Clustering Analysis Basics

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Outline

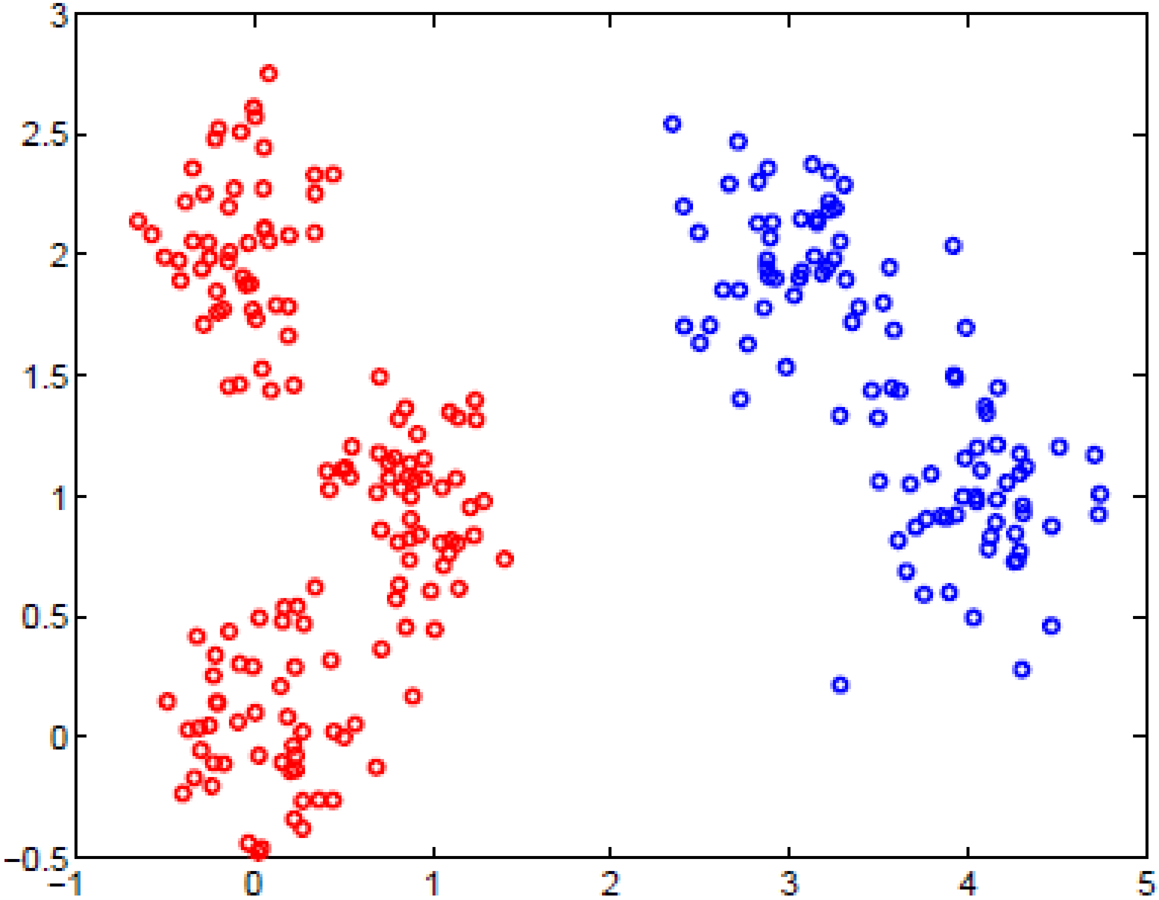
- Introduction
- Data Types and Representations
- Distance Measures
- Major Clustering Approaches
- Summary

Introduction

- Cluster: A collection/group of data objects/points
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis
  - find *similarities* between data according to characteristics underlying the data and grouping similar data objects into clusters
- Clustering Analysis: Unsupervised learning
  - no predefined classes for a training data set
  - Two general tasks: identify the "natural" clustering number and properly grouping objects into "sensible" clusters
- Typical applications
  - as a stand-alone tool to gain an insight into data distribution
  - as a preprocessing step of other algorithms in intelligent systems

Introduction

- Illustrative Example 1: how many clusters?



Introduction

- Illustrative Example 2: are they in the same cluster?

