Anomaly detection
    - Outliers
- Semi-supervised learning
    - Propagate limited labels
- Image segmentation
    - Object detection

Clustering

- Find natural groups of data
- Define a distance measure
- Group together data that is close together
- Top down
    - Partition data into clusters
- Bottom up
    - Group items into clusters

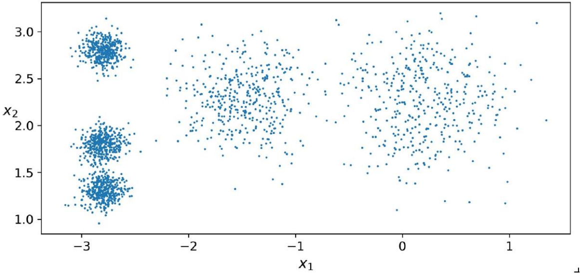


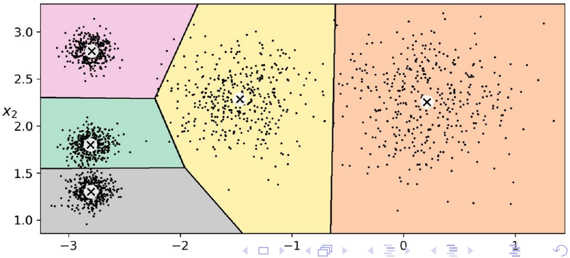


Top down clustering

K Means Clustering

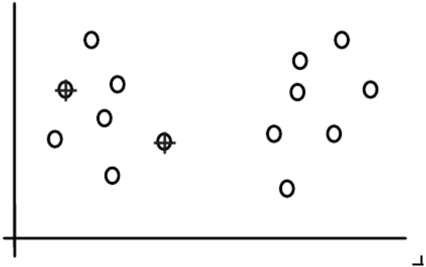
- Data items are points in n dimensions
    - $(x_1, x_2, \ldots, x_n)$
- Partition into K clusters
    - Fix K in advance
- Each cluster is represented by its geometric centre
    - *Centroid*, or *mean*
    - Hence "K means"





K Means Algorithm

- Choose K points initially as random centroids
- In each iteration
  - Assign each point to nearest centroid
  - Recompute centroids
- Termination
  - Clusters stabilize
  - Sum square distance is below threshold



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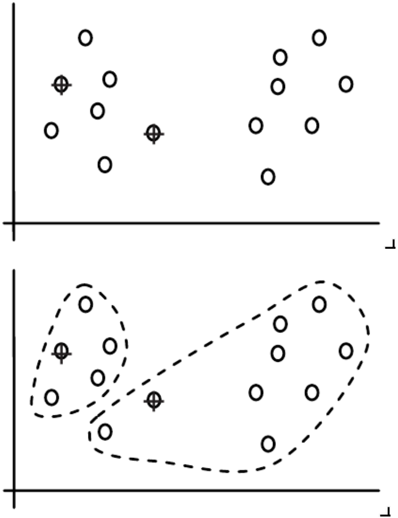

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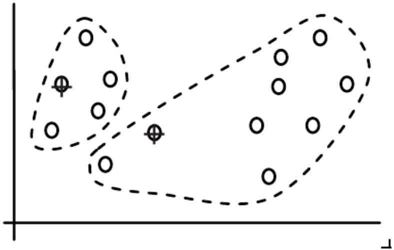

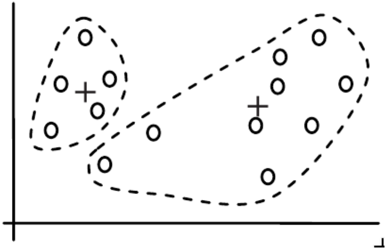

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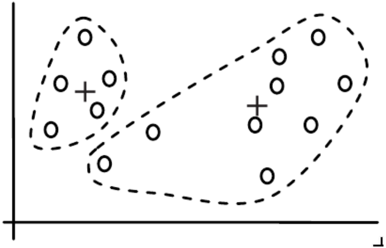

