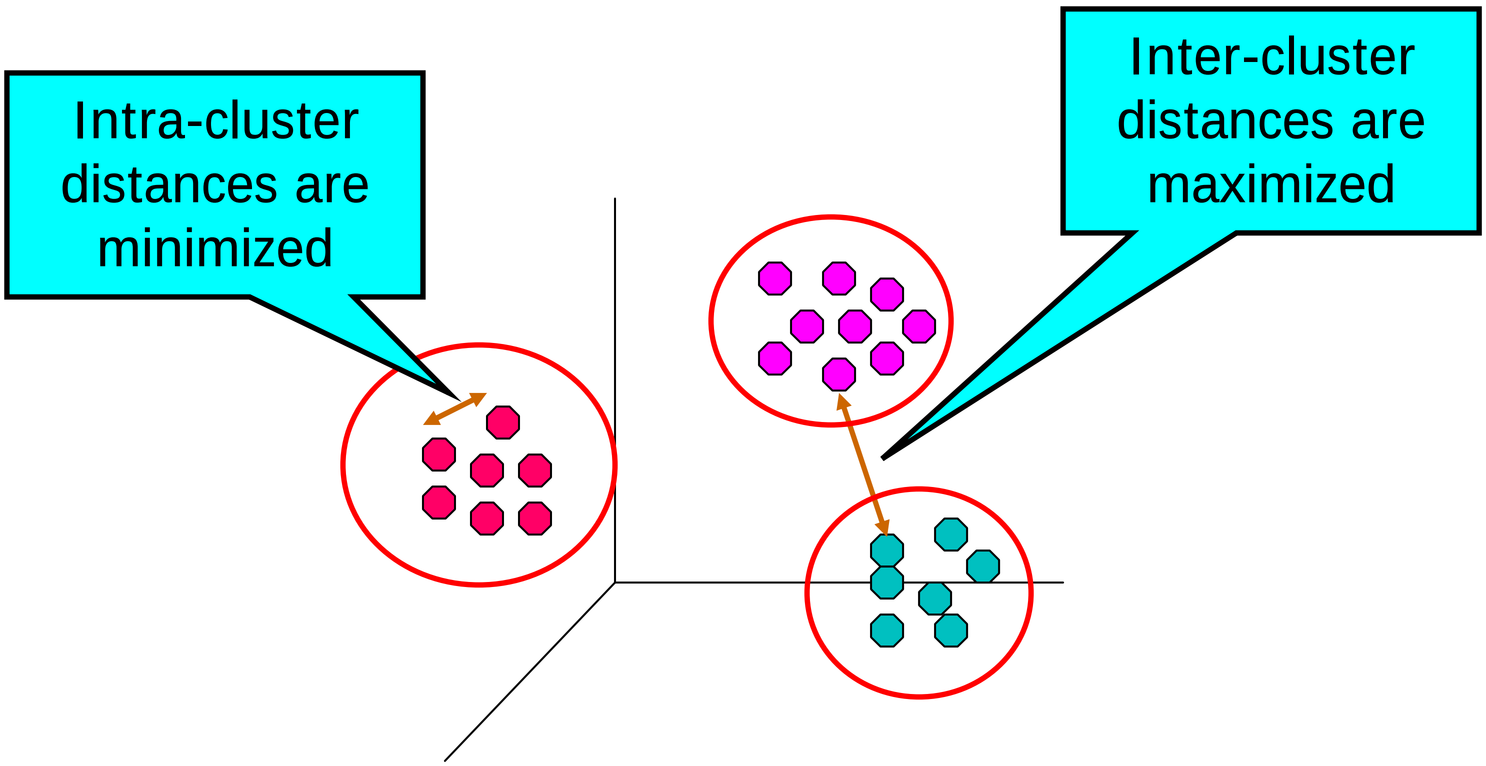
Lecture 14:

