Unsupervised Learning

Slides are taken from Dr. Bing Liu, UIC

Road map

Supervised learning vs. unsupervised learning

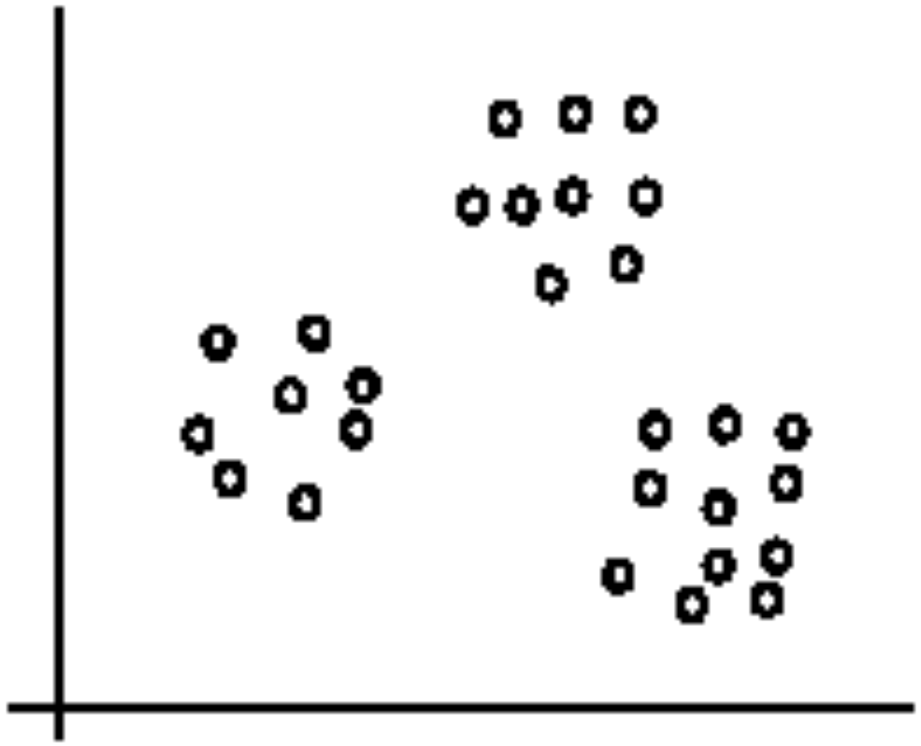
- Supervised learning: discover patterns in the data that relate data attributes with a target (class) attribute.
  - These patterns are then utilized to predict the values of the target attribute in future data instances.
- Unsupervised learning: The data have no target attribute.
  - We want to explore the data to find some intrinsic structures in them.

Clustering

- Clustering is a technique for finding similarity groups in data, called **clusters**. I.e.,
  - it groups data instances that are similar to (near) each other in one cluster and data instances that are very different (far away) from each other into different clusters.
- Clustering is often called an **unsupervised learning** task as no class values denoting an *a priori* grouping of the data instances are given, which is the case in supervised learning.
- Due to historical reasons, clustering is often considered synonymous with unsupervised learning.
  - In fact, association rule mining is also unsupervised
- This chapter focuses on clustering.

An illustration

- The data set has three natural groups of data points, i.e., 3 natural clusters.



What is clustering for?

- Let us see some real-life examples
- Example 1: groups people of similar sizes together to make “small”, “medium” and “large” T-Shirts.
    - Tailor-made for each person: too expensive
    - One-size-fits-all: does not fit all.
- Example 2: In marketing, segment customers according to their similarities
    - To do targeted marketing.

What is clustering for? (cont…)

- Example 3: Given a collection of text documents, we want to organize them according to their content similarities,
  - To produce a topic hierarchy
- In fact, clustering is one of the most utilized data mining techniques.
  - It has a long history, and used in almost every field, e.g., medicine, psychology, botany, sociology, biology, archeology, marketing, insurance, libraries, etc.
  - In recent years, due to the rapid increase of online documents, text clustering becomes important.

Aspects of clustering

- A clustering algorithm
  - Partitional clustering
  - Hierarchical clustering
  - …
- A distance (similarity, or dissimilarity) function
- Clustering quality
  - Inter-clusters distance $\Rightarrow$ maximized
  - Intra-clusters distance $\Rightarrow$ minimized
- The quality of a clustering result depends on the algorithm, the distance function, and the application.

Road map

- Basic concepts
- K-means algorithm
- Representation of clusters
- Hierarchical clustering
- Distance functions
- Data standardization
- Handling mixed attributes
- Which clustering algorithm to use?
- Cluster evaluation
- Discovering holes and data regions
- Summary

K-means clustering

- K-means is a partitional clustering algorithm
- Let the set of data points (or instances) *D* be

  $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$,

  where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ir})$ is a vector in a real-valued space $X \subseteq R^r$, and *r* is the number of attributes (dimensions) in the data.
- The *k*-means algorithm partitions the given data into *k* clusters.
  - Each cluster has a cluster **center**, called **centroid**.
  - *k* is specified by the user

K-means algorithm

- Given *k*, the *k-means* algorithm works as follows:
  1) Randomly choose *k* data points (seeds) to be the initial centroids, cluster centers
  2) Assign each data point to the closest centroid
  3) Re-compute the centroids using the current cluster memberships.
  4) If a convergence criterion is not met, go to 2).

K-means algorithm – (cont …)

```
Algorithm k-means(k, D)
  Choose k data points as the initial centroids (cluster centers)
  repeat
      for each data point x ∈ D do
          compute the distance from x to each centroid;
          assign x to the closest centroid          // a centroid represents a cluster
      endfor
      re-compute the centroids using the current cluster memberships
  until the stopping criterion is met
```

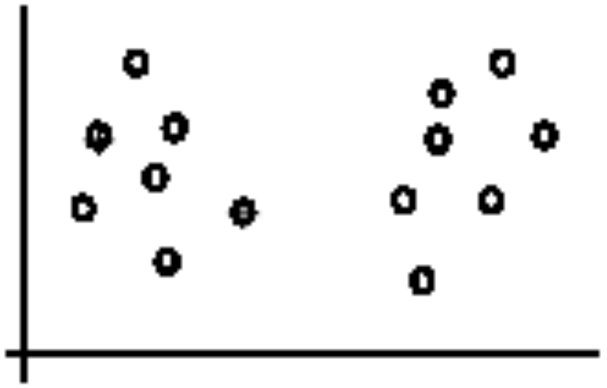
Stopping/convergence criterion

1. no (or minimum) re-assignments of data points to different clusters,
2. no (or minimum) change of centroids, or
3. minimum decrease in the **sum of squared error** (SSE),

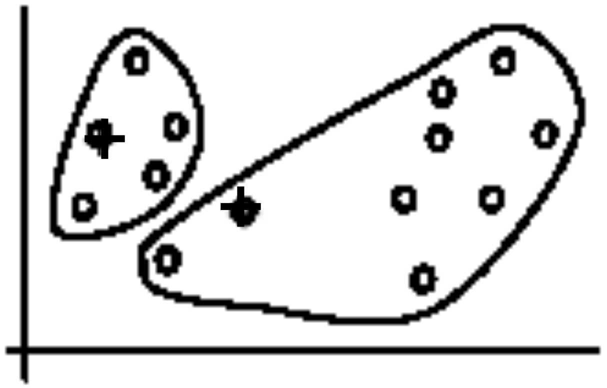
$$SSE = \sum_{j=1}^{k} \sum_{\mathbf{x} \in C_j} dist(\mathbf{x}, \mathbf{m}_j)^2 \qquad (1)$$

- C_i is the jth cluster, $\mathbf{m}_j$ is the centroid of cluster C_j (the mean vector of all the data points in C_j), and *dist*($\mathbf{x}$, $\mathbf{m}_j$) is the distance between data point $\mathbf{x}$ and centroid $\mathbf{m}_j$.

