

dm24s1

## Topic 11 : Clustering

### Part 01 : Overview

Preparation

Data Handling

Exploring Data 1

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Exploring Data 2

Building Models

Prediction

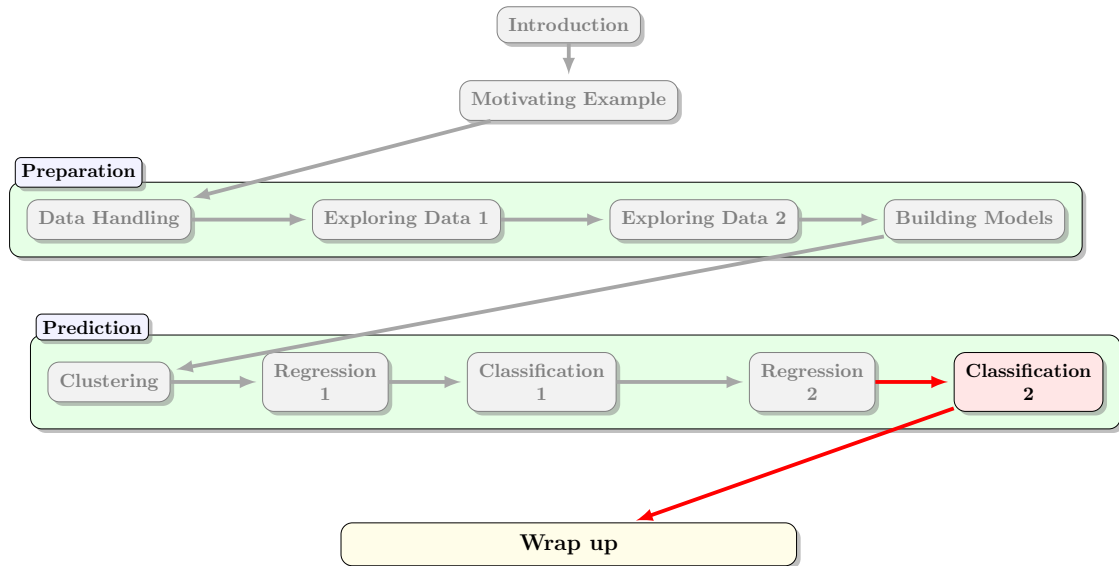
Autumn Semester, 2024

### Outline

- How to compute distances between instances
- Algorithms that partition the data

Wrap up

# Data Mining (Week 11)



# Overview — Summary

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1. Introduction	4
2. Distance Measures	9
3. Hierarchical Clustering	14
4. Partioning Algorithms	25
4.1. K-means	28
4.2. Soft clustering	34
4.3. Expectation Maximisation (EM) iterations	37
4.4. Density-based clustering	39
4.5. Choosing $k$ for centre-based clusters	44
5. Review and resources	50

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  - Iris data: predicting which of three species

Clustering is a long-established form of analysis, having much in common with exploratory data analysis. We look at the main concepts and algorithms today.

# Background: Unsupervised Learning

## Definition 1 (Unsupervised Learning)

With unsupervised learning, the system receives input instances  $x_1, x_2, \dots$  but obtains neither target outputs, nor rewards from its environment. Its goal is to build representations of the input that can be used for decision making, predicting future inputs, efficiently communicating the inputs to another machine, etc. It does this by finding patterns in the data beyond what would be considered pure unstructured noise (**Ghahramani2004**).

Regression and classification are examples of supervised learning because they require labeled *training* data.

We saw *dimensionality reduction* in Topic 8 (Regression 2). Other unsupervised learning techniques include *anomaly detection* and the very “hot” *Generative Adversarial Networks* of deep learning. We look at *clustering* today.

# Introduction to Clustering

## Definition 2 (Clustering)

Clustering is the operation of grouping objects into a smaller number of clusters (or segments), which have two properties. Firstly, they are not defined in advance by an analyst, but are discovered during the operation, unlike the classes used in classification. Secondly, the clusters combine objects having similar characteristics, which are separated from objects having different characteristics (resulting in *internal homogeneity* and *external heterogeneity* (**Tuffery2011**)).

Clustering is usually called *segmentation* in marketing studies.

Usually clustering is not an end in itself: it generates insights that are used to motivate and inform other analyses.

The “quality” of a cluster analysis is difficult to determine objectively - there is no equivalent of *recall*, say.

# Hierarchical versus Partitional techniques

## Hierarchical

- Intermediate steps are interpretable

## Partitional

- Interpret the final clustering only

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- relatively few parameters to specify
- more complex interpretation

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- more parameters to specify
- interpretation is relatively easy

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# Distance Measures and their role in clustering

## Definition 3 (Distance Measure)

A *distance measure* (c.f., its complement, a *similarity measure*) is a scalar number  $d(x_1, x_2)$  that quantifies the degree of agreement between two (usually vector-valued) observations  $x_1$  and  $x_2$ . When  $x_1 = x_2$ ,  $d(x_1, x_2) = 0$  and  $d(x_1, x_2) > 0$  otherwise. It increases as the difference in the observations increases.

By definition, clustering is based on within-cluster homogeneity (measured by small  $d$ ) versus large  $d$  between clusters. Thus choice of distance measure plays a critical part in generating useful clusters.