Cluster Analysis

What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups

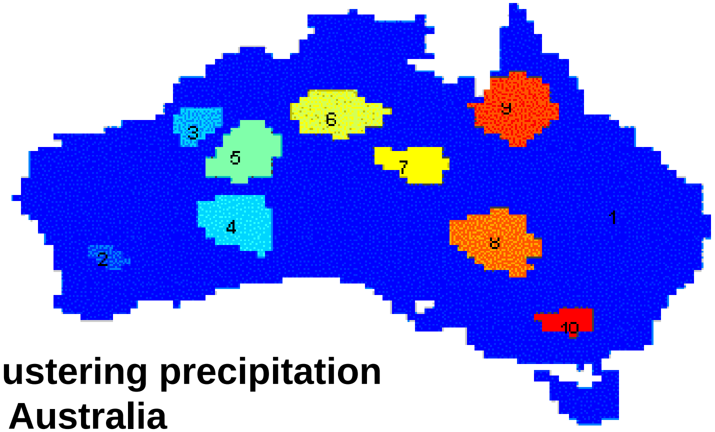


Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

	Discovered Clusters	*Industry Group*
1	Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP

- **Summarization**
  - Reduce the size of large data sets



Clustering precipitation in Australia

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

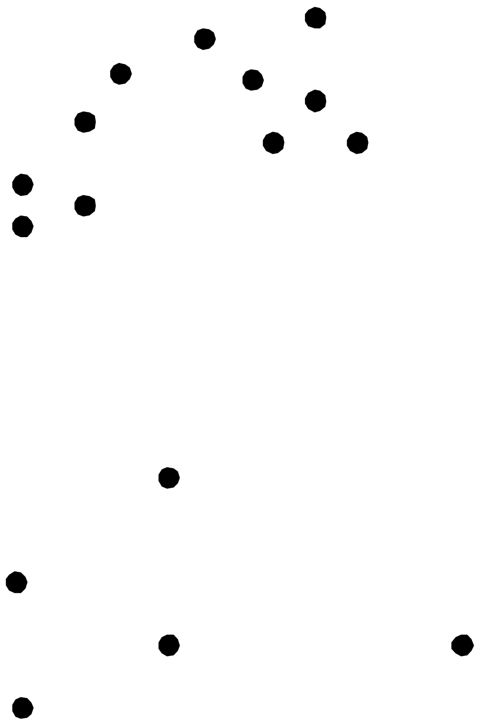
Two Clusters

Four Clusters

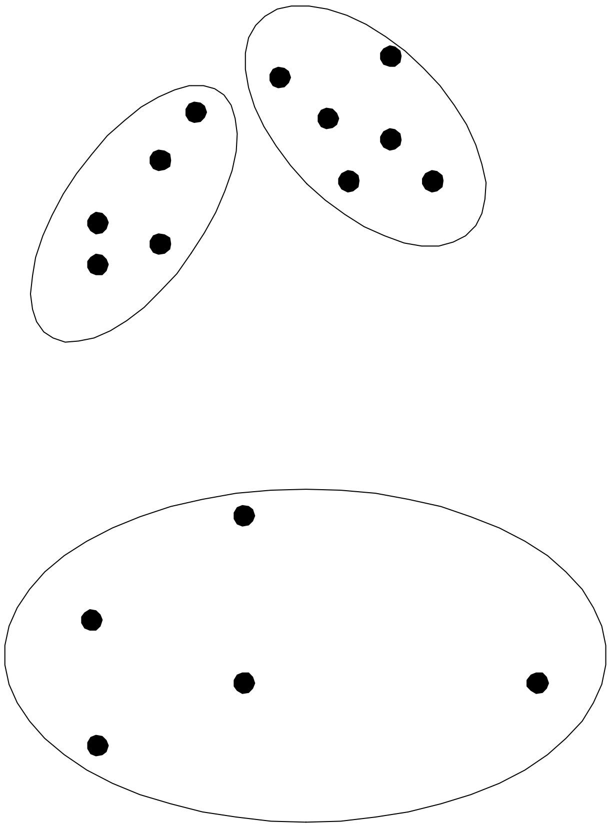
Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