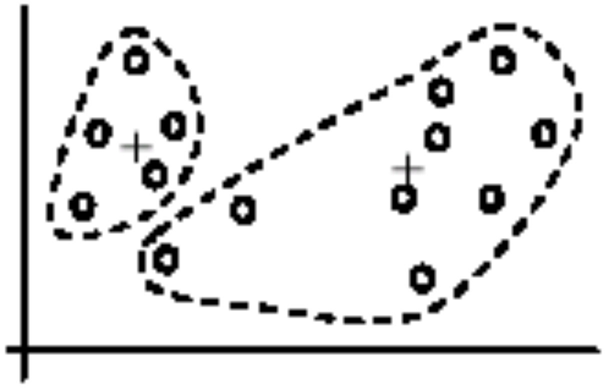
An example



(A). Random selection of *k* centers

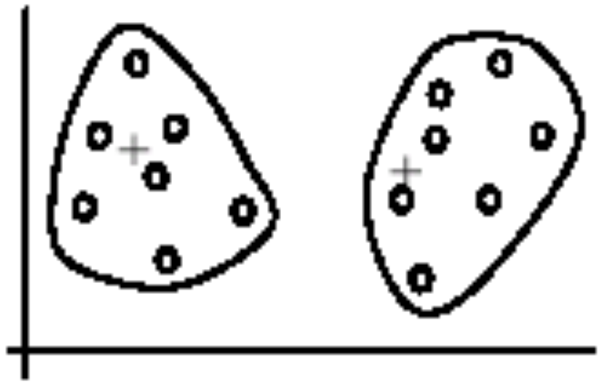


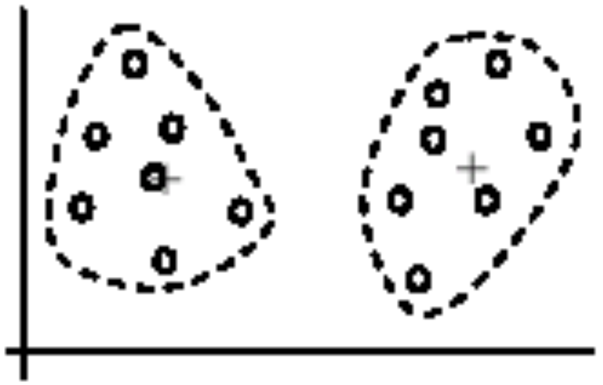
Iteration 1: (B). Cluster assignment

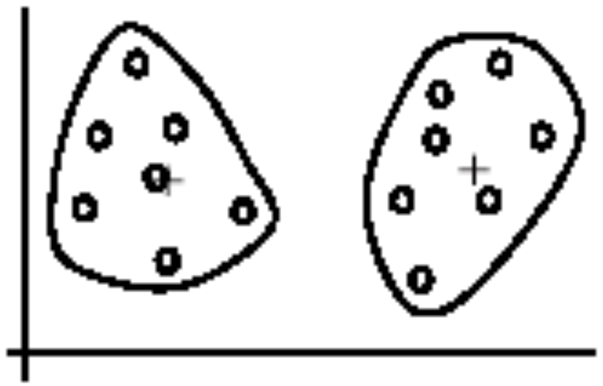


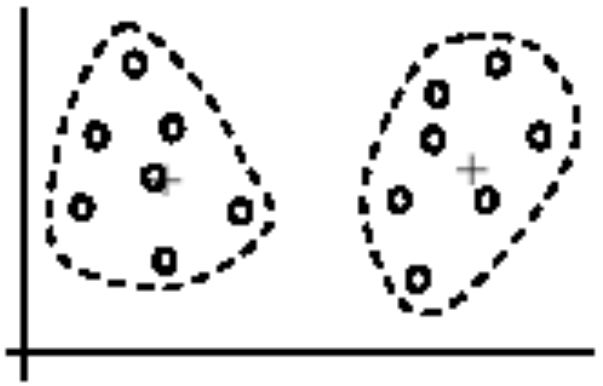
(C). Re-compute centroids

An example (cont …)


Iteration 2: (D). Cluster assignment


(E). Re-compute centroids


Iteration 3: (F). Cluster assignment


(G). Re-compute centroids

An example distance function

The *k*-means algorithm can be used for any application data set where the **mean** can be defined and computed. In the **Euclidean space**, the mean of a cluster is computed with:

$$\mathbf{m}_j = \frac{1}{|C_j|} \sum_{\mathbf{x}_i \in C_j} \mathbf{x}_i \qquad (2)$$

where $|C_j|$ is the number of data points in cluster C_j. The distance from one data point $\mathbf{x}_i$ to a mean (centroid) $\mathbf{m}_j$ is computed with

$$\begin{aligned} dist(\mathbf{x}_i, \mathbf{m}_j) &= \| \mathbf{x}_i - \mathbf{m}_j \| \\ &= \sqrt{(x_{i1} - m_{j1})^2 + (x_{i2} - m_{j2})^2 + \ldots + (x_{ir} - m_{jr})^2} \end{aligned} \qquad (3)$$

Strengths of k-means

- Strengths:
  - Simple: easy to understand and to implement
  - Efficient: Time complexity: $O(tkn)$,

    where n is the number of data points,

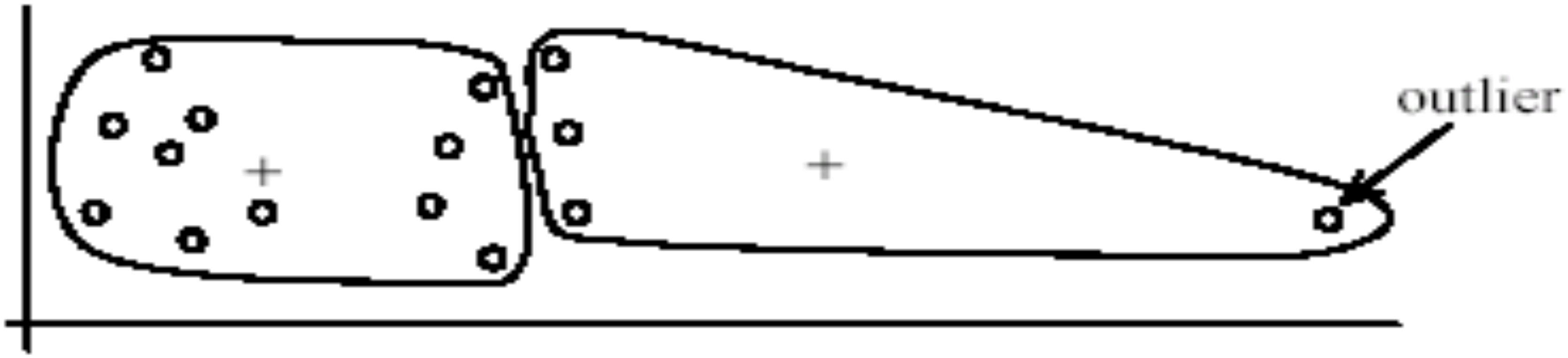
    k is the number of clusters, and

    t is the number of iterations.
  - Since both k and t are small. k-means is considered a linear algorithm.
- K-means is the most popular clustering algorithm.
- Note that: it terminates at a local optimum if SSE is used. The global optimum is hard to find due to complexity.