# Distance Measures for numeric data

## Definition 4 (Minkowski $p$ -norm)

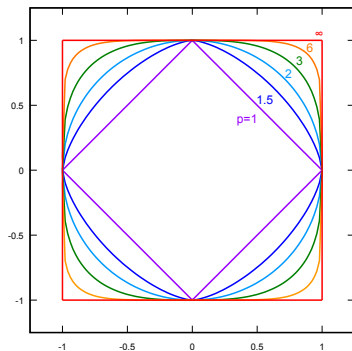
For a real number  $1 \leq p < \infty$ , the  $p$ -norm of  $\mathbf{x}$  is defined by

$$\|\mathbf{x}\|_p \equiv (|x_1|^p + |x_2|^p + \dots + |x_n|^p)^{\frac{1}{p}}.$$

The limiting case of  $p = \infty$  is defined as

$$\|\mathbf{x}\|_\infty \equiv \max\{|x_1|, |x_2|, \dots, |x_n|\}.$$

See the visualisation of the “unit balls” alongside, for  $p = 1, 1.5, 2, 3, 6, \infty$ .



Source: wikipedia

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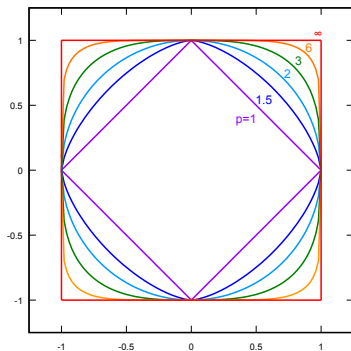
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The most common norms are when  $p = 1, 2$ , or  $\infty$ . Choice of  $p$  depends on the application scenario. Can you think of when you would use each?



Source: wikipedia

## (Selected) Distance Measures for categorical data

Let  $\mathbf{x}_1 = [e_{1,1}, e_{1,2}, \dots, e_{1,k}]^T$  and  $\mathbf{x}_2 = [e_{2,1}, e_{2,2}, \dots, e_{2,k}]^T$ . Furthermore let  $e_{1,j}e_{2,j} = 1$  if  $e_{1,j} = e_{2,j}$  and  $e_{1,j}e_{2,j} = 0$  otherwise. To compute  $s$ , the number of matching attributes between  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , we can just compute the dot product:

$$s = \mathbf{x}_1^T \mathbf{x}_2$$

and the number of mismatches is  $d = k - s$ , where  $k$  is the number of attributes in  $\mathbf{x}$ .



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### Definition 5 (Euclidean distance for categorical observations)

$\|\mathbf{x}_1 - \mathbf{x}_2\| = \sqrt{\mathbf{x}_1^T \mathbf{x}_1 - 2\mathbf{x}_1^T \mathbf{x}_2 + \mathbf{x}_2^T \mathbf{x}_2} = \sqrt{2(k - s)}$ . So the maximum distance occurs when  $s = 0$  ( $\mathbf{x}_1$  and  $\mathbf{x}_2$  share no attribute values in common, as expected).

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### Definition 6 (Hamming Distance)

This is the number of mismatched values  $k - s$ .

## (Selected) Distance Measures for categorical data - ratios

### Definition 7 (Cosine similarity)

$$\cos \theta_{1,2} = \frac{\mathbf{x}_1^T \mathbf{x}_2}{\|\mathbf{x}_1\| \|\mathbf{x}_2\|} = \frac{s}{\sqrt{k} \sqrt{k}} = \frac{s}{k}.$$

because  $\|\mathbf{x}\| \equiv \sqrt{\mathbf{x}^T \mathbf{x}} = \sqrt{k}$ .

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## Definition 8 (Jaccard Coefficient)

This is the ratio of the number of matching values  $s$  to the number of distinct values that appear in  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , across the  $d$  *distinct* attributes of both. It is  $J(\mathbf{x}_1, \mathbf{x}_2) = \frac{s}{2(k-s)+s} = \frac{s}{2k-s}$ .

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Note that all these distance measures are functions of  $s$  and  $k$ , where  $k$  is a constant and  $s$  is a count of the number of matching attribute values across the two observations in question.

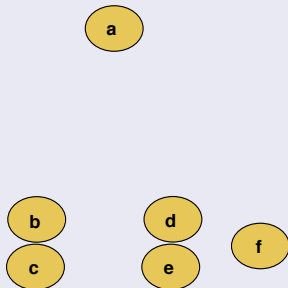
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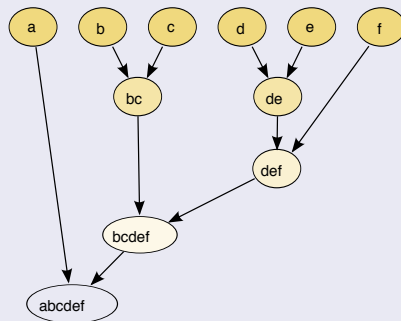
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# Simple example of data and its dendrogram

Data



Dendrogram



This illustrates how *agglomerative* clustering works. *Divisive* clustering works in the opposite direction, but the (flipped) dendrogram is the same in this case.

Sometimes, the vertical separation between Level  $i$  and  $i + 1$  of the tree indicates the distance between clusters that are merged at Level  $i + 1$ .