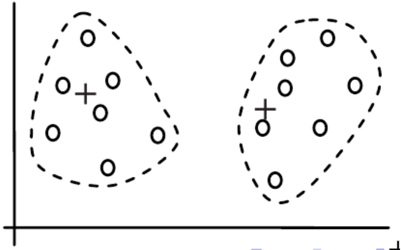

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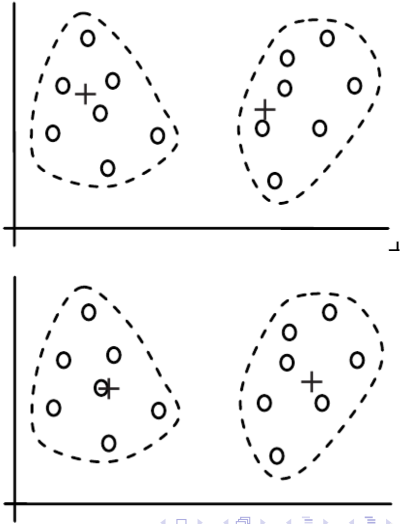

K Means Algorithm

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  - Clusters stabilize, or
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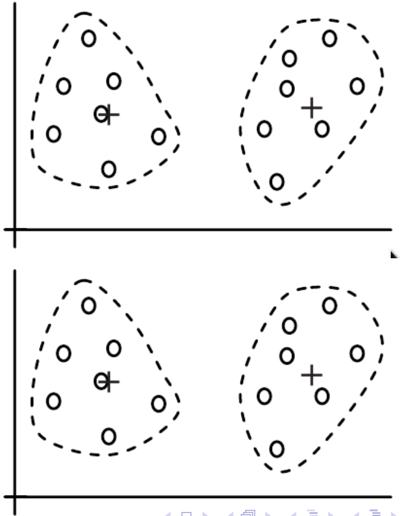
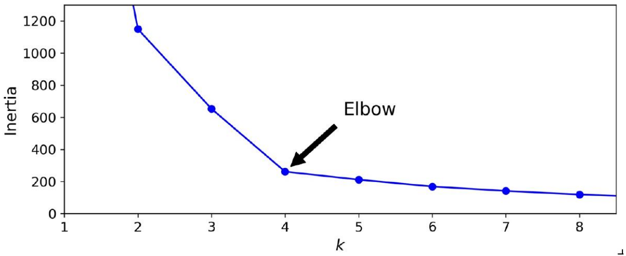


Evaluating clustering

- How "tight" are the clusters?
- Mean squared distance from centroids – *inertia*

$$\frac{1}{n}\sum_{j=1}^{K}\sum_{x\in C_j} dist(x, centroid_j)^2$$



- Plot inertia for different values of K and look for optimum
- Can also use change in inertia threshold to stop iterations