Blue shark, sheep, cat, dog

Lizard, sparrow, viper, seagull, gold fish, frog, red mullet

1. Two clusters
2. Clustering criterion: How animals bear their progeny

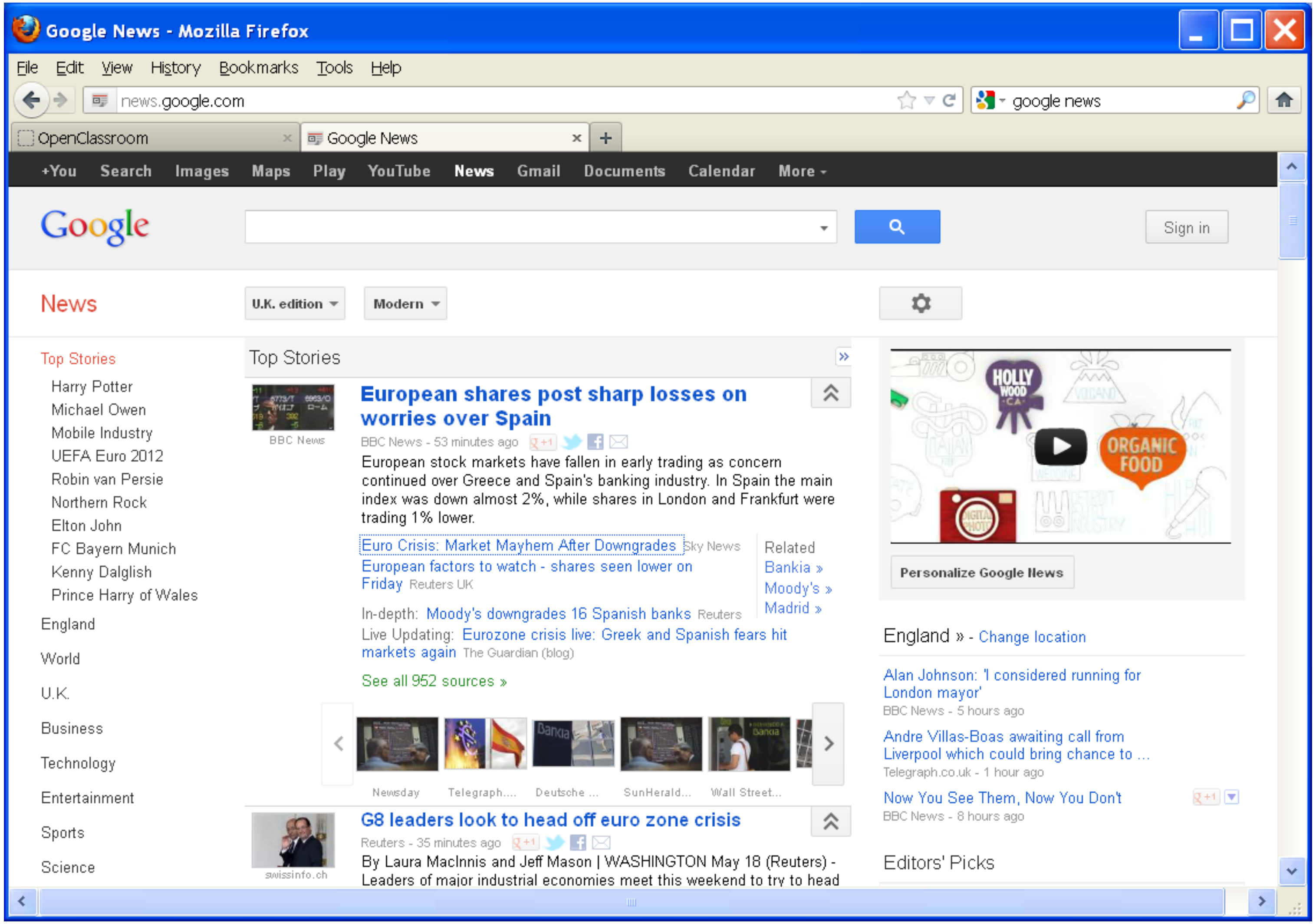
Gold fish, red mullet, blue shark

Sheep, sparrow, dog, cat, seagull, lizard, frog, viper

1. Two clusters
2. Clustering criterion: Existence of lungs

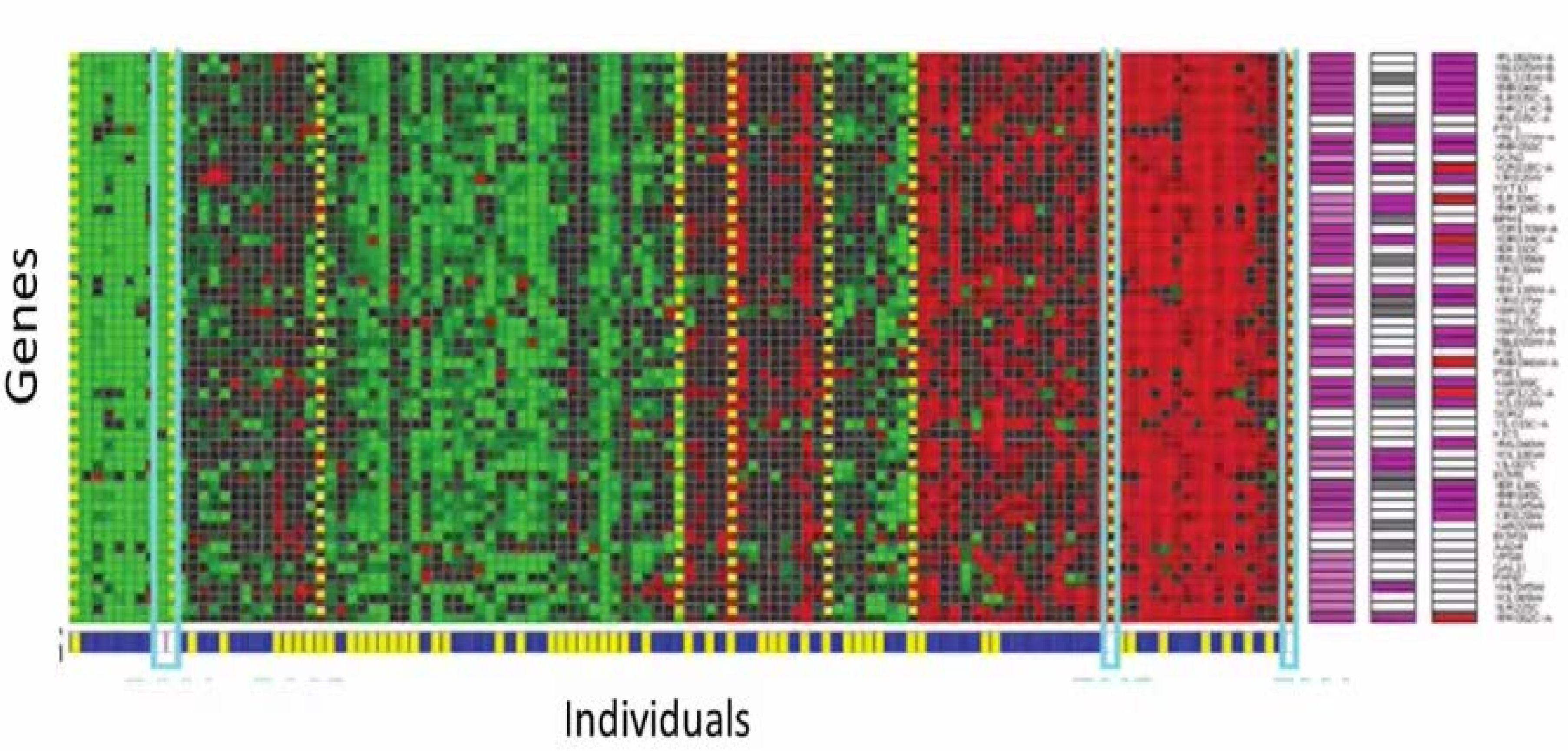
Introduction

- Real Applications: [Google News]



Introduction

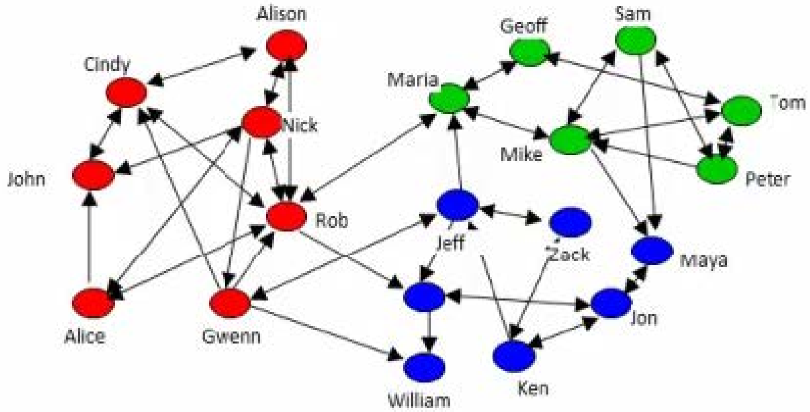
- Real Applications: Genetics Analysis



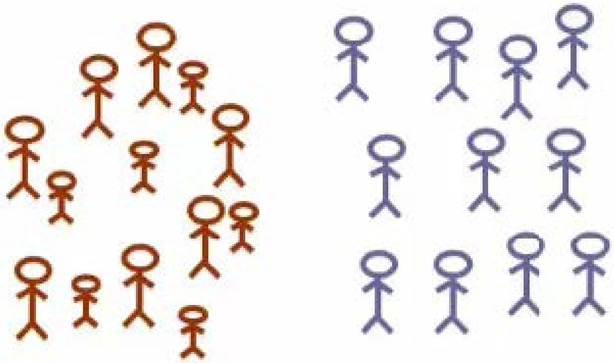
Introduction

- Real Applications: Emerging Applications

Organize computing clusters



Social network analysis



Market segmentation.

Astronomical data analysis

Introduction

- A technique demanded by many real world tasks
  - Bank/Internet Security: fraud/spam pattern discovery
  - Biology: taxonomy of living things such as kingdom, phylum, class, order, family, genus and species
  - City-planning: Identifying groups of houses according to their house type, value, and geographical location
  - Climate change: understanding earth climate, find patterns of atmospheric and ocean
  - Finance: stock clustering analysis to uncover correlation underlying shares
  - Image Compression/segmentation: coherent pixels grouped
  - Information retrieval/organisation: Google search, topic-based news
  - Land use: Identification of areas of similar land use in an earth observation database
  - Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
  - Social network mining: special interest group automatic discovery

Quiz

Of the following examples, which would you address using an unsupervised learning algorithm? (Check all that apply.)

- [ ] Given email labeled as spam/not spam, learn a spam filter.
- [x] Given a set of news articles found on the web, group them into set of articles about the same story.
- [x] Given a database of customer data, automatically discover market segments and group customers into different market segments.
- [ ] Given a dataset of patients diagnosed as either having diabetes or not, learn to classify new patients as having diabetes or not.

Data Types and Representations

- Discrete vs. Continuous
  - Discrete Feature
    - Has only a finite set of values
      e.g., zip codes, rank, or the set of words in a collection of documents
    - Sometimes, represented as integer variable
  - Continuous Feature
    - Has real numbers as feature values
      e.g, temperature, height, or weight
    - Practically, real values can only be measured and represented using a finite number of digits
    - Continuous features are typically represented as floating-point variables

Data Types and Representations

- Data representations
  - Data matrix (object-by-feature structure)

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- n data points (objects) with p dimensions (features)
- **Two modes**: row and column represent different entities