*Diagram Source:* wikipedia

# Dendrograms

## Definition 9 (dendrogram)

The dendrogram shows clusters and their subclusters, in the form of a tree. The root cluster contains all elements; each leaf contains a single element. Clusters are merged in order of their similarity.



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An alternative representation is to display the data as a point cloud and to overlay nested clusters over the data.

# Overview of Hierarchical Clustering Algorithm

## Method (Agglomerative hierarchical clustering (AGNES))

Initialise the Cluster set  $C = \{x_i\}, i = 1, \dots, n$ ;

$q \leftarrow |\{c_i\}| = n$ ;

Compute the  $n \times n$  proximity matrix  $D$  where  $D_{ij} = d(c_i, c_j)$ ;

**repeat**

Find  $i, j$  associated with  $\min_{i,j} D$ , where  $i, j$  are indices of clusters that are nearest each other;

Create the merged cluster  $c'_i$  containing the elements of cluster  $c_i$  and  $c_j$ ;

Record the merge operation so the dendrogram data structure can be built;

Drop the old  $c_j$  cluster since it is not needed any more;

Delete row  $D(j, :)$  and column  $D(:, j)$  from  $D$

$q \leftarrow q - 1$ ;

Update row  $D(i, :)$  and column  $D(:, i)$  to compute distance between new cluster  $c'_i$  and remaining  $q - 2$  clusters;

**until**  $q = 1$  and hence only one cluster remains;

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As can be seen, this is a deterministic search algorithm.

However, there is scope for different definitions of the distance function  $d(c_i, c_j)$  between clusters  $c_i$  and  $c_j$ .

## Distance between clusters: linkage

Earlier, we looked at different ways of computing the *distance between two points*.  
For hierarchical clustering, we need to compute the *distance between two clusters*.

### Definition 10 (Linkage function)

For Complete Linkage:  $D(X, Y) = \max_{x \in X, y \in Y} d(x, y)$ .

For Single Linkage:  $D(X, Y) = \min_{x \in X, y \in Y} d(x, y)$ .

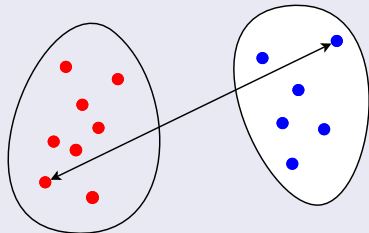
For Average Linkage:  $D(X, Y) = \frac{1}{|X||Y|} \sum_{x \in X, y \in Y} d(x, y)$ . This is also known as Unweighted Pair Group Method with Arithmetic Mean (UPGMA) linkage.

For Ward linkage: the initial (single-point) cluster distances are simply the Euclidean distances between the points. The clusters are merged based on a minimum variance criterion. The distance between any point and a merged cluster is calculated using a recursive formula of Lance-Williams type (**MurtaghLegendre2014**).

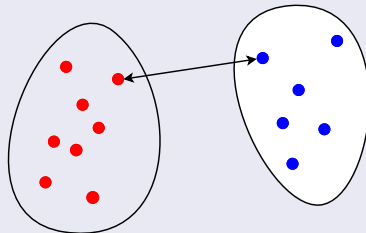
Generally, Complete Linkage and Ward's minimum variance linkage give the most balanced and useful clusters.

# Distance between clusters: linkage visualisation

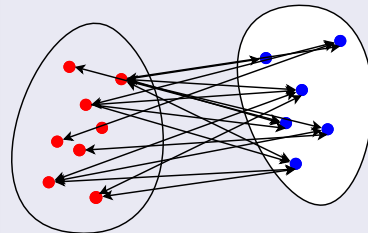
## Complete Linkage



## Single Linkage



## Average Linkage

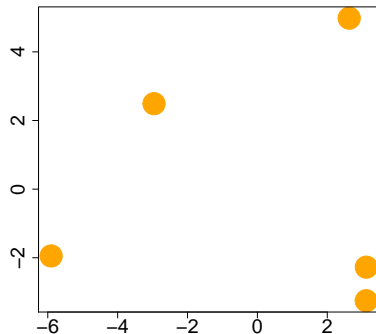


## AGNES worked example: setting the scene

Distance Matrix, Step 0

	A	B	C	D	E
A	0				
B	9	0			
C	3	7	0		
D	6	5	9	0	
E	11	10	2	8	0

MDS placement of points from distances



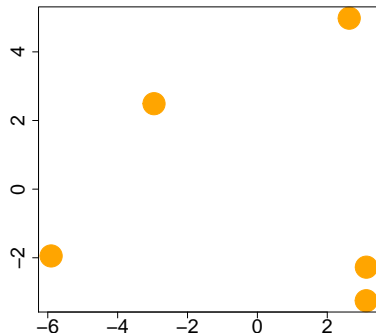


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## Use of distance matrices

Many algorithms in data mining either start from a distance matrix representation, or need to **create it themselves**. Reversing the process (from distances to locations) is not unique, but **MultiDimensional Scaling** often gives an attractive placement (as above, centred on origin).

# AGNES worked example: Initial iterations

## First clustering: CE, A, B, D

The smallest distance is 2 between C-E. We cluster these points and compute the distance of the remaining points from the CE cluster. Because of **single** linkage, we store the **minimum** such distance in the revised table beside.