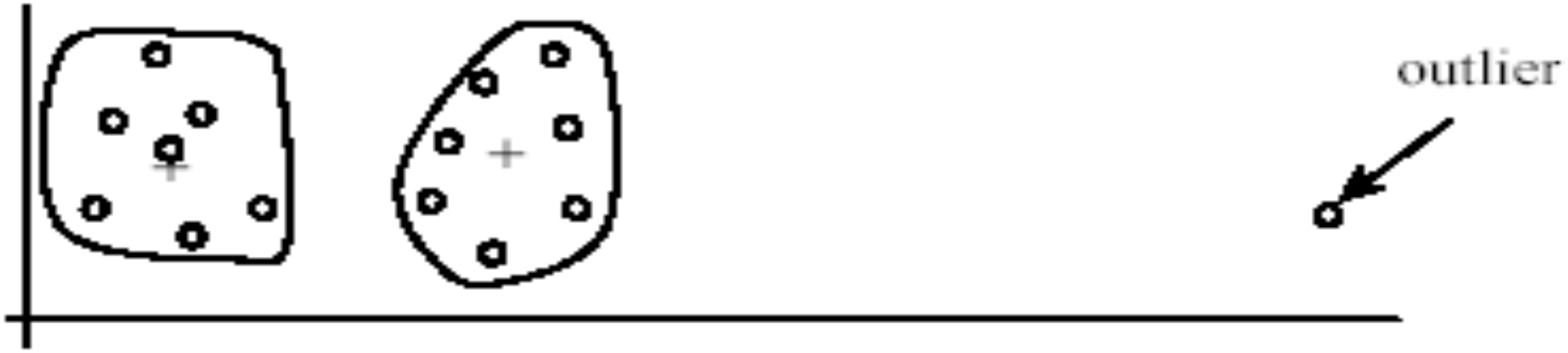
Weaknesses of k-means

- The algorithm is only applicable if the mean is defined.
    - For categorical data, *k*-mode - the centroid is represented by most frequent values.
- The user needs to specify *k*.
- The algorithm is sensitive to **outliers**
    - Outliers are data points that are very far away from other data points.
    - Outliers could be errors in the data recording or some special data points with very different values.

Weaknesses of k-means: Problems with outliers



(A): Undesirable clusters



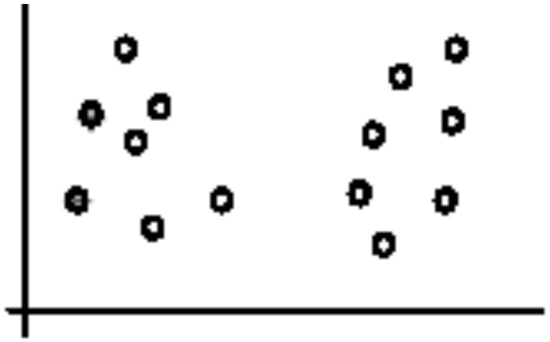
(B): Ideal clusters

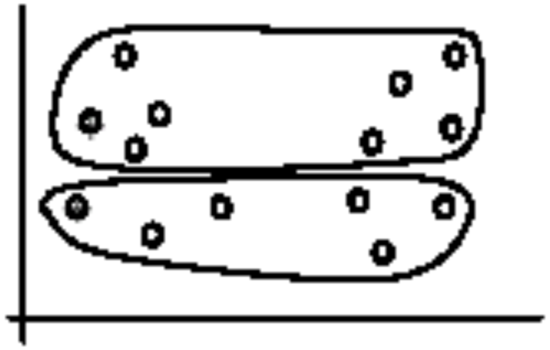
Weaknesses of k-means: To deal with outliers

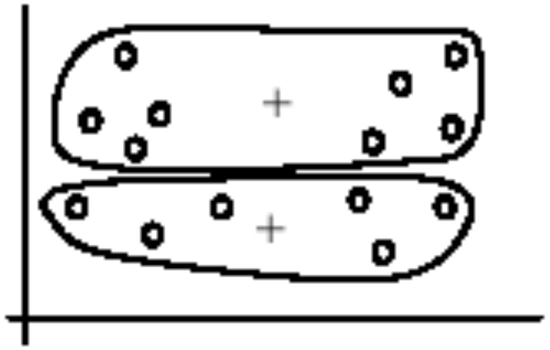
- One method is to remove some data points in the clustering process that are much further away from the centroids than other data points.
  - To be safe, we may want to monitor these possible outliers over a few iterations and then decide to remove them.
- Another method is to perform random sampling. Since in sampling we only choose a small subset of the data points, the chance of selecting an outlier is very small.
  - Assign the rest of the data points to the clusters by distance or similarity comparison, or classification

Weaknesses of k-means (cont …)

- The algorithm is sensitive to initial seeds.

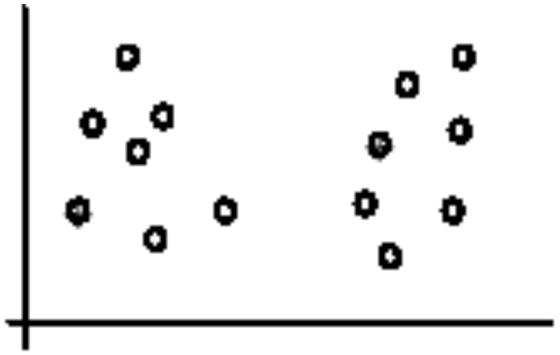

(A). Random selection of seeds (centroids)


(B). Iteration 1


(C). Iteration 2

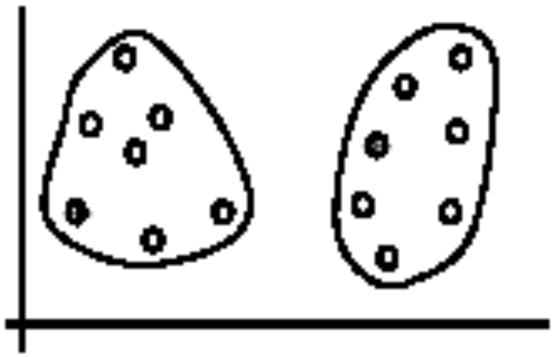
Weaknesses of k-means (cont …)

- If we use different seeds: good results

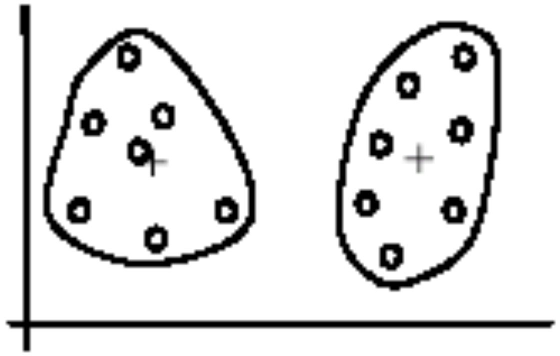


(A). Random selection of k seeds (centroids)

- There are some methods to help choose good seeds



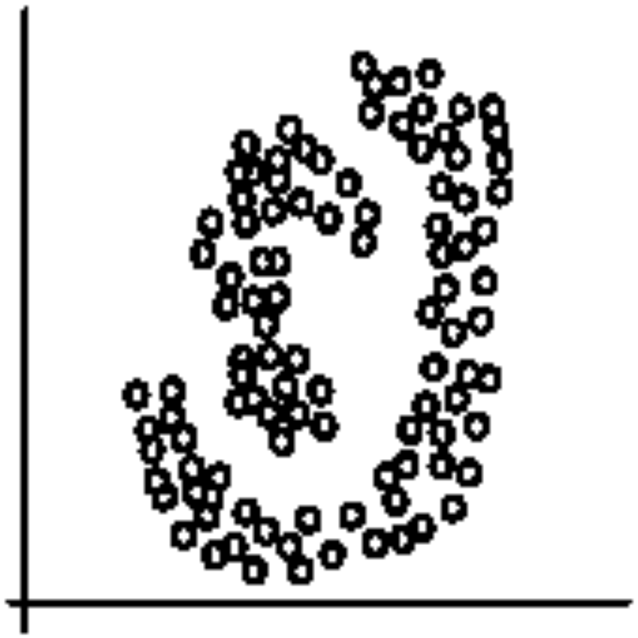
(B). Iteration 1

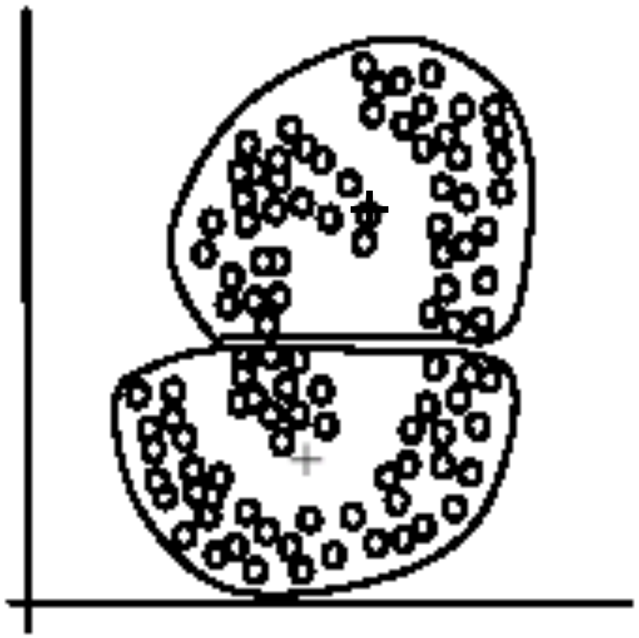


(C). Iteration 2

Weaknesses of k-means (cont …)

- The *k*-means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).