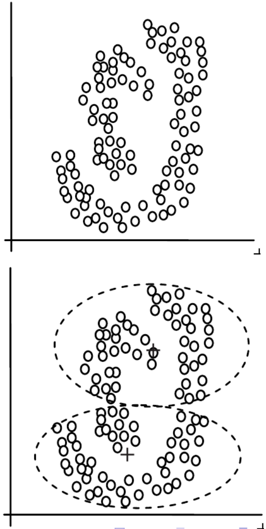
K Means Algorithm

Advantages

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

Disadvantages

- Can only find clusters that look like ellipses



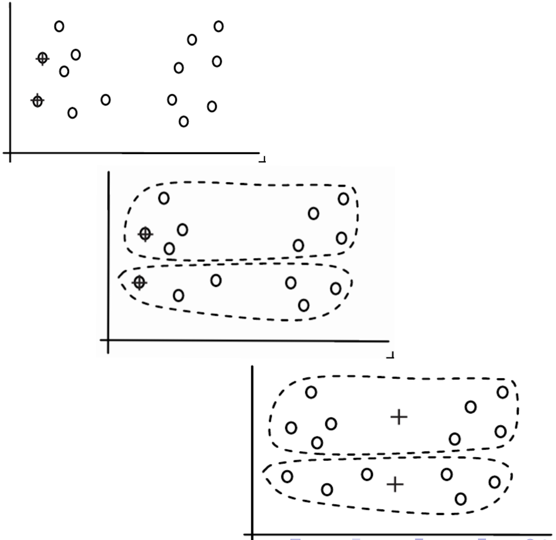
K Means Algorithm

Advantages

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

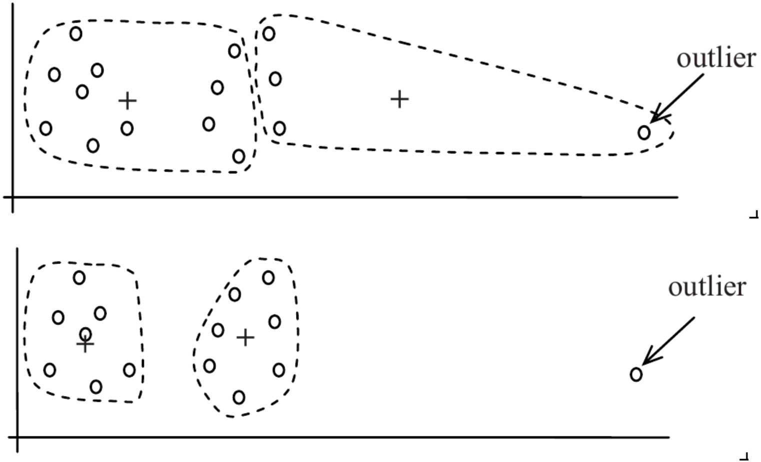
Disadvantages

- Can only find clusters that look like ellipses
- Choice of initial random centroid matters
  - Repeat and check



Outliers

- Anomalous values
  - Far away from all centroids
- But clustering with outliers distorts clusters
- How to identify outliers before clustering?

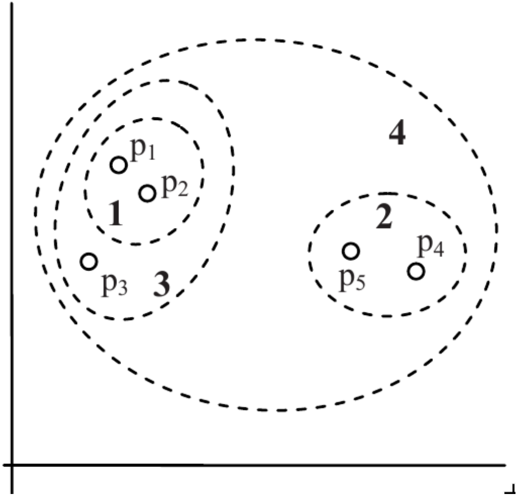


Clustering

- K Means clustering can only find clusters that look like ellipses
- Instead, build clusters bottom up, by merging clusters

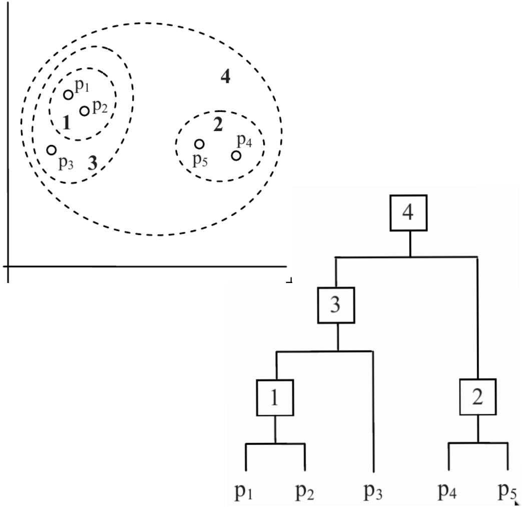
Hierarchical clustering

- Initially, each item is a singleton cluster
- At each step, merge nearest clusters