## Distance Matrix, Step 1

	CE	A	B	D
CE	0			
A	3	0		
B	7	9	0	
D	8	6	5	0

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## Distance Matrix, Step 1

	CE	A	B	D
CE	0			
A	3	0		
B	7	9	0	
D	8	6	5	0

## Second clustering: ACE, B, D

The smallest distance is 3 between A and CE. We cluster these points and compute the distance of the remaining points from the ACE cluster. For example  $d(B,A) = 9$ ,  $d(B,C) = 7$ ,  $d(B,E) = 10$ , so by single linkage  $d(B,ACE) = 7$  as in the revised table beside.

## Distance Matrix, Step 2

	ACE	B	D
ACE	0		
B	7	0	
D	6	5	0

Minimum distances so far: 2,3

# AGNES worked example: Final iterations

## Third clustering: CE, A, B, D

The smallest distance is 5, between B and D, so we create a BD cluster. The new distance matrix is shown alongside. The next step after this would be to merge ACE with BD, creating a single ABCDE cluster. The algorithm ends...

## Distance Matrix, Step 3

	ACE	BD
ACE	0	
BD	6	0

Minimum distances so far: 2,3,5,(6)

# AGNES worked example: Final iterations

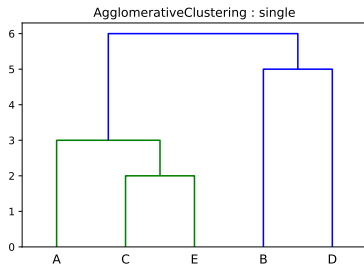
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## Distance Matrix, Step 3

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BD	6	0

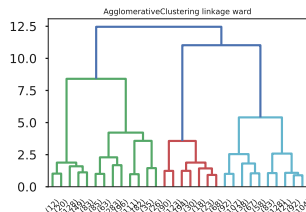
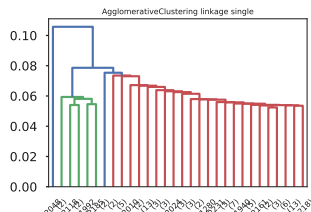
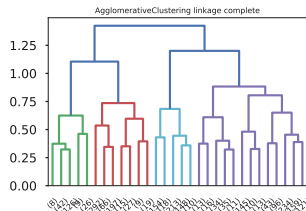
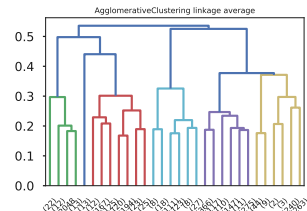
Minimum distances so far: 2,3,5,(6)



## Resulting Dendrogram

The resulting dendrogram summarises the hierarchical clustering. Note that the joins/splits occur at distances 2, 3, 5 and 6, as noted above.

# Comparison of Dendrograms



As can be seen, the choice of linkage function has a dramatic effect on cluster membership. The underlying data in this instance appeared to have 6 clusters. Can you see this in these dendrograms?

# Uses of hierarchical clustering

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- Since hierarchical clustering provides more than one candidate clustering, it can require more system resources (computation and memory) than other techniques. Thus it might not scale very well.
- We have seen agglomerative (bottom-up) clustering. Divisive (top-down) clustering (DIANA) is also available, but has worse scalability.

# Outline

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4.1. K-means	28
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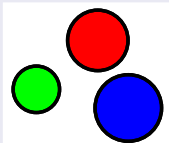
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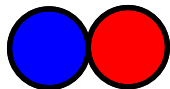
... looks for regions, possibly non-convex, where the data density is higher, and assigns observations in those regions to the relevant cluster. Any other observations are assumed to be either “noise” or “border” observations.

# Types of partitional clustering

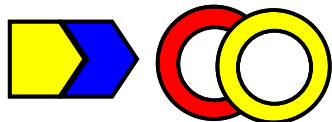
## Well-separated clusters



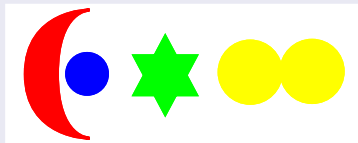
## Centre-based clusters



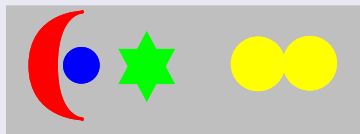
## Conceptual clusters



## Contiguity-based clusters



## Density-based clusters



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  - **k-medoids** : Manhattan ( $\ell_1$ ) distance is used instead of Euclidean ( $\ell_2$ ), and centres are constrained to be data points); PAM and CLARA algorithms.
- Generally Lloyd's algorithm is robust, although it is affected by the choice of initial centres, and care must be taken to avoid empty clusters

# K-means algorithm: Detail

## Method (k-means algorithm)

$t \leftarrow 0$ ;

Initialise centres  $\{\mu_j^t, j = 1, \dots, k\}$ : choose  $k$  points randomly, without replacement;

**repeat**

$t \leftarrow t + 1$ ;

$C_j \leftarrow \emptyset, \forall j = 1, \dots, k$ ;

▷ Cluster Assignment Step E

**for all**  $\mathbf{x}$  **do**

▷ Assign  $\mathbf{x}_j$  to the nearest centroid from the previous iteration

$j^* \leftarrow \arg \min_i \left\{ \|\mathbf{x}_j - \mu_i^{t-1}\|^2 \right\}$ ;

$C_{j^*} \leftarrow C_{j^*} \cup \{\mathbf{x}_j\}$ ;

**end for**

▷ Centroid Update Step M

**for all**  $i = 1$  to  $k$  **do**

$\mu_i^t \leftarrow \frac{1}{|C_i|} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$ ;

**end for**

**until**  $\sum_{i=1}^k \|\mu_i^t - \mu_i^{t-1}\|^2 \leq \epsilon$

The termination condition is that the difference in centre positions should not exceed a small tolerance  $\epsilon$ . This happens when points stay in their cluster from iteration  $p$  to  $p + 1$ , so cluster centre stays same.