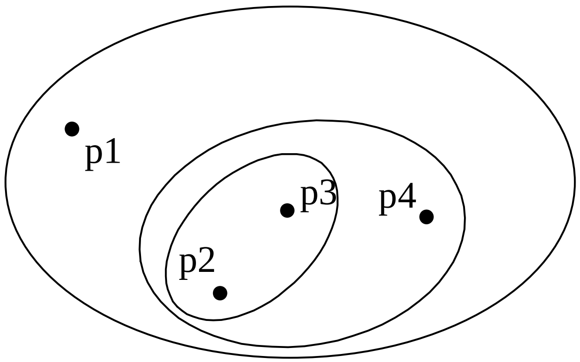


Original Points

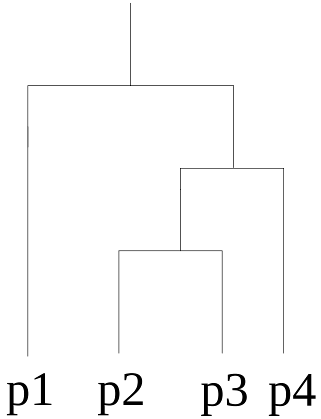


A Partitional Clustering

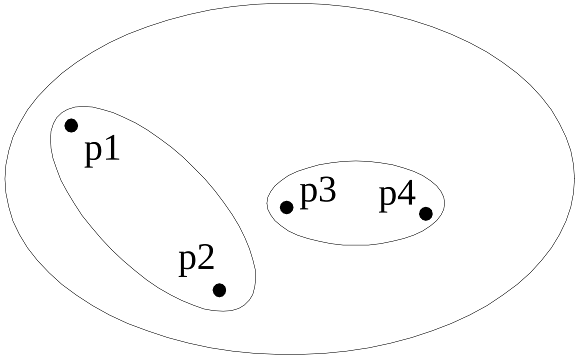
Hierarchical Clustering



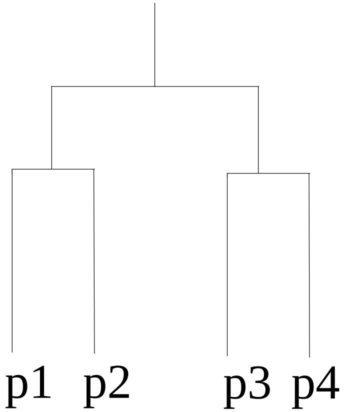
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

- Exclusive versus non-exclusive
  - In non-exclusive clusterings, points may belong to multiple clusters.
  - Can represent multiple classes or ‘border’ points
- Fuzzy versus non-fuzzy
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
  - Weights must sum to 1
  - Probabilistic clustering has similar characteristics
- Partial versus complete
  - In some cases, we only want to cluster some of the data