Hierarchical Clustering

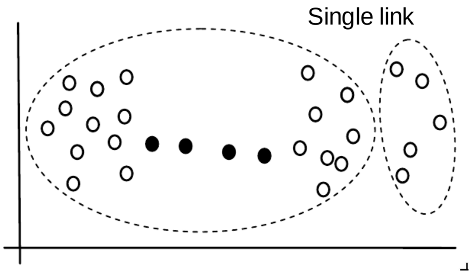
- Initially, each item is a singleton cluster
- At each step, merge nearest clusters
- Can represent process using a tree – dendrogram
- Choose appropriate level in dendrogram for final clustering

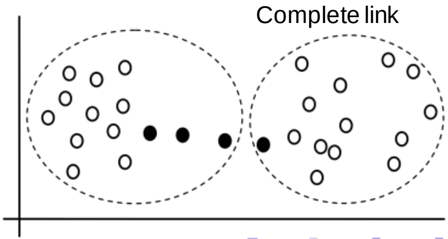


Hierarchical Clustering

To merge clusters, define distance between clusters

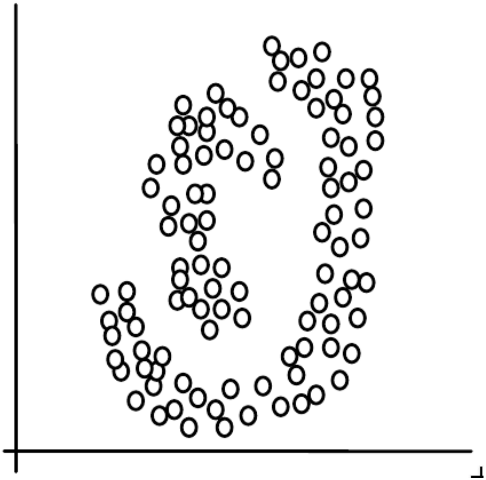
- Single link: distance between closest points
    - Creates chain effect
- Complete link: maximum of pairwise distances
- Average link: mean of pairwise distances
- All require $O(n^2)$ computation - expensive





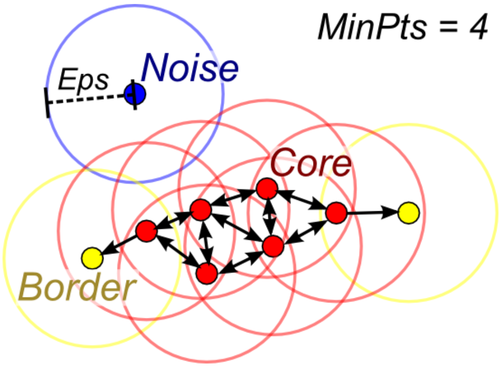
Clustering

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



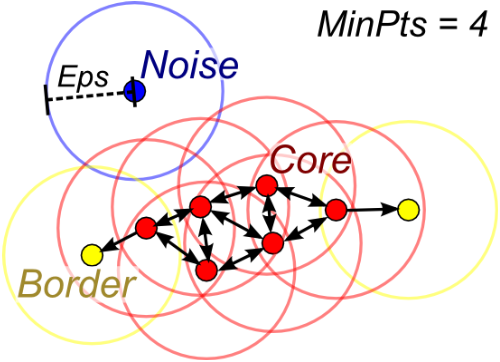
Density based clustering

- Construct a small ball around each point, radius *Eps*
- Identify a threshold for neighbours within ball, *MinPts*
- Core point – has at least *MinPts* neighbours inside *Eps* ball
- Connect each core point to all its neighbours
- Border points – attached to core points but not core themselves
- Noise – disconnected points