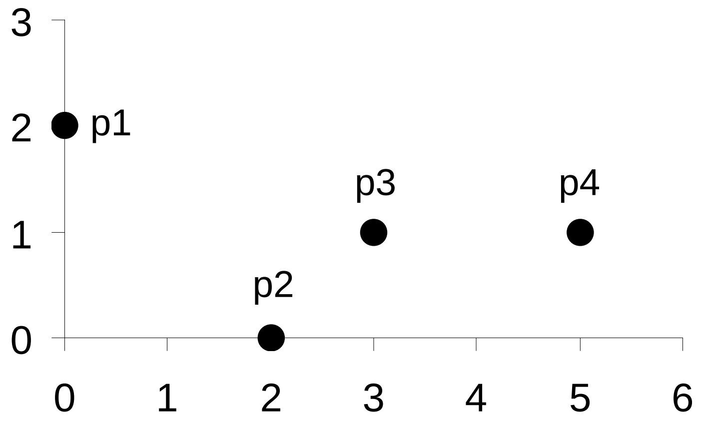
  - Distance/dissimilarity matrix (object-by-object structure)

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

- n data points, but registers only the distance
- A symmetric/triangular matrix
- **Single mode**: row and column for the same entity (distance)

Data Types and Representations

- Examples



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

Data Matrix

	p1	**p2**	**p3**	**p4**
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix (i.e., Dissimilarity Matrix) for Euclidean Distance

Distance Measures

- Minkowski Distance (http://en.wikipedia.org/wiki/Minkowski_distance)

  For $\mathbf{x} = (x_1\ x_2 \cdots x_n)$ and $\mathbf{y} = (y_1\ y_2 \cdots y_n)$

$$d(\mathbf{x}, \mathbf{y}) = \left(|x_1 - y_1|^p + |x_2 - y_2|^p \cdots + |x_n - y_n|^p\right)^{\frac{1}{p}}, \quad p > 0$$

  – $p = 1$: Manhattan (city block) distance

$$d(\mathbf{x}, \mathbf{y}) = |x_1 - y_1| + |x_2 - y_2| \cdots + |x_n - y_n|$$

  – $p = 2$: Euclidean distance

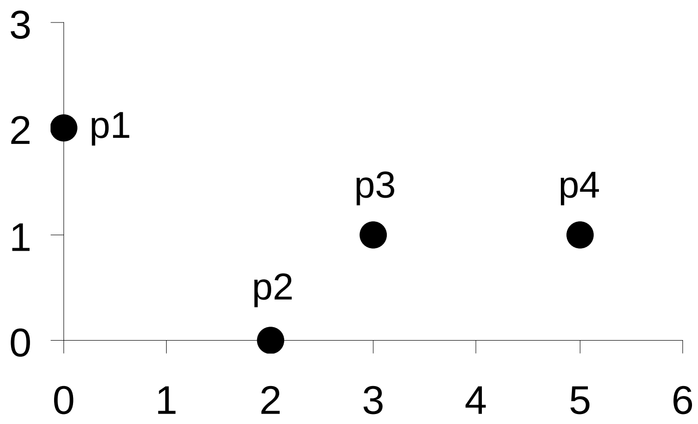
$$d(\mathbf{x}, \mathbf{y}) = \sqrt{|x_1 - y_1|^2 + |x_2 - y_2|^2 \cdots + |x_n - y_n|^2}$$

  – Do not confuse p with n, i.e., all these distances are defined based on all numbers of features (dimensions).

  – A generic measure: use appropriate p in different applications

Distance Measures

- Example: Manhatten and Euclidean distances



L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

Distance Matrix for Manhattan Distance

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

Data Matrix

L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix for Euclidean Distance

Distance Measures

- Cosine Measure (Similarity vs. Distance)

  For $\mathbf{x} = (x_1\ x_2 \cdots x_n)$ and $\mathbf{y} = (y_1\ y_2 \cdots y_n)$

$$\cos(\mathbf{x}, \mathbf{y}) = \frac{x_1 y_1 + \cdots + x_n y_n}{\sqrt{x_1^2 + \cdots + x_n^2}\sqrt{y_1^2 + \cdots + y_n^2}}$$

$$d(\mathbf{x}, \mathbf{y}) = 1 - \cos(\mathbf{x}, \mathbf{y})$$

  – Property: $0 \le d(\mathbf{x}, \mathbf{y}) \le 2$
  – Nonmetric vector objects: keywords in documents, gene features in micro-arrays, ...
  – Applications: information retrieval, biologic taxonomy, ...

Distance Measures

- Example: Cosine measure

$$\mathbf{x}_1 = (3, 2, 0, 5, 2, 0, 0),\ \mathbf{x}_2 = (1, 0, 0, 0, 1, 0, 2)$$

$$3\times1+2\times0+0\times0+5\times0+2\times1+0\times0+0\times2=5$$

$$\sqrt{3^2+2^2+0^2+5^2+2^2+0^2+0^2}=\sqrt{42}\approx 6.48$$

$$\sqrt{1^2+0^2+0^2+0^2+1^2+0^2+2^2}=\sqrt{6}\approx 2.45$$

$$\cos(\mathbf{x}_1,\mathbf{x}_2)=\frac{5}{6.48\times2.45}\approx 0.32$$

$$d(\mathbf{x}_1,\mathbf{x}_2)=1-\cos(\mathbf{x}_1,\mathbf{x}_2)=1-0.32=0.68$$

Distance Measures

- Distance for Binary Features
  - For binary features, their value can be converted into 1 or 0.
  - Contingency table for binary feature vectors, $\mathbf{x}$ and $\mathbf{y}$

