Clustering

Part 1

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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.
  - Based on information found in the data that describes the objects and their relationships.
  - Also known as unsupervised classification.
- Many applications
  - Understanding: group related documents for browsing or to find genes and proteins that have similar functionality.
  - Summarization: Reduce the size of large data sets.

What is not Cluster Analysis?

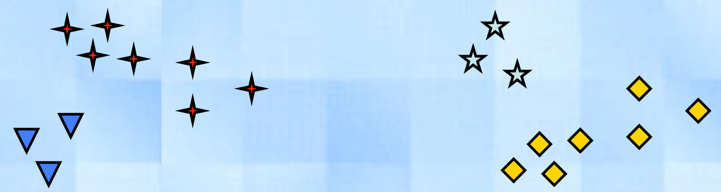
- Supervised classification.
  - Have class label information.
- Simple segmentation.
  - Dividing students into different registration groups alphabetically, by last name.
- Results of a query.
  - Groupings are a result of an external specification.
- Graph partitioning
  - Some mutual relevance and synergy, but areas are not identical.

Notion of a Cluster is Ambiguous

Initial points.

Six Clusters

Two Clusters

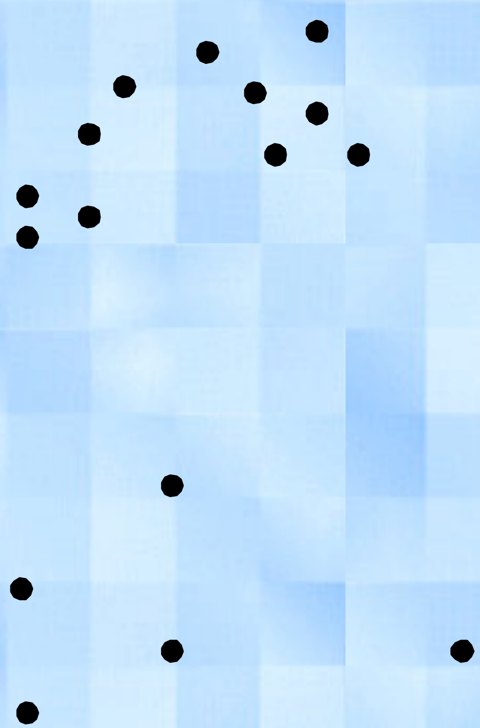


Four Clusters

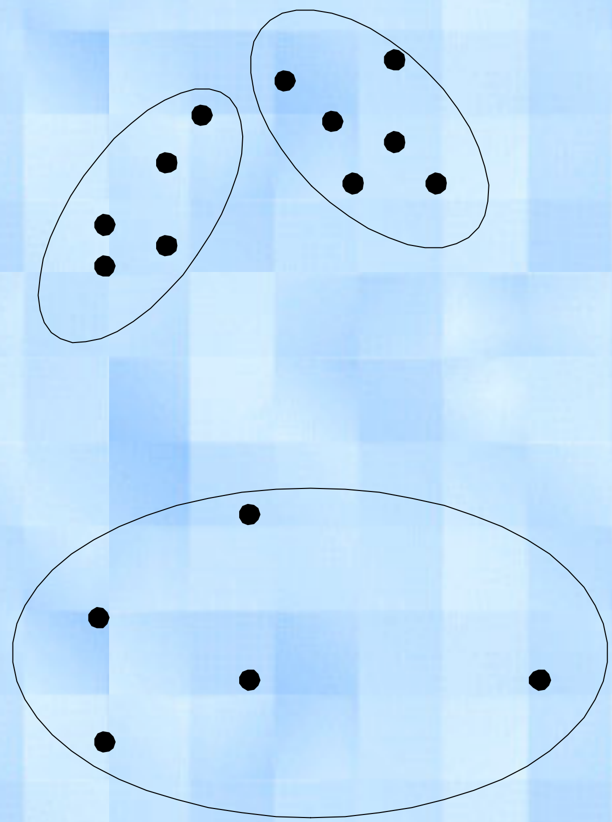
Types of Clusterings

- A *clustering* is a set of clusters.
- One important distinction is 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