(A): Two natural clusters


(B): *k*-means clusters

K-means summary

- Despite weaknesses, *k*-means is still the most popular algorithm due to its simplicity, efficiency and
  - other clustering algorithms have their own lists of weaknesses.
- No clear evidence that any other clustering algorithm performs better in general
  - although they may be more suitable for some specific types of data or applications.
- Comparing different clustering algorithms is a difficult task. No one knows the correct clusters!

Road map

- Basic concepts
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- Representation of clusters
- Hierarchical clustering
- Distance functions
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- Which clustering algorithm to use?
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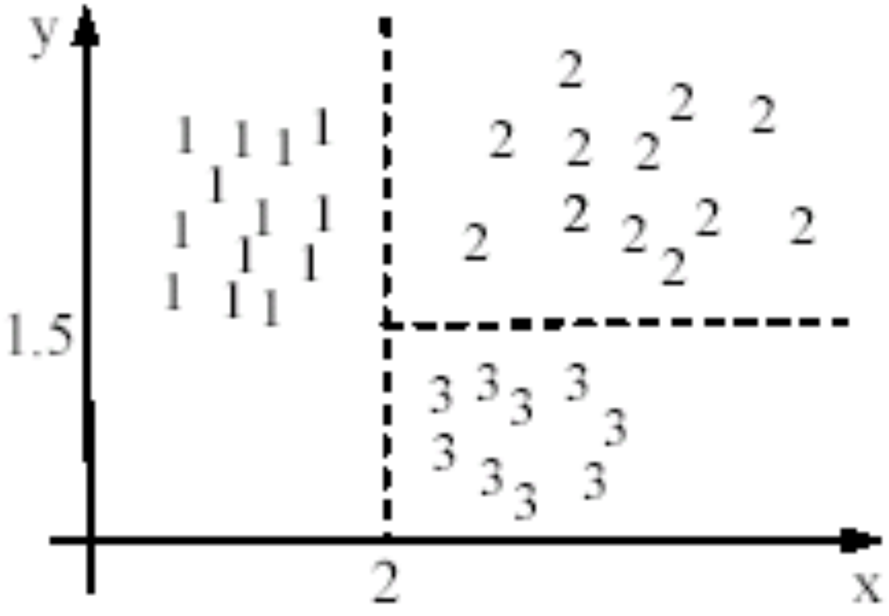
Common ways to represent clusters

- Use the centroid of each cluster to represent the cluster.
  - compute the radius and
  - standard deviation of the cluster to determine its spread in each dimension
  - The centroid representation alone works well if the clusters are of the hyper-spherical shape.
  - If clusters are elongated or are of other shapes, centroids are not sufficient

Using classification model

- All the data points in a cluster are regarded to have the same class label, e.g., the cluster ID
  - run a supervised learning algorithm on the data to find a classification model.



$x \leq 2 \rightarrow$ cluster 1

$x > 2, y > 1.5 \rightarrow$ cluster 2

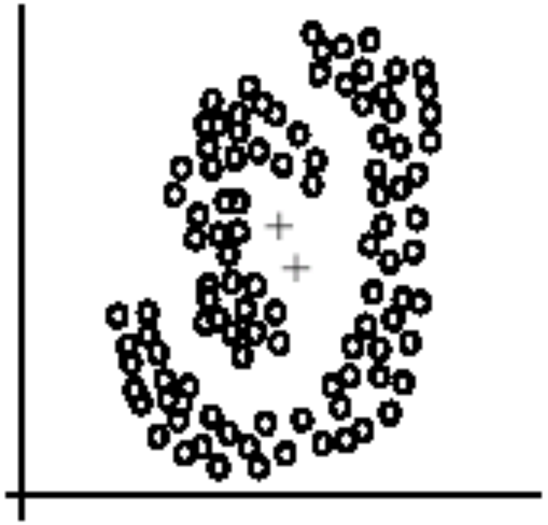
$x > 2, y \leq 1.5 \rightarrow$ cluster 3

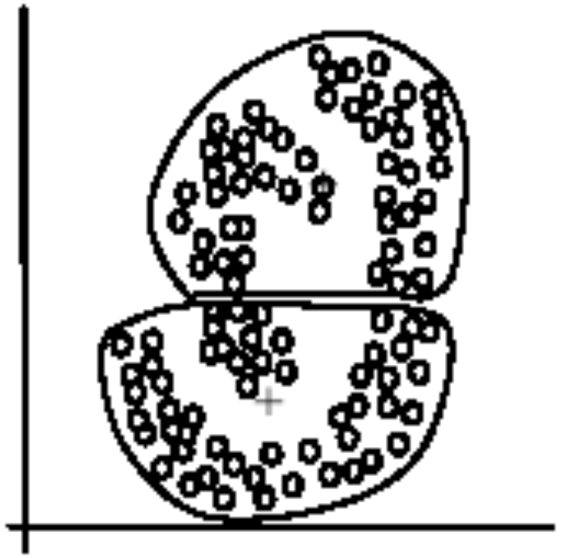
Use frequent values to represent cluster

- This method is mainly for clustering of categorical data (e.g., *k*-modes clustering).
- Main method used in text clustering, where a small set of frequent words in each cluster is selected to represent the cluster.

Clusters of arbitrary shapes

- Hyper-elliptical and hyper-spherical clusters are usually easy to represent, using their centroid together with spreads.
- Irregular shape clusters are hard to represent. They may not be useful in some applications.
  - Using centroids are not suitable (upper figure) in general
  - K-means clusters may be more useful (lower figure), e.g., for making 2 size T-shirts.





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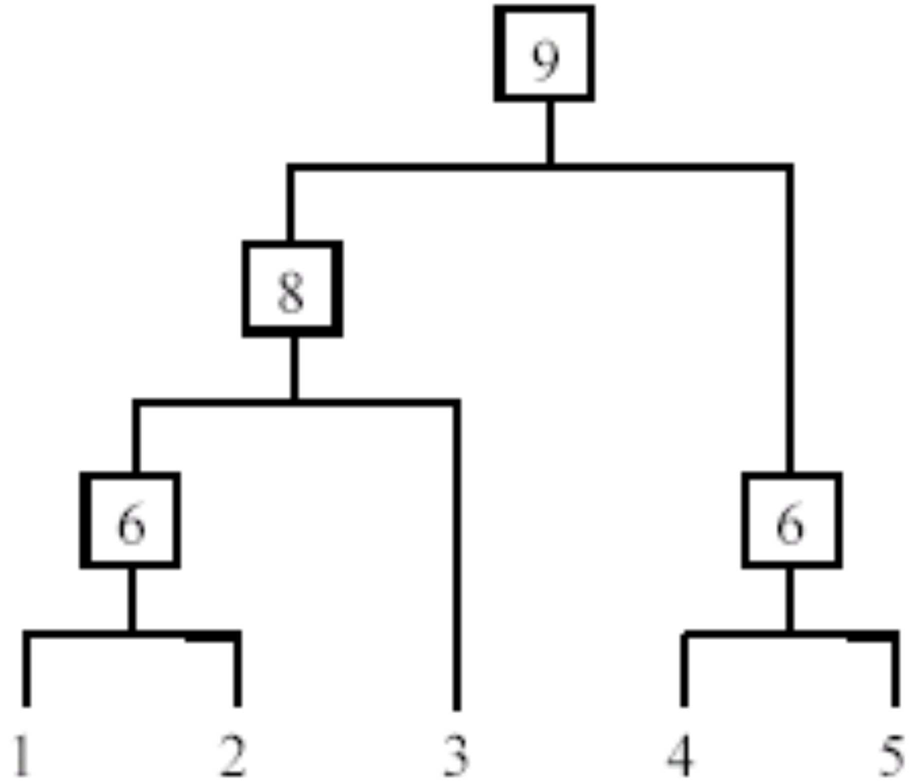
Hierarchical Clustering

- Produce a nested sequence of clusters, a tree, also called Dendrogram.