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  - **Or** Use k-prototypes on the original data if some data is categorical and some is numerical

## “K-means” for categorical data: k-modes

➤ k-means uses **centroids** and **Euclidean** distance; k-modes uses **modes** and **Hamming** distance ➤

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## Implementation

Installation: `conda install -c conda-forge kmodes`

```
from kmodes.kmodes import KModes
import pandas as pd
import numpy as np
data=pd.read_csv("studentGrades.csv", index_col=["Student"])
# n_init=4 means rerun with 4 random starts, take the overall best
untrainedModel=KModes(n_clusters=3, random_state=42, n_init=4)
trainedModel=untrainedModel.fit(data)
unseenStudents = [['A', 'B', 'A'], ['C', 'A', 'B']]
clusters=trainedModel.predict(unseenStudents)
print(clusters)
```



# “K-means” for numerical and categorical data: k-prototypes

Combine k-means (on numerical data) and k-modes (on categorical data) in one clustering algorithm.

## Intuition

- A **prototype** instance has representative values of numerical and categorical features.

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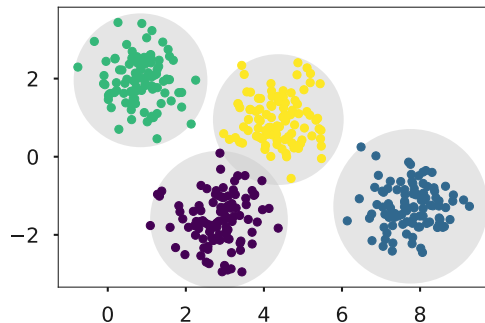
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from kmodes.kprototypes import KPrototypes