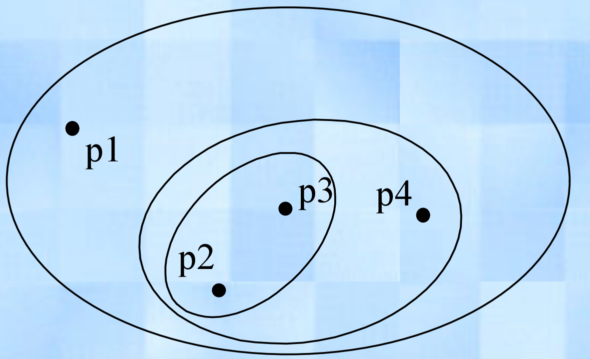


Original Points

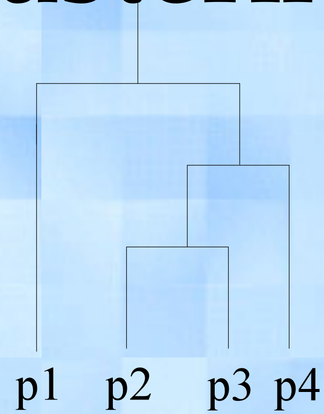


A Partitional Clustering

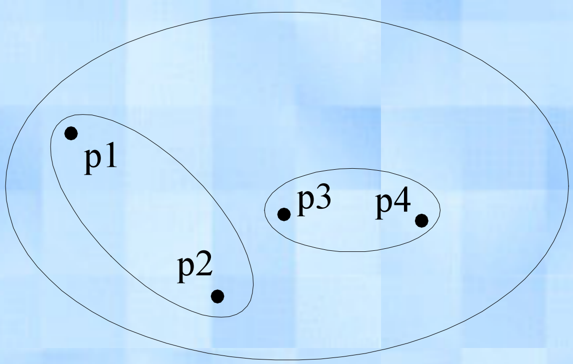
Hierarchical Clustering



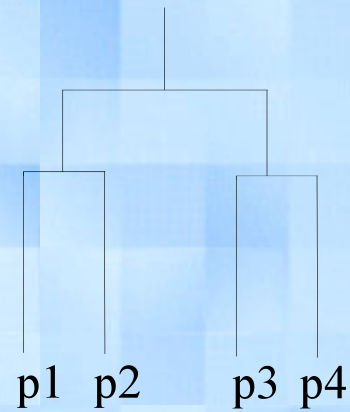
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



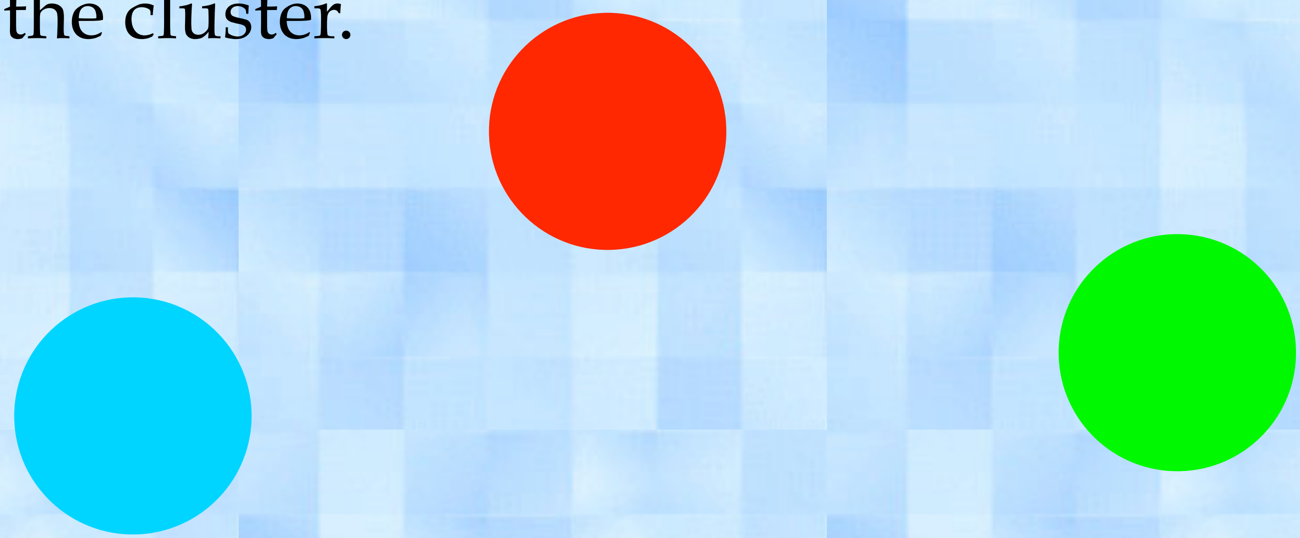
Non-traditional Dendrogram

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 clusterings, 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.

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.



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.

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.