		$\mathbf{y}$: 1	$\mathbf{y}$: 0
$\mathbf{x}$	1	a	b
	0	c	d

a : number of features that equal 1 for both $\mathbf{x}$ and $\mathbf{y}$

b : number of features that equal 1 for $\mathbf{x}$ but that are 0 for $\mathbf{y}$

c : number of features that equal 0 for $\mathbf{x}$ but that are 1 for $\mathbf{y}$

d : number of features that equal 0 for both $\mathbf{x}$ and $\mathbf{y}$

Distance Measures

- Distance for Binary Features
  - Distance for symmetric binary features

    Both of their states equally valuable and carry the same weight; i.e., no preference on which outcome should be coded as 1 or 0 , e.g. gender

$$d(\mathbf{x}, \mathbf{y}) = \frac{b + c}{a + b + c + d}$$

  - Distance for asymmetric binary features

    Outcomes of the states not equally important, e.g., the *positive* and *negative* outcomes of a disease test ; the rarest one is set to 1 and the other is 0.

$$d(\mathbf{x}, \mathbf{y}) = \frac{b + c}{a + b + c}$$

Distance Measures

- Example: Distance for binary features

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	**1**	**0**	**1**	**0**	**0**	**0**
Mary	F	**1**	**0**	**1**	**0**	**1**	**0**
Jim	M	**1**	**1**	**0**	**0**	**0**	**0**

- "Y": yes
- "P": positive
- "N": negative

  – gender is a symmetric feature (less important)
  – the remaining features are asymmetric binary
  – set the values "Y" and "P" to 1, and the value "N" to 0

	Mary	
Jack	2	0
	1	3

$$d(\text{Jack}, \text{Mary}) = \frac{0+1}{2+0+1} = 0.33$$

	Jim	
Jack	1	1
	1	3

$$d(\text{Jack}, \text{Jim}) = \frac{1+1}{1+1+1} = 0.67$$

	Mary	
Jim	1	1
	2	2

$$d(\text{Jim}, \text{Mary}) = \frac{1+2}{1+1+2} = 0.75$$

Distance Measures

- Distance for nominal features
  - A generalization of the binary feature so that it can take more than two states/values, e.g., red, yellow, blue, green, ...
  - There are two methods to handle variables of such features.
    - **Simple mis-matching**

$$d(\mathbf{x}, \mathbf{y}) = \frac{\text{number of mis-matching features between } \mathbf{x} \text{ and } \mathbf{y}}{\text{total number of features}}$$

    - **Convert it into binary variables**

creating new binary features for all of its nominal states

e.g., if an feature has three possible nominal states: red, yellow and blue, then this feature will be expanded into three binary features accordingly. Thus, distance measures for binary features are now applicable!

Distance Measures

- Distance for nominal features (cont.)
  - Example: Play tennis

	Outlook	Temperature	Humidity	Wind
D_1	010	100	10	10
D_2	100	100	01	10

- **Simple mis-matching**

$$d(D_1, D_2) = \frac{2}{4} = 0.5$$

- **Creating new binary features**
  - **Using the same number of bits as those features can take**

$$\text{Outlook} = \{\text{Sunny, Overcast, Rain}\} \Longrightarrow (100, 010, 001)$$

$$\text{Temperature} = \{\text{High, Mild, Cool}\} \Longrightarrow (100, 010, 001)$$

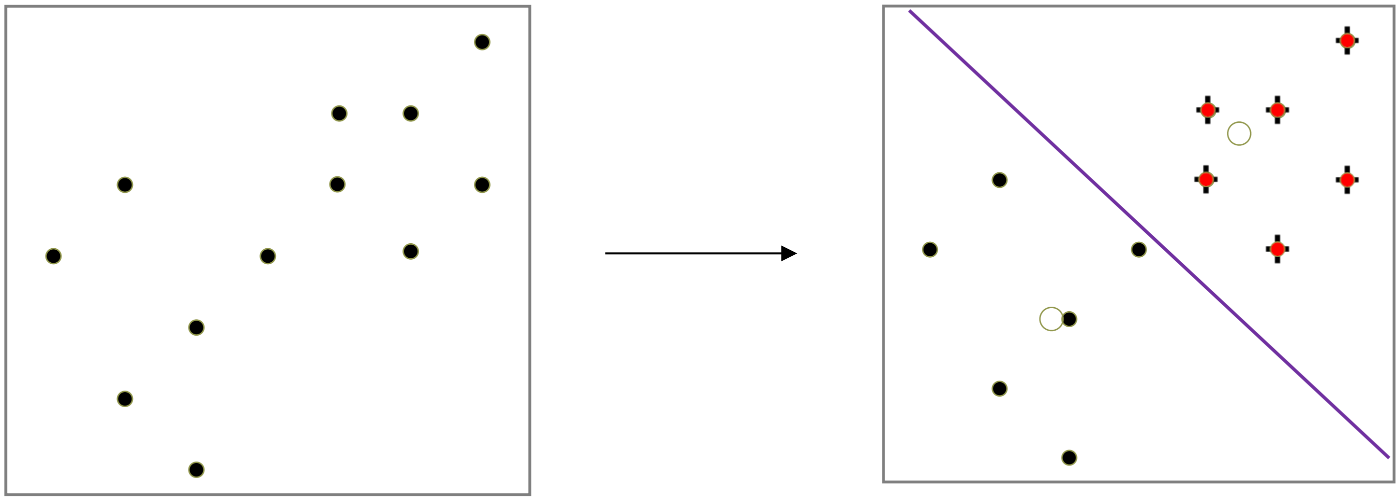
$$\text{Humidity} = \{\text{High, Normal}\} \Longrightarrow (10, 01)$$