Types of hierarchical clustering

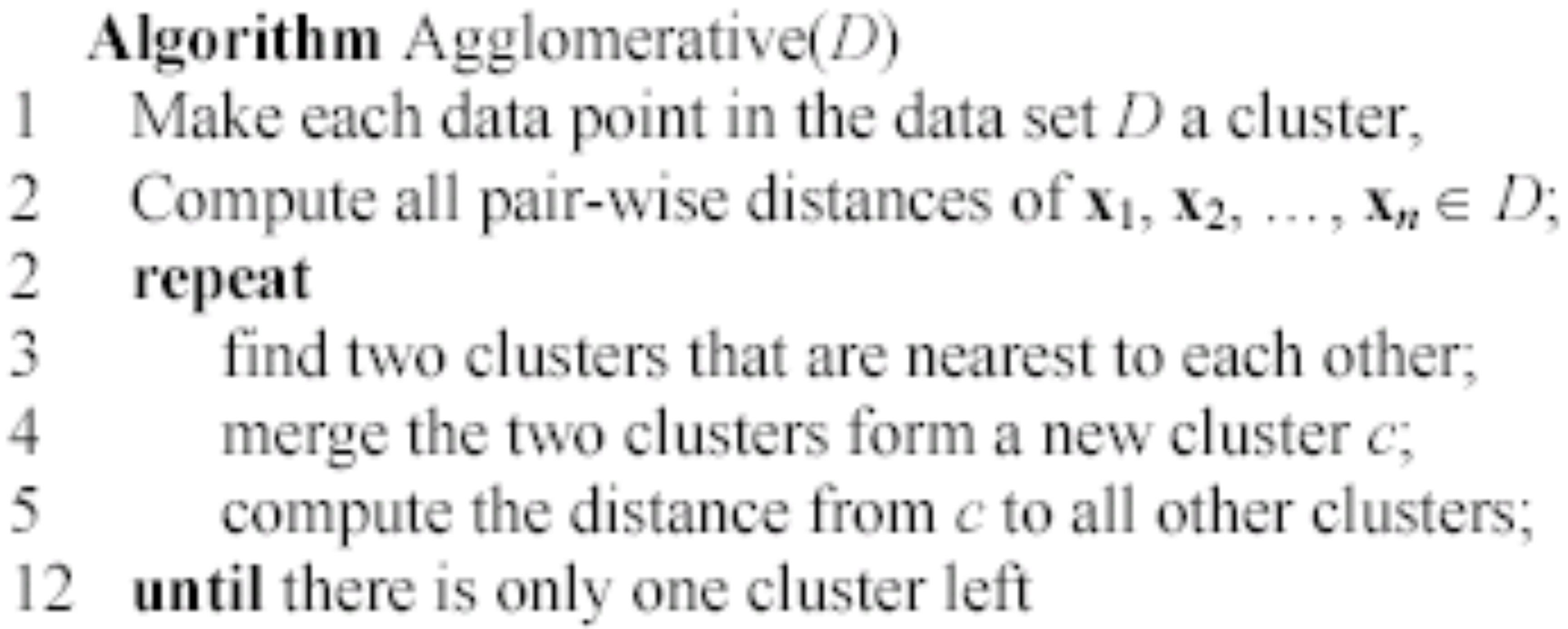
- Agglomerative (bottom up) clustering: It builds the dendrogram (tree) from the bottom level, and
  - merges the most similar (or nearest) pair of clusters
  - stops when all the data points are merged into a single cluster (i.e., the root cluster).
- Divisive (top down) clustering: It starts with all data points in one cluster, the root.
  - Splits the root into a set of child clusters. Each child cluster is recursively divided further
  - stops when only singleton clusters of individual data points remain, i.e., each cluster with only a single point

Agglomerative clustering

It is more popular then divisive methods.

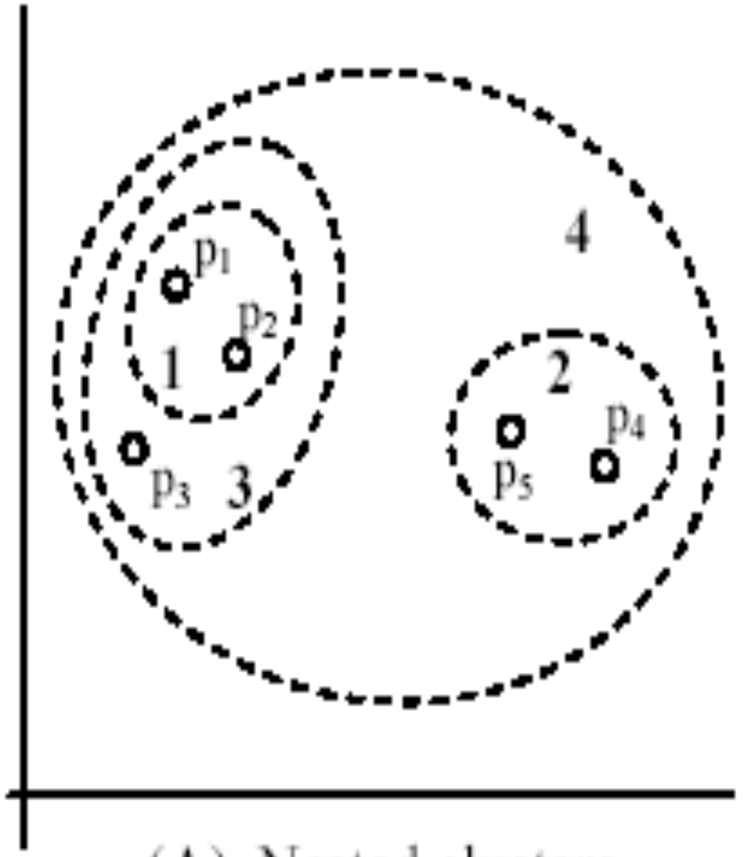
- At the beginning, each data point forms a cluster (also called a node).
- Merge nodes/clusters that have the least distance.
- Go on merging
- Eventually all nodes belong to one cluster