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.
  - The three curves don’t form clusters since they fade into the noise, as does the bridge between the two small circular 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 two data objects are.
  - Is lower when objects are more alike.
  - Minimum dissimilarity is often 0.
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Summary of 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	$d = \frac{\|p-q\|}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\|p-q\|}{n-1}$
Interval or Ratio	$d = \|p - q\|$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Euclidean Distance

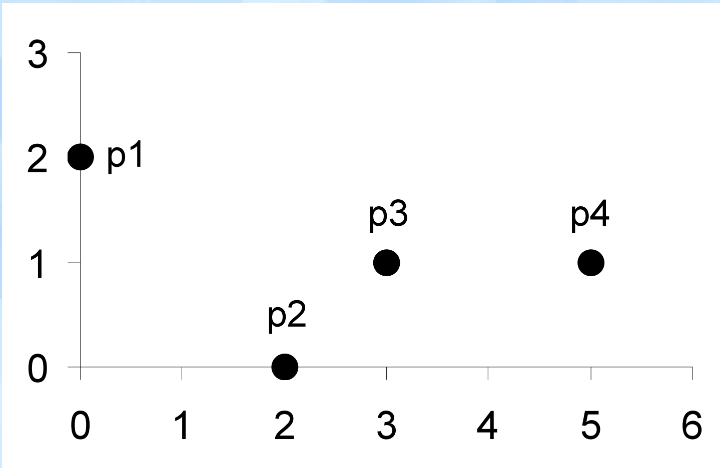
- Euclidean Distance

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

  - 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 k^{th} 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.
- $r \rightarrow \infty$. "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

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 • 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**

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

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

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

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

Correlation

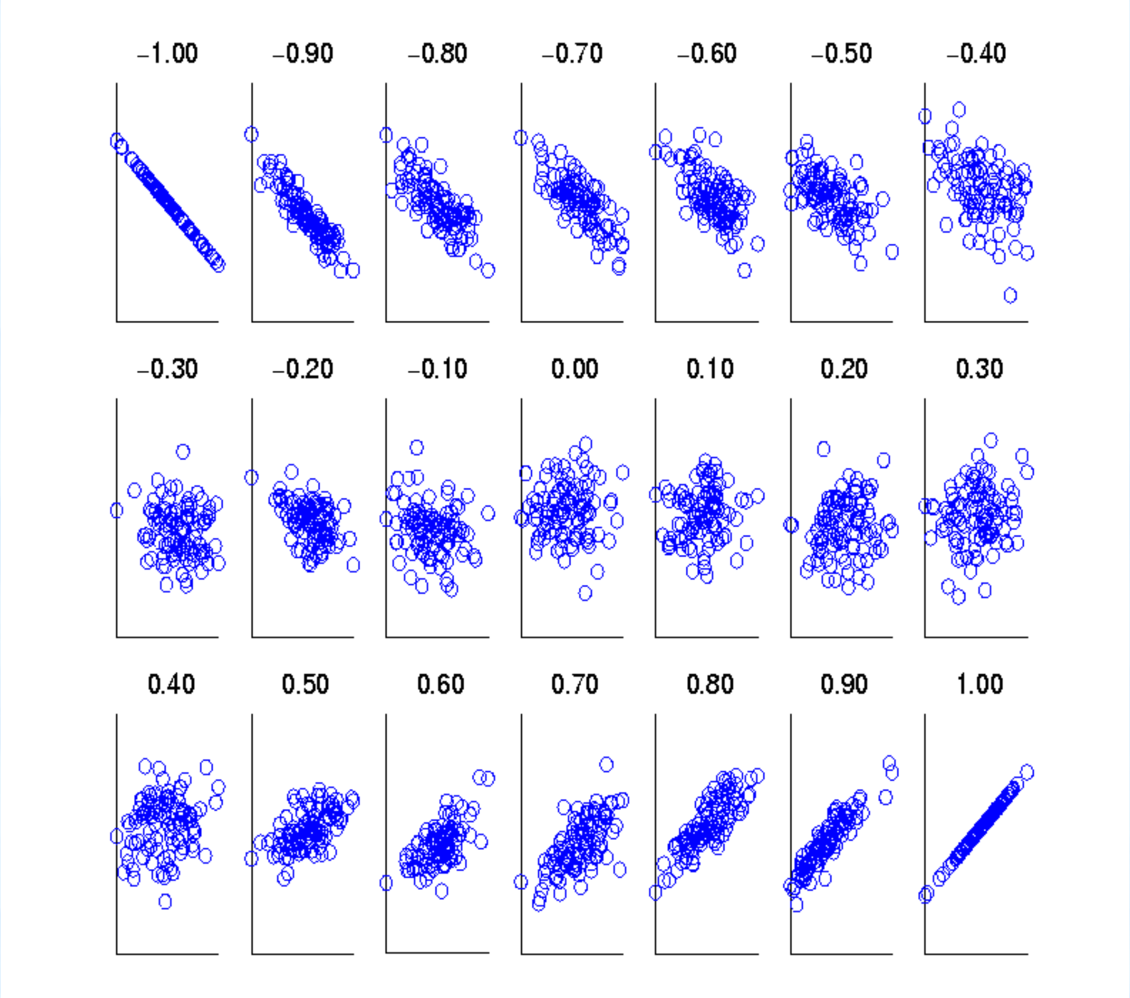
- Correlation measure the linear relationship between objects.
- To compute correlation, we standardize data objects, *p* and *q*, and then take the dot product.