$$\text{Wind} = \{\text{Strong, Weak}\} \Longrightarrow (10, 01)$$

$$d(D_1, D_2) = \frac{2+2}{10} = 0.4$$

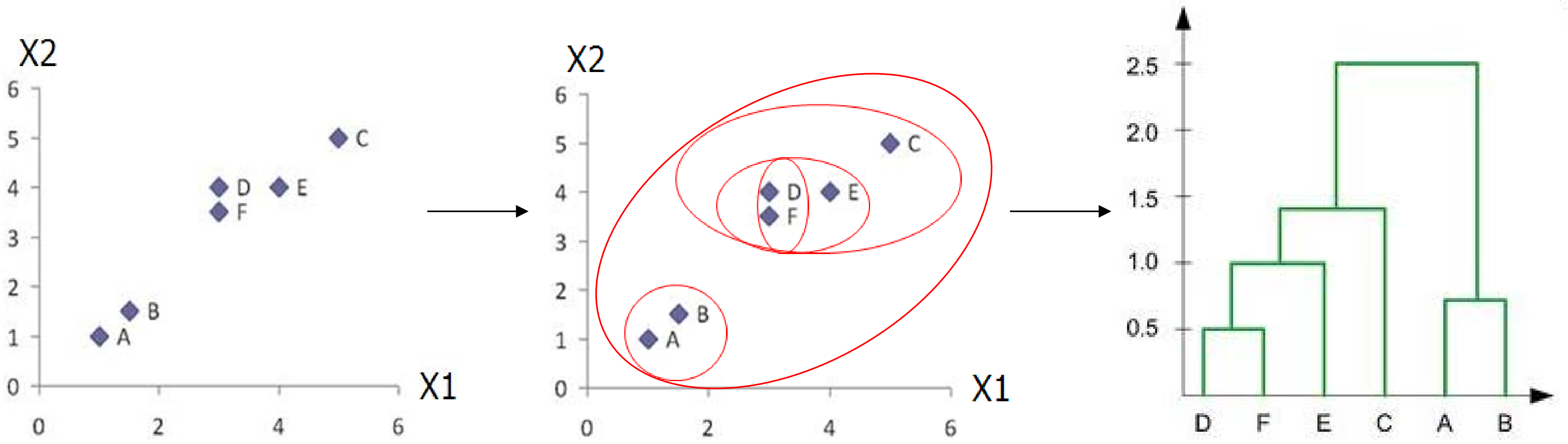
Major Clustering Approaches

- Partitioning approach
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square distance cost
  - Typical methods: k-means, k-medoids, CLARANS, ...



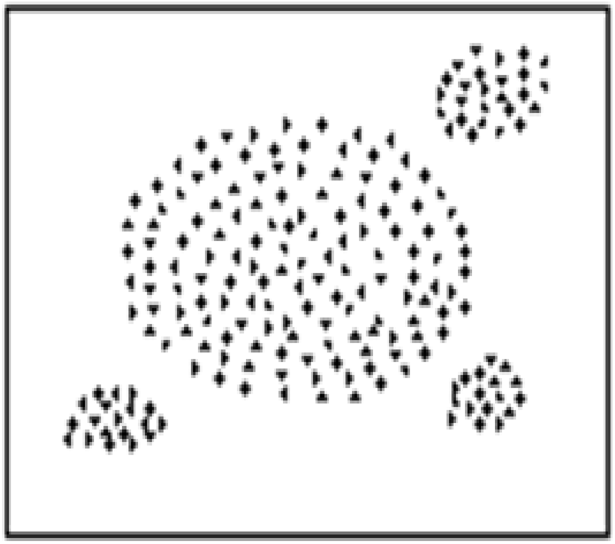
Major Clustering Approaches

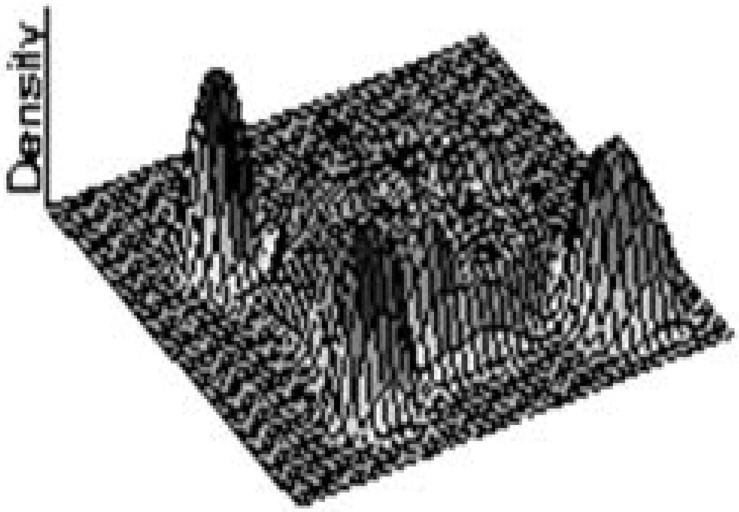
- Hierarchical approach
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Agglomerative, Diana, Agnes, BIRCH, ROCK, ...