Agglomerative clustering algorithm

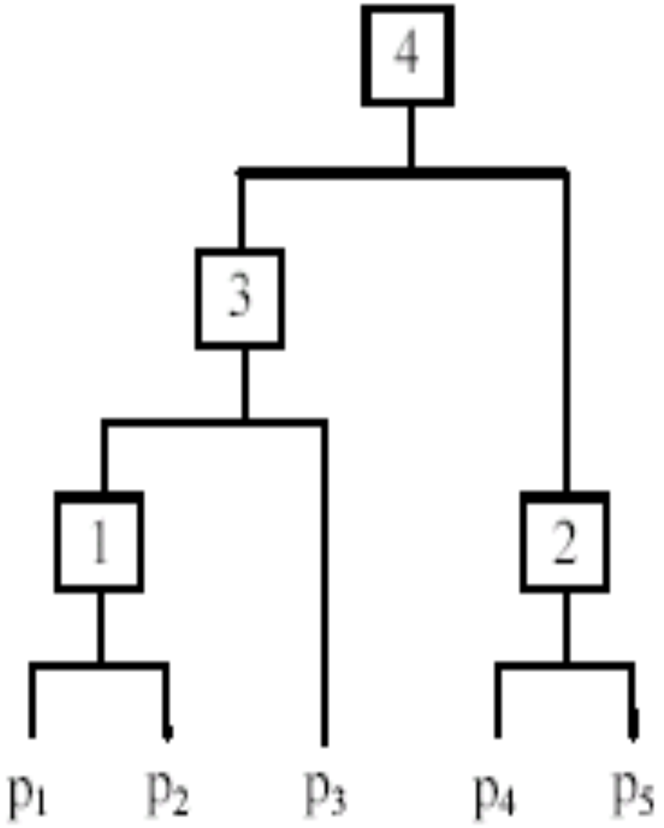


```
Algorithm Agglomerative($D$)
  Make each data point in the data set $D$ a cluster,
  Compute all pair-wise distances of $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in D$;
  repeat
      find two clusters that are nearest to each other;
      merge the two clusters form a new cluster $c$;
      compute the distance from $c$ to all other clusters;
  until there is only one cluster left
```

An example: working of the algorithm



(A). Nested clusters



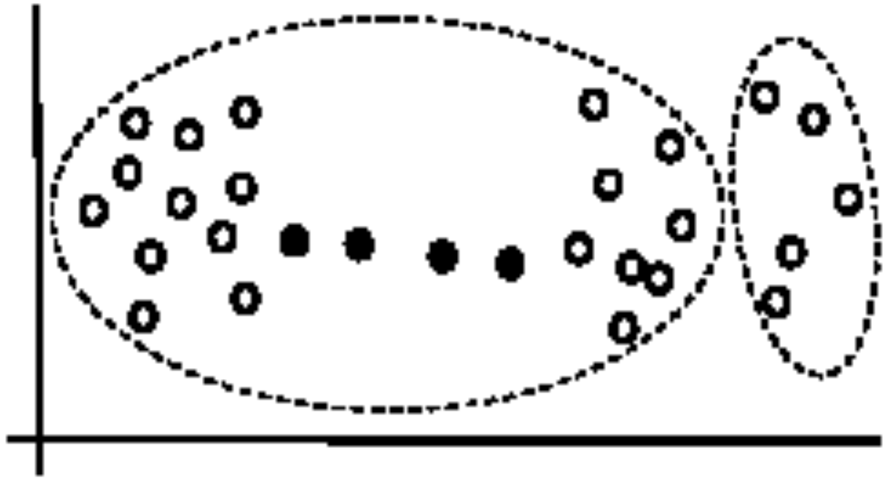
(B) Dendrogram

Measuring the distance of two clusters

- A few ways to measure distances of two clusters.
- Results in different variations of the algorithm.
  - Single link
  - Complete link
  - Average link
  - Centroids
  - …

Single link method

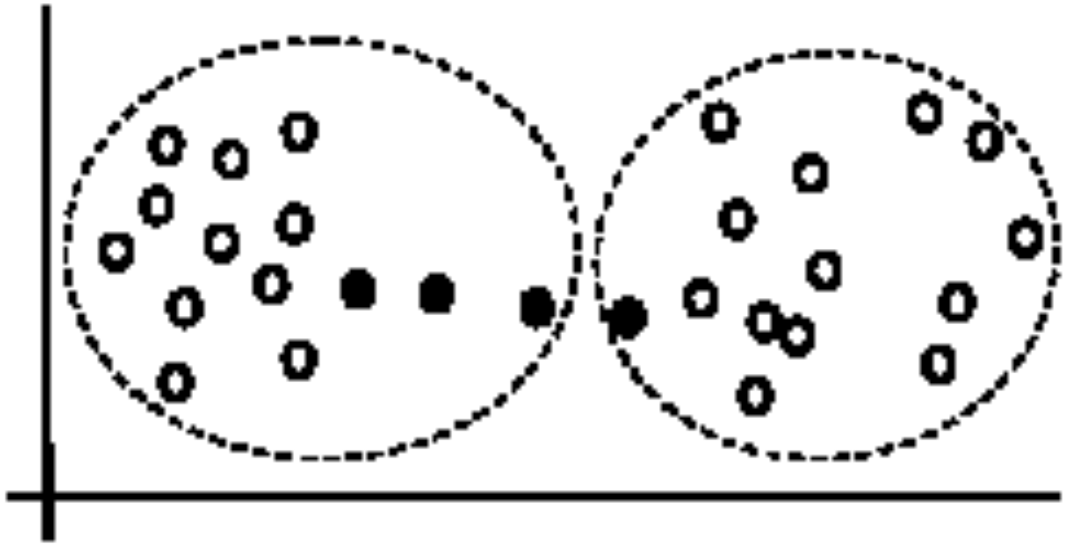
- The distance between two clusters is the distance between two closest data points in the two clusters, one data point from each cluster.
- It can find arbitrarily shaped clusters, but
  - It may cause the undesirable "chain effect" by noisy points



Two natural clusters are split into two

Complete link method

- The distance between two clusters is the distance of two furthest data points in the two clusters.
- It is sensitive to outliers because they are far away



Average link and centroid methods

- Average link: A compromise between
  - the sensitivity of complete-link clustering to outliers and
  - the tendency of single-link clustering to form long chains that do not correspond to the intuitive notion of clusters as compact, spherical objects.
  - In this method, the distance between two clusters is the average distance of all pair-wise distances between the data points in two clusters.
- Centroid method: In this method, the distance between two clusters is the distance between their centroids

The complexity

- All the algorithms are at least $O(n^2)$. n is the number of data points.
- Single link can be done in $O(n^2)$.
- Complete and average links can be done in $O(n^2 \log n)$.
- Due the complexity, hard to use for large data sets.
  - Sampling
  - Scale-up methods (e.g., BIRCH).

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Distance functions

- Key to clustering. “similarity” and “dissimilarity” can also commonly used terms.
- There are numerous distance functions for
  - Different types of data
    - Numeric data
    - Nominal data
  - Different specific applications

Distance functions for numeric attributes

- Most commonly used functions are
  - Euclidean distance and
  - Manhattan (city block) distance
- We denote distance with: *dist*($\mathbf{x}_i$, $\mathbf{x}_j$), where $\mathbf{x}_i$ and $\mathbf{x}_j$ are data points (vectors)
- They are special cases of Minkowski distance. h is positive integer.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = ((x_{i1} - x_{j1})^h + (x_{i2} - x_{j2})^h + \ldots + (x_{ir} - x_{jr})^h)^{\frac{1}{h}}$$

Euclidean distance and Manhattan distance

- If *h* = 2, it is the Euclidean distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + ... + (x_{ir} - x_{jr})^2}$$

- If *h* = 1, it is the Manhattan distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = | x_{i1} - x_{j1} | + | x_{i2} - x_{j2} | + ... + | x_{ir} - x_{jr} |$$

- Weighted Euclidean distance

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{w_1(x_{i1} - x_{j1})^2 + w_2(x_{i2} - x_{j2})^2 + ... + w_r(x_{ir} - x_{jr})^2}$$

Squared distance and Chebychev distance

- Squared Euclidean distance: to place progressively greater weight on data points that are further apart.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + ... + (x_{ir} - x_{jr})^2$$

- Chebychev distance: one wants to define two data points as "different" if they are different on any one of the attributes.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \max(|x_{i1} - x_{j1}|, |x_{i2} - x_{j2}|, ..., |x_{ir} - x_{jr}|)$$

Distance functions for binary and nominal attributes

- Binary attribute: has two values or states but no ordering relationships, e.g.,
  - Gender: male and female.
- We use a confusion matrix to introduce the distance functions/measures.
- Let the *i*th and *j*th data points be $\mathbf{x}_i$ and $\mathbf{x}_j$ (vectors)

Confusion matrix

$$\begin{array}{cc|c|c|c}
 & & \multicolumn{2}{c}{\text{Data point } j} & \\
 & & 1 & 0 & \\
\hline
 & 1 & a & b & a+b \\
\hline
\text{Data point } i & 0 & c & d & c+d \\
\hline
 & & a+c & b+d & a+b+c+d
\end{array} \qquad (10)$$

a: the number of attributes with the value of 1 for both data points.

b: the number of attributes for which $x_{if} = 1$ and $x_{jf} = 0$, where x_{if} (x_{jf}) is the value of the *f*th attribute of the data point $\mathbf{x}_i$ ($\mathbf{x}_j$).

c: the number of attributes for which $x_{if} = 0$ and $x_{jf} = 1$.

d: the number of attributes with the value of 0 for both data points.