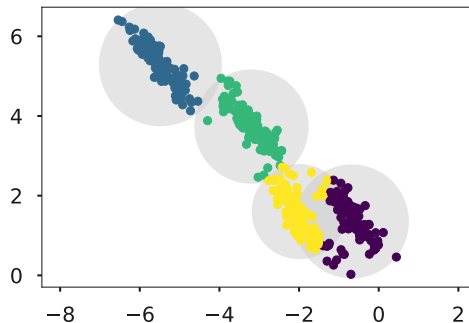
# Configure the clustering algorithm
kproto = KPrototypes(n_clusters=4, init='Cao')
# Indicate which columns are categorical, and apply to data
clusters = kproto.fit_predict(X, categorical=[1, 2])
```

# K-means algorithm: In practice



With the original globular clusters,  $k$ -means was able to find the centres and clusters easily.

$k$ -means minimises the within-cluster sum of squared distances (also known as *inertia*) so the choice of distance function is critical.



With the stretched clusters,  $k$ -means had more difficulty, e.g., with the yellow and purple clusters.

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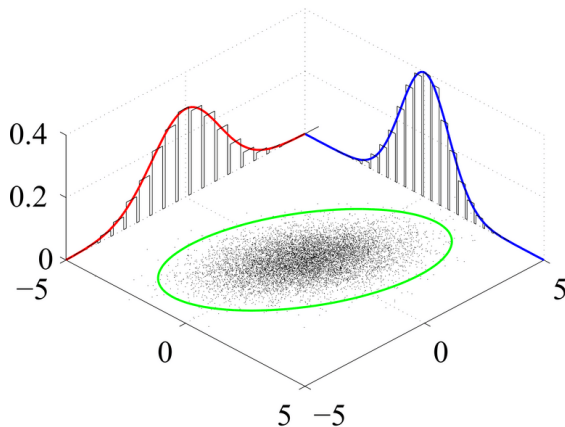
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- $P$  is a function of the relative Euclidean distances to the cluster centres  $\{\mu_j\}$
- This probability function can be generalised, notably to take account of the *shape* of the clusters and not just their centres, leading to *Gaussian Mixture Model* (GMM) probabilistic clustering

# Review: Multivariate (2D) Gaussian/Normal distribution



- The distribution can have different dimensions that do not need to align with the coordinate axes; captured as a  $2 \times 2$  covariance matrix  $\mathbf{C}$
- The distribution stretches to infinity in the plane, but points far from the centre of the distribution have very low probability.
- A collection of clusters can be modelled by overlaying a *mixture* of such Gaussian distributions on the plane.

Source: Wikipedia

# Review of Bayes Theorem

## Use of Bayes Theorem in Classification

**Likelihood** is the probability of the data given the label. **Prior** measures our belief about how likely each label is *before* we have seen any data. The **Posterior** includes influences of both the Prior and the Likelihood.

$$P(y = c|x) = \frac{P(x|y = c)P(y = c)}{P(x)}$$

The Posterior here is  $P(y = c|x)$ , the Likelihood is  $P(x|y = c)$  and the Prior is  $P(y = c)$ .  $P(x)$  is a normalizing constant that measures how likely the observed data  $x$  is.

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When used for Gaussian Mixture Models, there is not just a *single* cluster label  $c$ , but a linear combination of many.

# Overview of EM algorithm for GMM clustering

**E-step** For each  $x_i$ , calculate the probability that  $x_i$  belongs to the  $j^{\text{th}}$  distribution

$$P(\Theta_j|x_i, \Theta) = \frac{P(x_i|\Theta_j)}{\sum_{l=1}^k P(x_i|\Theta_l)},$$

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Lloyd's k-means algorithm is equivalent: the membership probability is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point. The M-step re-computes the cluster centres based on all the points and their cluster assignment.

# GMM compared with k-means

	k-means	GMM
E-step	Compute membership probability which is either 1 (allocated to this cluster) or 0 (not allocated to this cluster) for each point	Compute membership probability for each point based on all the Gaussian models and their parameters.

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Use for	Well-separated	Centre-based or well-separated
Shape	nondirectional (“spherical”)	directional (“ellipsoidal”) or nondirectional

# Relaxing the constraints: density-based clustering

k-means and GMM are both characterised by the following properties:

- the number of clusters  $k$  must be specified beforehand
- clusters have a convex shape
- they work best when the clusters are linearly separable
- all points are assigned to clusters, so can be sensitive to outliers

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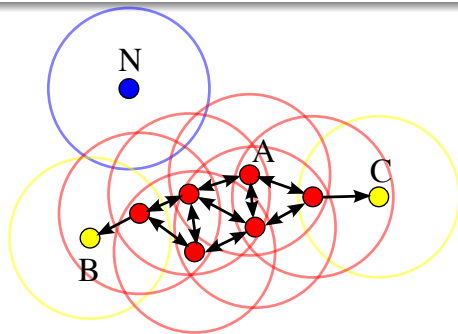
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## Density-based clustering relaxes these conditions

It uses the heuristic that clusters are (arbitrarily-shaped) contiguous regions with high datapoint density. Datapoints outside these regions represent *noise* and are ignored. Rather than specifying  $k$ , the user specifies density thresholds.

# Relaxing the constraints: density-based clustering

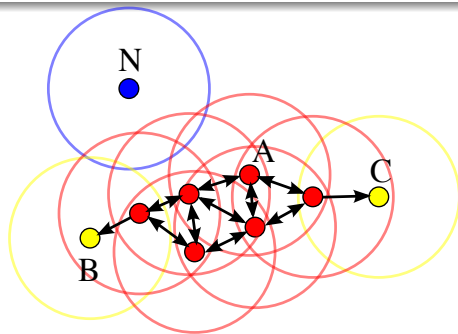


*Source: wikipedia*

- A, B and C are directly connected points.



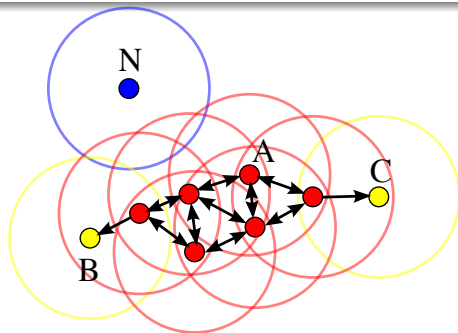
# Relaxing the constraints: density-based clustering



*Source: wikipedia*

- A, B and C are directly connected points.
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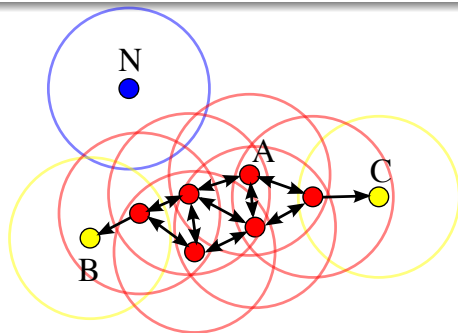