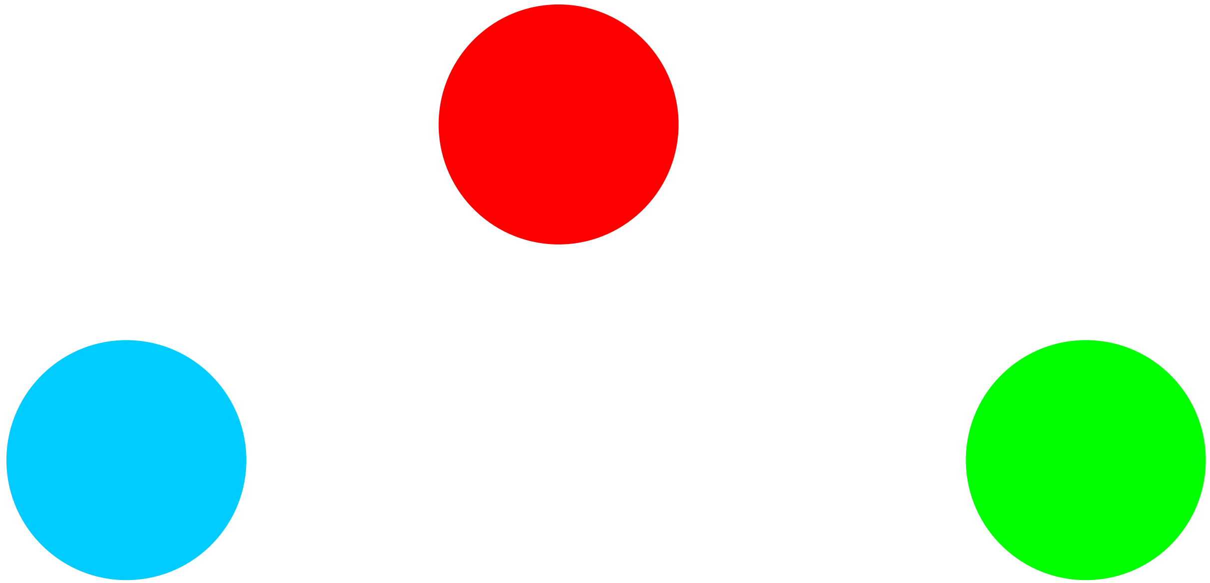
Elements of A Clustering Problem

- Input:
  - Almost any object can be clustered:
    - Continuous-valued data points in multi-dimensional space
    - People, with heterogeneous attributes (salary, age, sex, level of education, marital status, etc)
    - Time series
    - Sequences (Web click-streams, gene, events)
    - Graphs (XML structures, molecules, etc)
    - Patterns and Models (association rules, classification models, clusters of clusters, etc)
  - Similarity or dissimilarity measure

- Output:
  - A set of clusters:
    - well-separated clusters
    - center-based clusters
    - contiguous clusters
    - density-based clusters

Types of Clusters: Well-Separated

- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

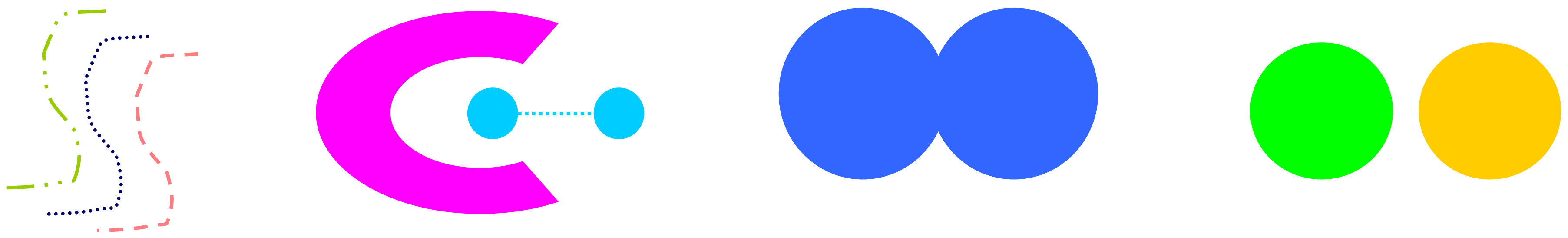
Types of Clusters: Center-Based

- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative" point of a cluster

4 center-based clusters

Types of Clusters: Contiguity-Based

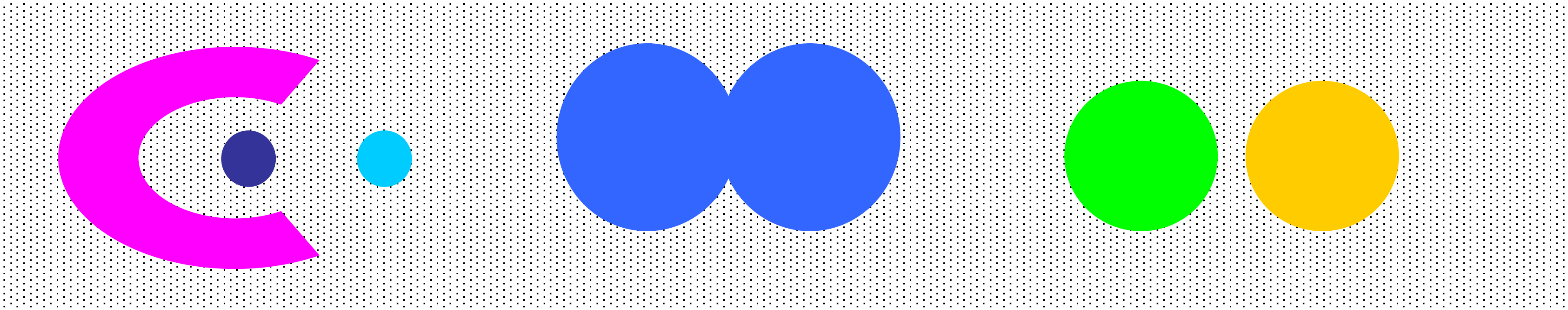
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters: Density-Based

- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Similarity and Dissimilarity

- Similarity
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity
  - Numerical measure of how different are two data objects
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

p and *q* are the attribute values for two data objects.

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Euclidean Distance

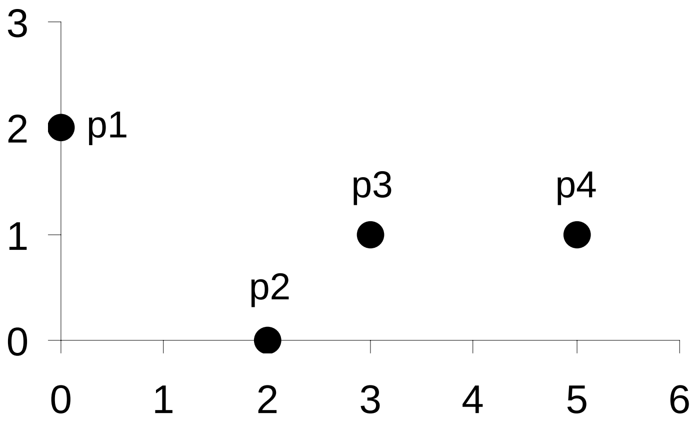
- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Where n is the number of dimensions (attributes) and p_k and q_k are, respectively, the k^th^ attributes (components) or data objects p and q.

- Standardization is necessary, if scales differ.

Euclidean Distance



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

	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

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

Where r is a parameter, n is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L_1 norm) distance.
  - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- $r = 2$. Euclidean distance
- $r \to \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors
- Do not confuse *r* with *n*, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance

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

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

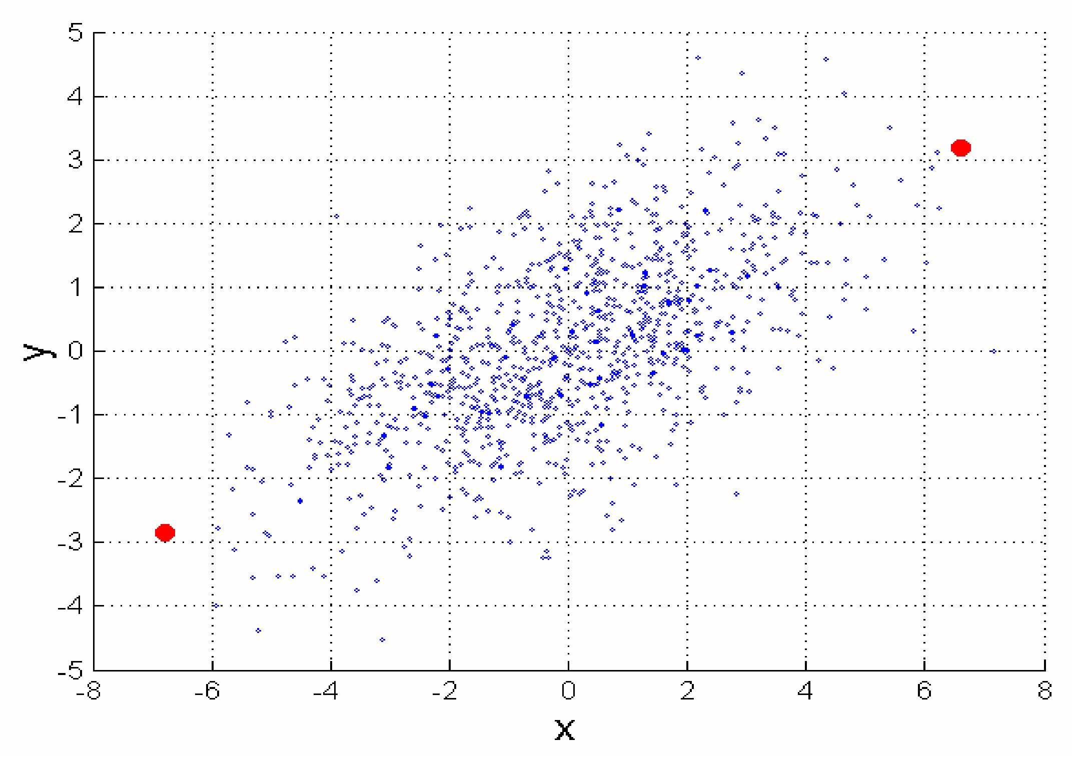
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