Symmetric binary attributes

- A binary attribute is **symmetric** if both of its states (0 and 1) have equal importance, and carry the same weights, e.g., male and female of the attribute Gender
- Distance function: Simple Matching Coefficient, proportion of mismatches of their values

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

Symmetric binary attributes: example

$\mathbf{x}_1$	1	1	1	0	1	0	0
$\mathbf{x}_2$	0	1	1	0	0	1	0

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{2+1}{2+2+1+2} = \frac{3}{7} = 0.429$$

Asymmetric binary attributes

- Asymmetric: if one of the states is more important or more valuable than the other.
  - By convention, state 1 represents the more important state, which is typically the rare or infrequent state.
  - Jaccard coefficient is a popular measure

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b+c}{a+b+c}$$

  - We can have some variations, adding weights

Nominal attributes

- Nominal attributes: with more than two states or values.
  - the commonly used distance measure is also based on the simple matching method.
  - Given two data points $\mathbf{x}_i$ and $\mathbf{x}_j$, let the number of attributes be r, and the number of values that match in $\mathbf{x}_i$ and $\mathbf{x}_j$ be q.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{r - q}{r}$$

Distance function for text documents

- A text document consists of a sequence of sentences and each sentence consists of a sequence of words.
- To simplify: a document is usually considered a "bag" of words in document clustering.
    - Sequence and position of words are ignored.
- A document is represented with a vector just like a normal data point.
- It is common to use similarity to compare two documents rather than distance.
    - The most commonly used similarity function is the **cosine similarity**. We will study this later.

Road map

Data standardization

- In the Euclidean space, standardization of attributes is recommended so that all attributes can have equal impact on the computation of distances.
- Consider the following pair of data points
  - $\mathbf{x}_i$: (0.1, 20) and $\mathbf{x}_j$: (0.9, 720).

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{(0.9 - 0.1)^2 + (720 - 20)^2} = 700.000457,$$

- The distance is almost completely dominated by (720-20) = 700.
- Standardize attributes: to force the attributes to have a common value range

Interval-scaled attributes

- Their values are real numbers following a linear scale.
  - The difference in Age between 10 and 20 is the same as that between 40 and 50.
  - The key idea is that intervals keep the same importance through out the scale
- Two main approaches to standardize interval scaled attributes, **range** and **z-score**. *f* is an attribute

$$range(x_{if}) = \frac{x_{if} - \min(f)}{\max(f) - \min(f)},$$

Interval-scaled attributes (cont …)

- Z-score: transforms the attribute values so that they have a mean of zero and a **mean absolute deviation** of 1. The mean absolute deviation of attribute *f*, denoted by s_f, is computed as follows

$$s_f = \frac{1}{n}\left(| x_{1f} - m_f | + | x_{2f} - m_f | + \ldots + | x_{nf} - m_f |\right),$$

$$m_f = \frac{1}{n}\left(x_{1f} + x_{2f} + \ldots + x_{nf}\right),$$

Z-score: $$z(x_{if}) = \frac{x_{if} - m_f}{s_f}.$$

Ratio-scaled attributes

- Numeric attributes, but unlike interval-scaled attributes, their scales are exponential,
- For example, the total amount of microorganisms that evolve in a time *t* is approximately given by

  Ae^{Bt},

  - where *A* and *B* are some positive constants.
- Do log transform: $\log(x_{if})$
  - Then treat it as an interval-scaled attribuete

Nominal attributes

- Sometime, we need to transform nominal attributes to numeric attributes.
- Transform nominal attributes to binary attributes.
  - The number of values of a nominal attribute is *v*.
  - Create *v* binary attributes to represent them.
  - If a data instance for the nominal attribute takes a particular value, the value of its binary attribute is set to 1, otherwise it is set to 0.
- The resulting binary attributes can be used as numeric attributes, with two values, 0 and 1.

Nominal attributes: an example

- Nominal attribute *fruit*: has three values,
  - Apple, Orange, and Pear
- We create three binary attributes called, Apple, Orange, and Pear in the new data.
- If a particular data instance in the original data has Apple as the value for *fruit*,
  - then in the transformed data, we set the value of the attribute Apple to 1, and
  - the values of attributes Orange and Pear to 0

Ordinal attributes

- Ordinal attribute: an ordinal attribute is like a nominal attribute, but its values have a numerical ordering. E.g.,
  - Age attribute with values: Young, MiddleAge and Old. They are ordered.
  - Common approach to standardization: treat is as an interval-scaled attribute.

Road map

- Basic concepts
- K-means algorithm
- Representation of clusters
- Hierarchical clustering
- Distance functions
- Data standardization
- Handling mixed attributes
- Which clustering algorithm to use?
- Cluster evaluation
- Discovering holes and data regions
- Summary

Mixed attributes

- Our distance functions given are for data with all numeric attributes, or all nominal attributes, etc.
- Practical data has different types:
  - Any subset of the 6 types of attributes,
    - **interval-scaled**,
    - **symmetric binary**,
    - **asymmetric binary**,
    - **ratio-scaled**,
    - **ordinal** and
    - **nominal**

Convert to a single type

- One common way of dealing with mixed attributes is to
  - Decide the dominant attribute type, and
  - Convert the other types to this type.
- E.g, if most attributes in a data set are interval-scaled,
  - we convert ordinal attributes and ratio-scaled attributes to interval-scaled attributes.
  - It is also appropriate to treat symmetric binary attributes as interval-scaled attributes.

Convert to a single type (cont …)

- It does not make much sense to convert a nominal attribute or an asymmetric binary attribute to an interval-scaled attribute,
  - but it is still frequently done in practice by assigning some numbers to them according to some hidden ordering, e.g., prices of the fruits
- Alternatively, a nominal attribute can be converted to a set of (symmetric) binary attributes, which are then treated as numeric attributes.

Combining individual distances

- This approach computes individual attribute distances and then combine them.

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{f=1}^{r} \delta_{ij}^f d_{ij}^f}{\sum_{f=1}^{r} \delta_{ij}^f}$$

This distance value is between 0 and 1. r is the number of attributes in the data set. The indicator δ_{ij}^f is 1 when both values x_{if} and x_{jf} for attribute f are non-missing, and it is set to 0 otherwise. It is also set to 0 if attribute f is asymmetric and the match is 0-0. Equation (25) cannot be computed if all δ_{ij}^f 's are 0. In such a case, some default value may be used or one of the data points is removed.

d_{ij}^f is the distance contributed by attribute f, and it is in the 0-1 range.

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How to choose a clustering algorithm

- Clustering research has a long history. A vast collection of algorithms are available.
  - We only introduced several main algorithms.
- Choosing the "best" algorithm is a challenge.
  - Every algorithm has limitations and works well with certain data distributions.
  - It is very hard, if not impossible, to know what distribution the application data follow. The data may not fully follow any "ideal" structure or distribution required by the algorithms.
  - One also needs to decide how to standardize the data, to choose a suitable distance function and to select other parameter values.

Choose a clustering algorithm (cont …)

- Due to these complexities, the common practice is to
  - run several algorithms using different distance functions and parameter settings, and
  - then carefully analyze and compare the results.
- The interpretation of the results must be based on insight into the meaning of the original data together with knowledge of the algorithms used.
- Clustering is highly application dependent and to certain extent subjective (personal preferences).