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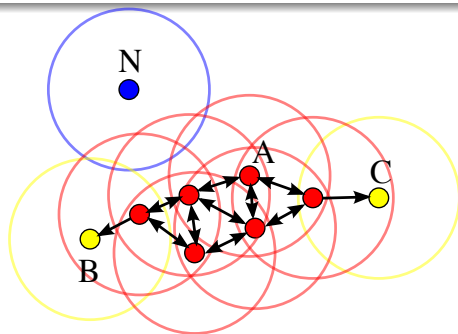
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- A, B and C are directly connected points.
- A is a **core** point
- B and C are **border** points.
- N is a **noise** point and so is not assigned to a cluster.
- The connected component of the 8 points (6 red, 2 yellow; including A,B,C) forms a cluster.

# DBSCAN algorithm and its concepts

## Definition 13 (DBSCAN)

Density-Based Spatial Clustering of Applications with Noise (DBSCAN): an algorithm for deriving clusters in areas of high data density.

## Definition 14 (eps-neighbourhood)

Epsilon  $\epsilon$  parameter defines a region of points  $\mathbf{t}$  around a point  $\mathbf{x}$  where  $\|\mathbf{t} - \mathbf{x}\| < \epsilon$ .

## Definition 15 (core point)

Point with at least  $\text{MinPts}-1$  other points in its eps-neighbourhood.

## Definition 16 (border point)

Point with less than  $\text{MinPts}-1$  other points in its eps-neighbourhood, but at least one is a core point.

## Definition 17 (noise point)

Point with less than  $\text{MinPts}-1$  other non-core points in its eps-neighbourhood.

# Development of the algorithm

## Definition 18 (Direct density reachable)

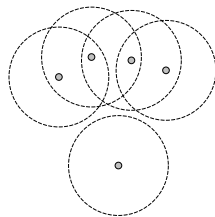
Point  $\mathbf{x}_A$  is directly density reachable from  $\mathbf{x}_B$  iff  $\mathbf{x}_A$  is in the eps-neighborhood of  $\mathbf{x}_B$  and  $\mathbf{x}_B$  is a *core point*.

## Definition 19 (Density reachable)

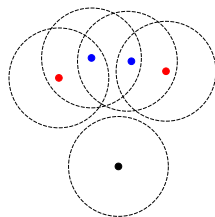
Point  $\mathbf{x}_A$  is density reachable from  $\mathbf{x}_B$  if there is a set of core points in each other's eps-neighbourhood between  $\mathbf{x}_A$  and  $\mathbf{x}_B$ .

## Definition 20 (Density connected)

Points  $\mathbf{x}_A$  and  $\mathbf{x}_B$  are density connected if there exists a core point  $\mathbf{x}_C$  so that both  $\mathbf{x}_A$  and  $\mathbf{x}_B$  are density reachable from  $\mathbf{x}_C$ .



Core, border and noise points are coloured blue, red and black below.



# Steps of the DBSCAN algorithm

## Method (DBSCAN)

- ➊ Find the  $\epsilon$  neighbors of every point.
  - ➋ Identify the core points with more than  $\text{minPts}$  neighbors.
  - ➌ Derive the *connected component* graphs of core points, assigning edges between core points that are less than  $\epsilon$  apart.
  - ➍ Identify the border points and assign them to their nearest cluster.
  - ➎ Label any remaining points as *noise*.
- A variant (HDBSCAN) excludes border points from the cluster, treating them as noise points (can be more robust).
  - Another variant (OPTICS) places the points in a priority queue, ordered by reachability distance (updating is slower, but handles varying density better).

# Choosing $k$ , the number of clusters

How can we decide on  $k$  for k-means and GMM?

- We can do this *graphically* (plot clusters for each  $k$ ) or by using *scores*.



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- Use `kmeans.inertia_` as the score for a given instance of the kmeans classifier.
- Can also compute inertia for other partitioning clustering techniques, but this is more work and interpretation is more difficult.

# Silhouette scores - derivation

How much is any point in a cluster nearer its peers than it is to points in the nearest of the other clusters?

## Method (Silhouette score)

**Require:** Clustering where the  $i$  point is assigned to cluster  $C(i)$  and there are  $k$  such clusters

**for all** point  $i$  in cluster  $C(i)$  **do**

    Calculate  $a(i)$ , the mean distance between  $i$  and all the other points in  $C(i)$ .  $\triangleright a(i) \equiv 0$  if there is no other point in  $C(i)$ .

    Calculate  $b(i)$ , minimum of the mean distances between  $i$  and all the other points in each of  $C(j)$  where  $j \neq i$ .

    Silhouette  $s(i) = 1 - a(i)/b(i)$  if  $a(i) < b(i)$ ,  $s(i) = 0$  if  $a(i) = b(i)$  and  $s(i) = b(i)/s(i) - 1$  if  $a(i) > b(i)$ .

**end for**

The mean of  $s(i)$  over all points ( $\bar{s}_k$ ) is a measure of the clustering efficiency for that value of  $k$ .

The  $k$  associated with the *maximum* of these  $\bar{s}_k$  silhouette scores is the best choice of  $k$ .

There are many other scores but they require more advanced mathematics and are out of scope for this module.

# Silhouette scores - examples

*Code to create silhouette plots*