L_∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

Mahalanobis Distance

$$mahalanobis(p,q) = (p-q)\Sigma^{-1}(p-q)^T$$

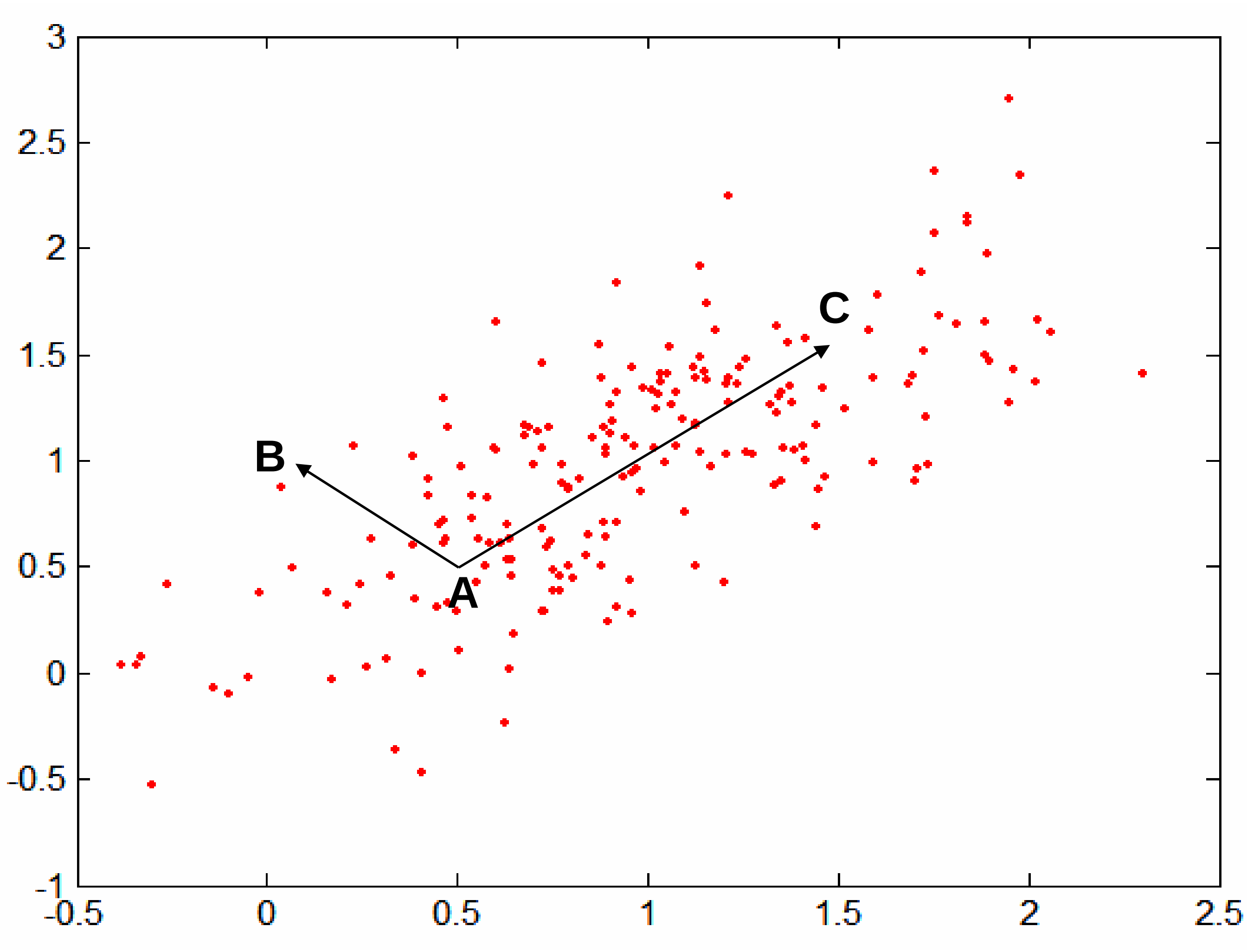


Σ is the covariance matrix of the input data X

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij} - \overline{X}_j)(X_{ik} - \overline{X}_k)$$

For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Mahalanobis Distance



Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well known properties.

  1. $d(p, q) \geq 0$ for all p and q and $d(p, q) = 0$ only if $p = q$. (Positive definiteness)
  2. $d(p, q) = d(q, p)$ for all p and q. (Symmetry)
  3. $d(p, r) \leq d(p, q) + d(q, r)$ for all points p, q, and r. (Triangle Inequality)

  where $d(p, q)$ is the distance (dissimilarity) between points (data objects), p and q.

- A distance that satisfies these properties is a metric

Common Properties of a Similarity

- Similarities, also have some well known properties.

  1. $s(p, q) = 1$ (or maximum similarity) only if $p = q$.
  2. $s(p, q) = s(q, p)$ for all p and q. (Symmetry)

  where $s(p, q)$ is the similarity between points (data objects), p and q.

Similarity Between Binary Vectors

- Common situation is that objects, *p* and *q*, have only binary attributes

- Compute similarities using the following quantities

  M_{01} = the number of attributes where p was 0 and q was 1

  M_{10} = the number of attributes where p was 1 and q was 0

  M_{00} = the number of attributes where p was 0 and q was 0

  M_{11} = the number of attributes where p was 1 and q was 1