$$p'_k = (p_k - mean(p)) / std(p)$$

$$q'_k = (q_k - mean(q)) / std(q)$$

$$correlation(p, q) = p' \bullet q'$$

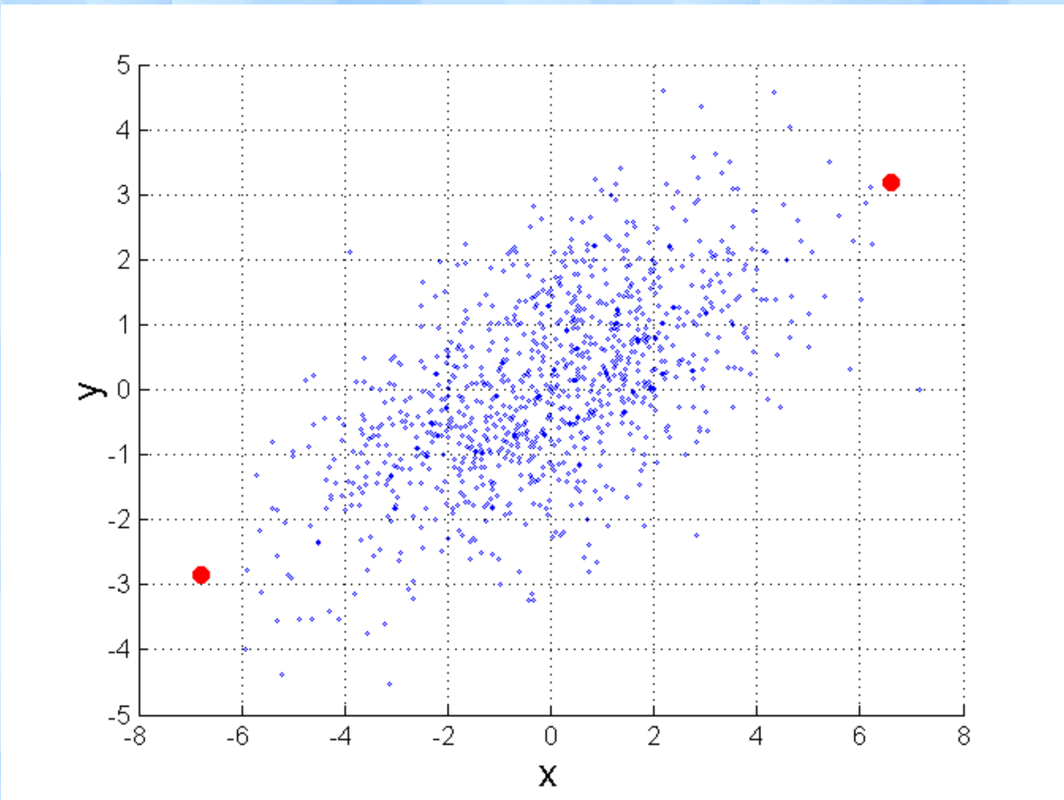
Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1

Mahalanobis Distance

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



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

A General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1. For the k^{th} attribute, compute a similarity, s_k, in the range $[0, 1]$.

2. Define an indicator variable, δ_k, for the k_{th} attribute as follows:

$$\delta_k = \begin{cases} 0 & \text{if the } k^{th} \text{ attribute is a binary asymmetric attribute and both objects have} \\ & \text{a value of } 0\text{, or if one of the objects has a missing values for the } k^{th} \text{ attribute} \\ 1 & \text{otherwise} \end{cases}$$

3. Compute the overall similarity between the two objects using the following formula:

$$similarity(p, q) = \frac{\sum_{k=1}^{n} \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use weights w_k which are between 0 and 1 and sum to 1.

$$similarity(p,q) = \frac{\sum_{k=1}^{n} w_k \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

$$distance(p,q) = \left(\sum_{k=1}^{n} w_k |p_k - q_k|^r \right)^{1/r}$$