```
from sklearn.metrics import silhouette_samples, silhouette_score

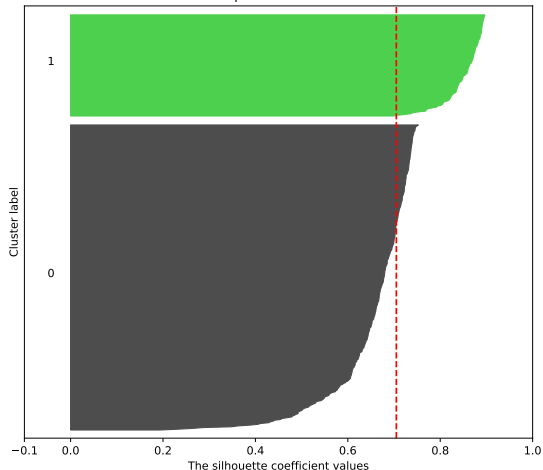
clusterer = KMeans(n_clusters=n_clusters, random_state=10)
cluster_labels = clusterer.fit_predict(X)

# The silhouette_score gives the average value for all the samples.
silhouette_avg = silhouette_score(X, cluster_labels)
```

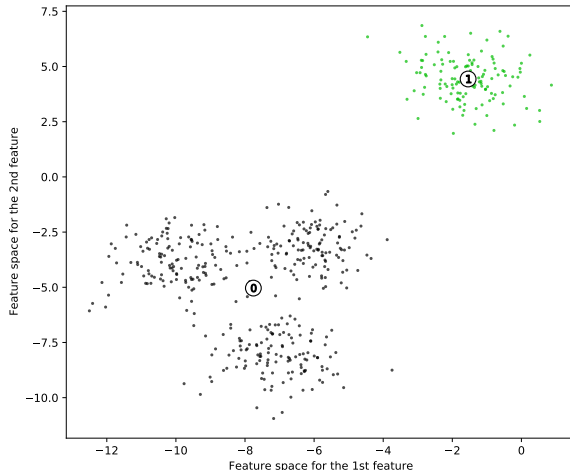
# Silhouette score with $k = 2$ - looking good

## Silhouette analysis for KMeans clustering on sample data with $n\_clusters = 2$

The silhouette plot for the various clusters.



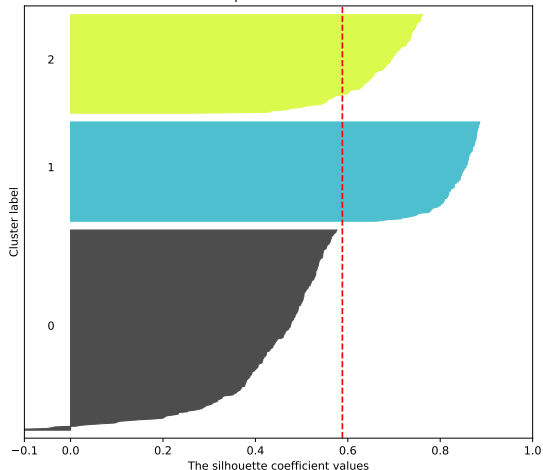
The visualization of the clustered data.



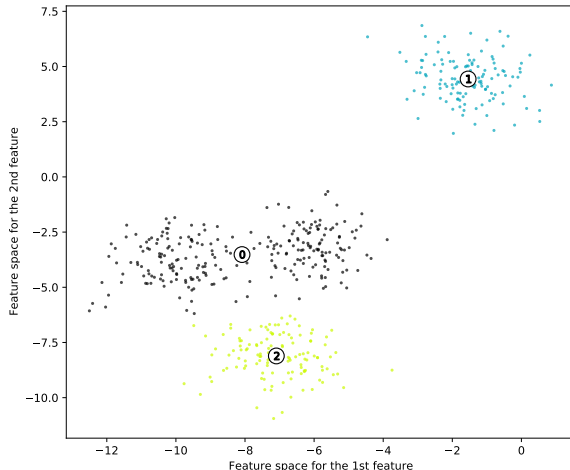
# Silhouette score with $k = 3$ - not looking good

## Silhouette analysis for KMeans clustering on sample data with $n\_clusters = 3$

The silhouette plot for the various clusters.



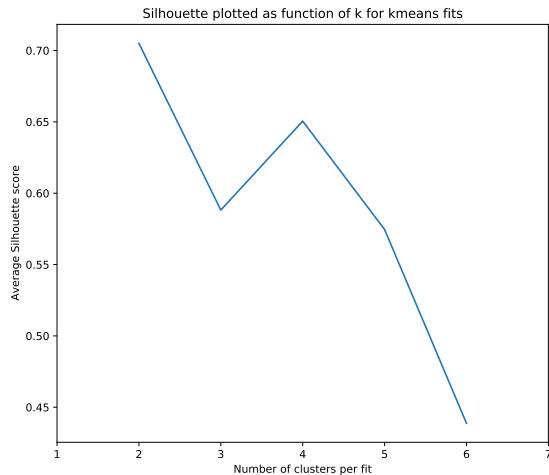
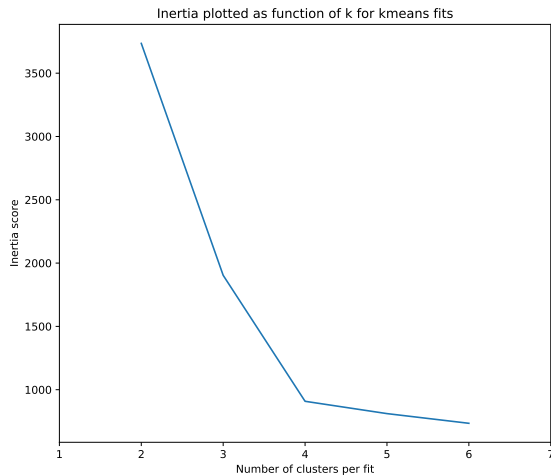
The visualization of the clustered data.



# Comparing both scoring systems

## *Inertia/elbow plot and silhouette plot on the same data*

Comparison of inertia and silhouette scores for estimating  $k$





# Outline

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## Tips

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- Can be good idea to transform data before clustering.
- Dendrogram is good for visualising structure when data is more than 3-D.



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- Hierarchical clustering can provide insights into the structure of a data set - very useful when exploring data for other techniques
- Partitional clustering can be used to label points according to which cluster they belong to
- Partitional classification has many approaches: centre-based and density based are most common
- Clustering can be used to help create training data for classification purposes (c.f., the digits notebook used in the practical)