- Simple Matching and Jaccard Coefficients

  SMC = number of matches / number of attributes

  $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})$

  J = number of 11 matches / number of not-both-zero attributes values

  $= (M_{11}) / (M_{01} + M_{10} + M_{11})$

SMC versus Jaccard: Example

$p =$ 1 0 0 0 0 0 0 0 0 0

$q =$ 0 0 0 0 0 0 1 0 0 1

$M_{01} = 2$ (the number of attributes where p was 0 and q was 1)

$M_{10} = 1$ (the number of attributes where p was 1 and q was 0)

$M_{00} = 7$ (the number of attributes where p was 0 and q was 0)

$M_{11} = 0$ (the number of attributes where p was 1 and q was 1)

$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$

$J = (M_{11}) / (M_{01} + M_{10} + M_{11}) = 0 / (2 + 1 + 0) = 0$

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

$$\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1|| \, ||d_2|| \,,$$

where $\bullet$ indicates vector dot product and $|| d ||$ is the length of vector d.

- Example:

d_1 = **3 2 0 5 0 0 0 2 0 0**

d_2 = **1 0 0 0 0 0 0 1 0 2**

$d_1 \bullet d_2$= 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5

$||d_1||$ = $(3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5}$ = $(42)^{0.5}$ = 6.481

$||d_2||$ = $(1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5}$ = $(6)^{0.5}$ = 2.245

$\cos(d_1, d_2) = .3150$

Extended Jaccard Coefficient (Tanimoto)

- Variation of Jaccard for continuous or count attributes
  - Reduces to Jaccard for binary attributes

$$T(p,q) = \frac{p \bullet q}{\|p\|^2 + \|q\|^2 - p \bullet q},$$