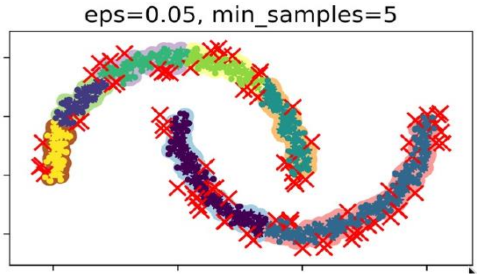
Density based clustering

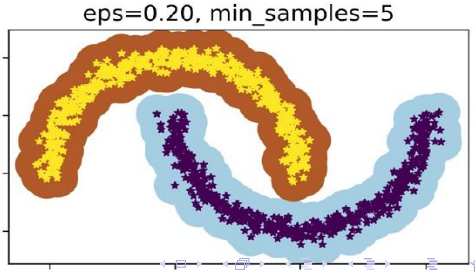
- Formally, edges from core points to neighbours define a directed graph
- Border points are part of this graph, but cannot add edges to extend the graph
- Discard the edge directions
- Connected components are clusters



Dbscan

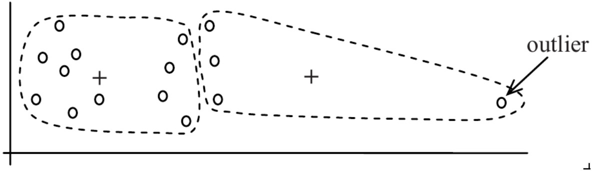
- Implementation of density based clustering available in Python and R
- Smaller value of *Eps* subdivides into small clusters
- Larger *Eps* groups larger clusters

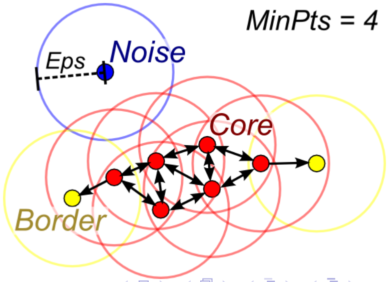




Outliers and clustering

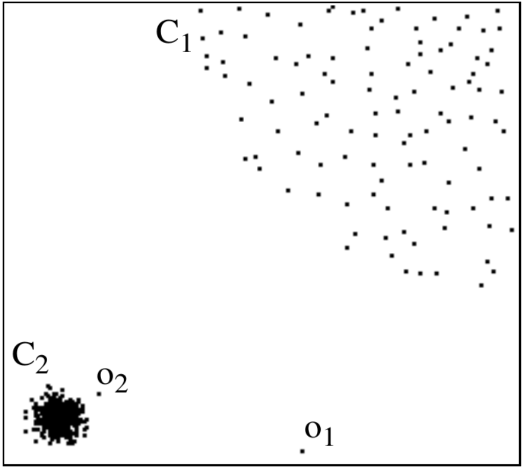
- Outliers are points that lie outside natural clusters
- K Means – far away from all centroids
    - But outliers can distort the clustering process
- Density based clustering – not connected to any core point
    - But density is applied uniformly





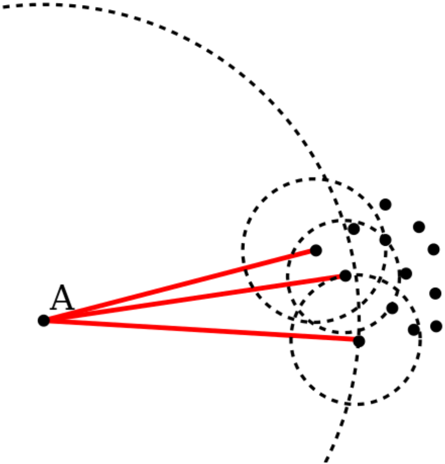
Outliers and density

- An outlier is less dense than its nearest neighbours
- But difference in density may be local
- 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



Outliers and density

- For clustering, we defined a radius *Eps* and looked for *MinPts* neighbours within that ball
- Instead, fix *MinPts* and find smallest ball with that many neighbours
- 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)*

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

- 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