Major Clustering Approaches

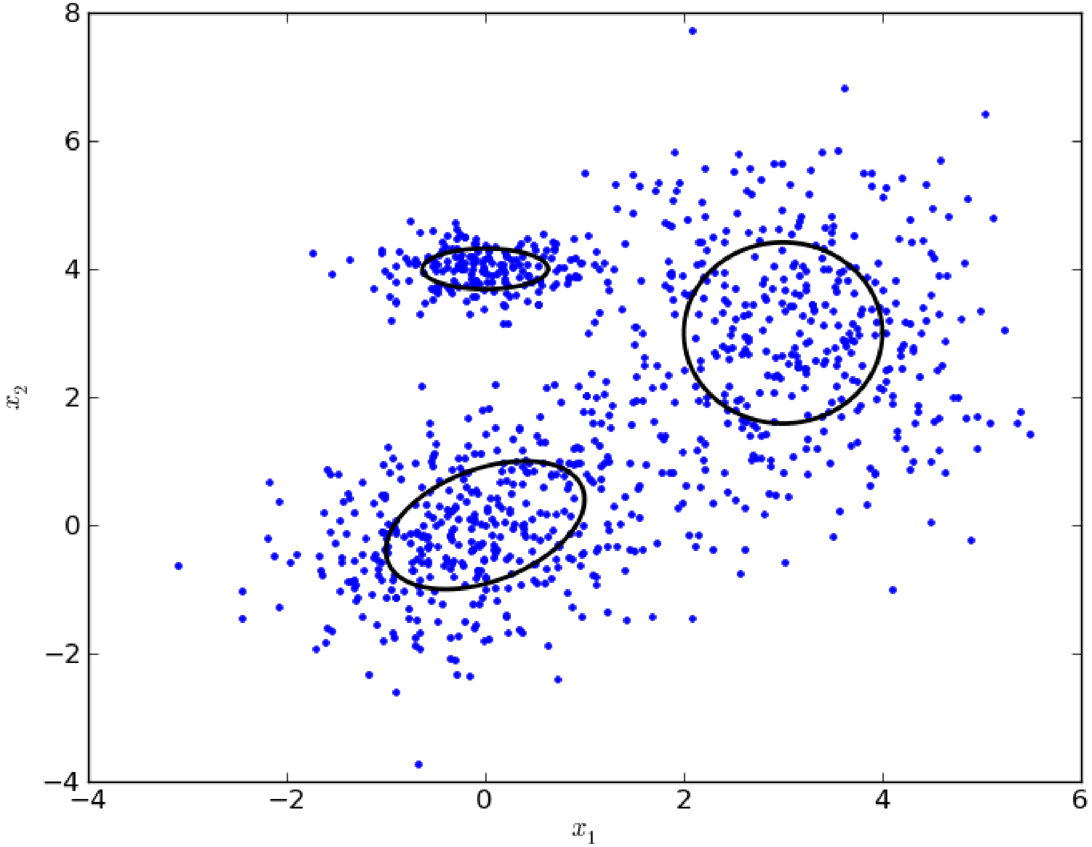
- Density-based approach
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue, ...





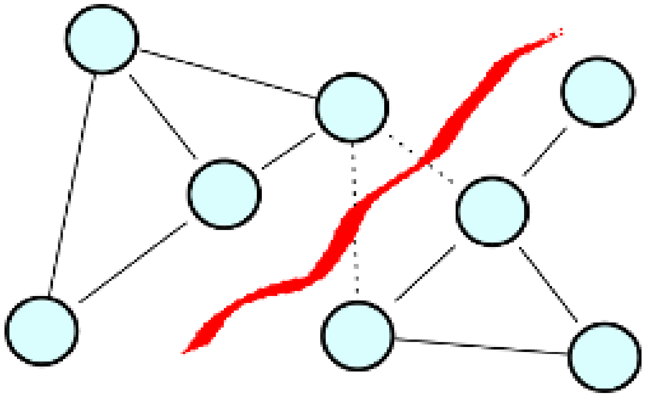
Major Clustering Approaches

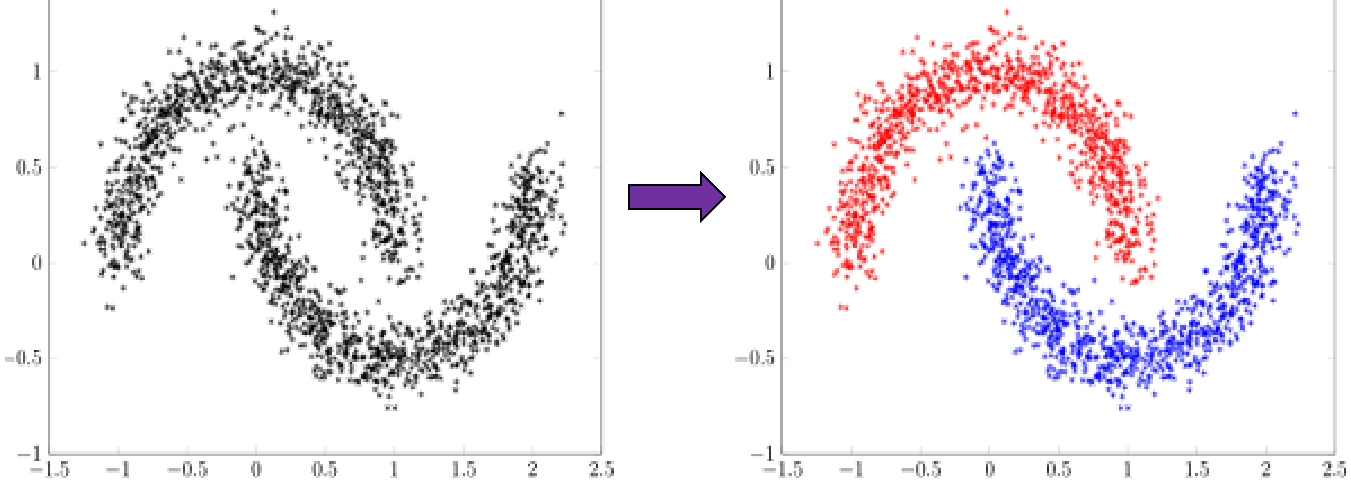
- Model-based approach
  - A generative model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: Gaussian Mixture Model (GMM), COBWEB, ...



Major Clustering Approaches

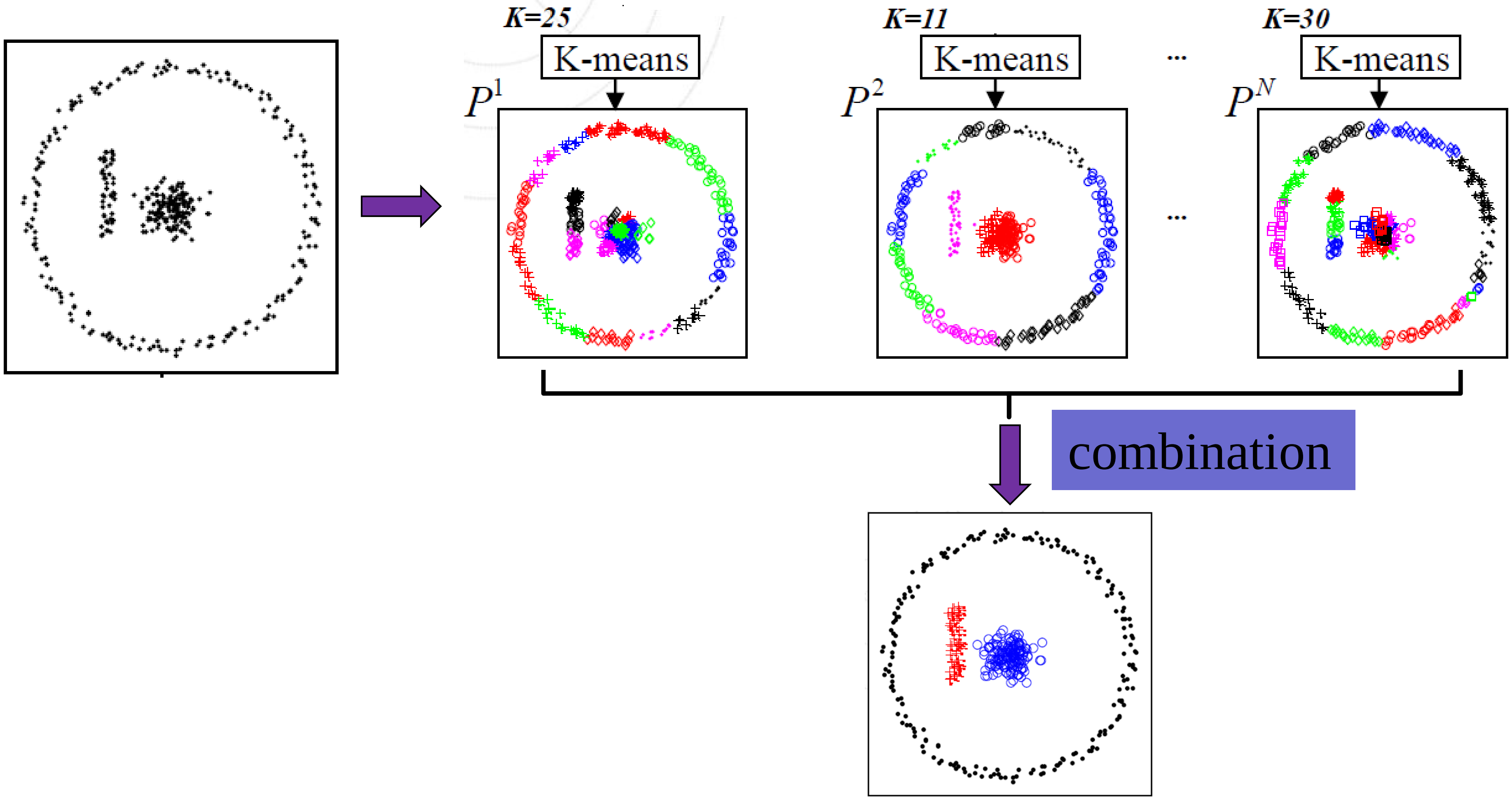
- Spectral clustering approach
  - Convert data set into weighted graph (vertex, edge), then cut the graph into sub-graphs corresponding to clusters via spectral analysis
  - Typical methods: Normalised-Cuts ......





Major Clustering Approaches

- Clustering ensemble approach
  - Combine multiple clustering results (different partitions)
  - Typical methods: Evidence-accumulation based, graph-based ……



MANCHESTER 1824

The University of Manchester

Summary

- Clustering analysis groups objects based on their (dis)similarity and has a broad range of applications.
- Measure of distance (or similarity) plays a critical role in clustering analysis and distance-based learning.
- Clustering algorithms can be categorized into partitioning, hierarchical, density-based, model-based, spectral clustering as well as ensemble approaches.
- There are still lots of research issues on cluster analysis;
  - finding the number of "natural" clusters with arbitrary shapes
  - dealing with mixed types of features
  - handling massive amount of data – Big Data
  - coping with data of high dimensionality
  - performance evaluation (especially when no ground-truth available)