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Cluster Evaluation: hard problem

- The quality of a clustering is very hard to evaluate because
  - We do not know the correct clusters
- Some methods are used:
  - User inspection
    - Study centroids, and spreads
    - Rules from a decision tree.
    - For text documents, one can read some documents in clusters.

Cluster evaluation: ground truth

- We use some labeled data (for classification)
- Assumption: Each class is a cluster.
- After clustering, a confusion matrix is constructed. From the matrix, we compute various measurements, entropy, purity, precision, recall and F-score.
  - Let the classes in the data D be $C = (c_1, c_2, \ldots, c_k)$. The clustering method produces k clusters, which divides D into k disjoint subsets, $D_1, D_2, \ldots, D_k$.

Evaluation measures: Entropy

Entropy: For each cluster, we can measure its entropy as follows:

$$entropy(D_i) = -\sum_{j=1}^{k} \Pr_i(c_j) \log_2 \Pr_i(c_j), \qquad (29)$$

where $\Pr_i(c_j)$ is the proportion of class c_j data points in cluster i or D_i. The total entropy of the whole clustering (which considers all clusters) is

$$entropy_{total}(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \times entropy(D_i) \qquad (30)$$

Evaluation measures: purity

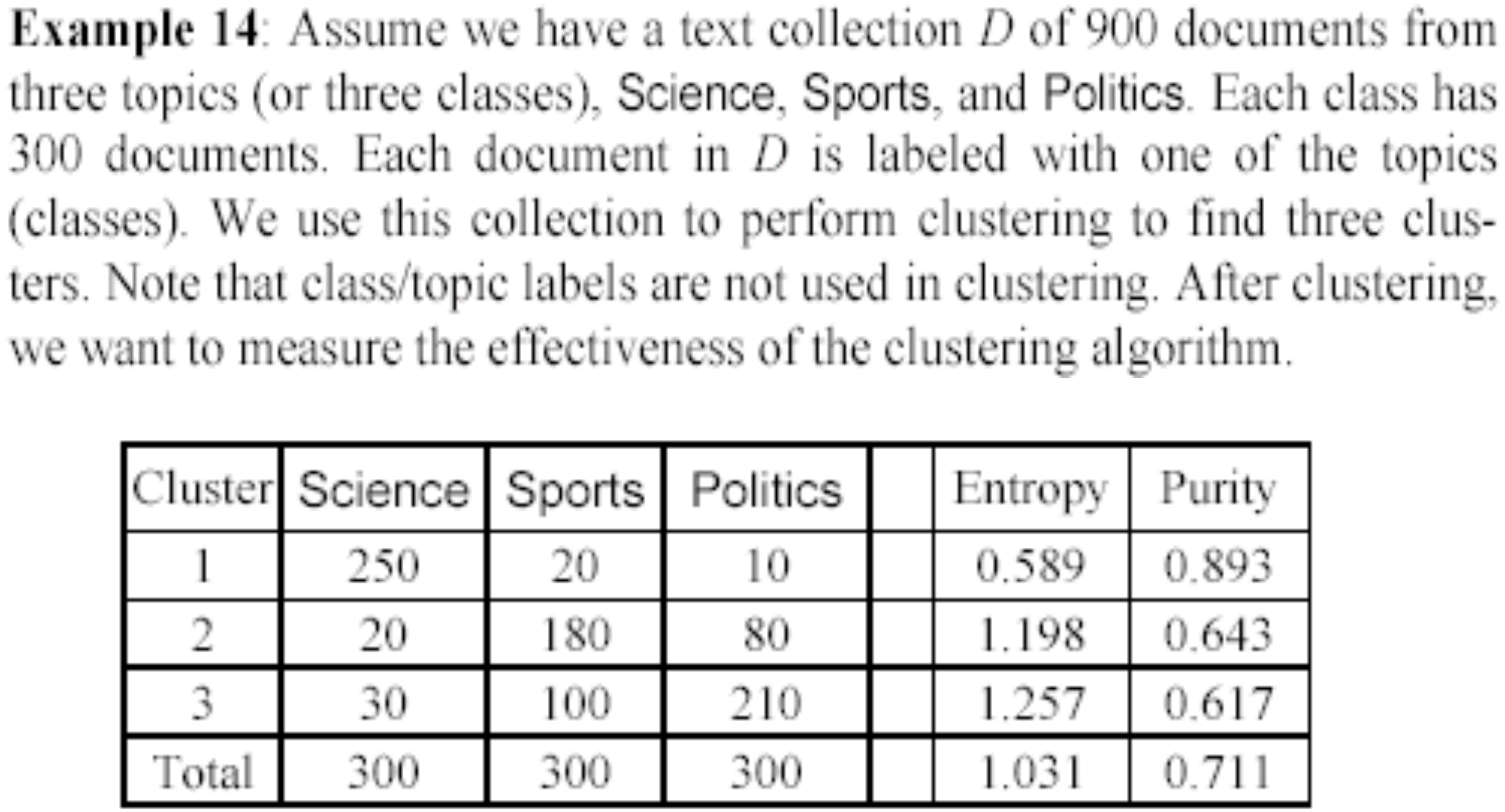
Purity: This again measures the extent that a cluster contains only one class of data. The purity of each cluster is computed with

$$purity(D_i) = \max_j(\Pr_i(c_j)) \quad (31)$$

The total purity of the whole clustering (considering all clusters) is

$$purity_{total}(D) = \sum_{i=1}^{k} \frac{|D_i|}{|D|} \times purity(D_i) \quad (32)$$

An example



Example 14: Assume we have a text collection *D* of 900 documents from three topics (or three classes), Science, Sports, and Politics. Each class has 300 documents. Each document in *D* is labeled with one of the topics (classes). We use this collection to perform clustering to find three clusters. Note that class/topic labels are not used in clustering. After clustering, we want to measure the effectiveness of the clustering algorithm.

Cluster	Science	Sports	Politics		Entropy	Purity
1	250	20	10		0.589	0.893
2	20	180	80		1.198	0.643
3	30	100	210		1.257	0.617
Total	300	300	300		1.031	0.711

A remark about ground truth evaluation

- Commonly used to compare different clustering algorithms.
- A real-life data set for clustering has no class labels.
  - Thus although an algorithm may perform very well on some labeled data sets, no guarantee that it will perform well on the actual application data at hand.
- The fact that it performs well on some label data sets does give us some confidence of the quality of the algorithm.
- This evaluation method is said to be based on **external data** or information.

Evaluation based on internal information

- **Intra-cluster cohesion** (compactness):
  - Cohesion measures how near the data points in a cluster are to the cluster centroid.
  - Sum of squared error (SSE) is a commonly used measure.
- **Inter-cluster separation** (isolation):
  - Separation means that different cluster centroids should be far away from one another.
- In most applications, expert judgments are still the key.

Indirect evaluation

- In some applications, clustering is not the primary task, but used to help perform another task.
- We can use the performance on the primary task to compare clustering methods.
- For instance, in an application, the primary task is to provide recommendations on book purchasing to online shoppers.
  - If we can cluster books according to their features, we might be able to provide better recommendations.
  - We can evaluate different clustering algorithms based on how well they help with the recommendation task.
  - Here, we assume that the recommendation can be reliably evaluated.

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Holes in data space

- All the clustering algorithms only group data.
- Clusters only represent one aspect of the knowledge in the data.
- Another aspect that we have not studied is the **holes**.
  - A hole is a region in the data space that contains no or few data points. Reasons:
    - insufficient data in certain areas, and/or
    - certain attribute-value combinations are not possible or seldom occur.

Holes are useful too

- Although clusters are important, holes in the space can be quite useful too.
- For example, in a disease database
  - we may find that certain symptoms and/or test values do not occur together, or
  - when a certain medicine is used, some test values never go beyond certain ranges.
- Discovery of such information can be important in medical domains because
  - it could mean the discovery of a cure to a disease or some biological laws.

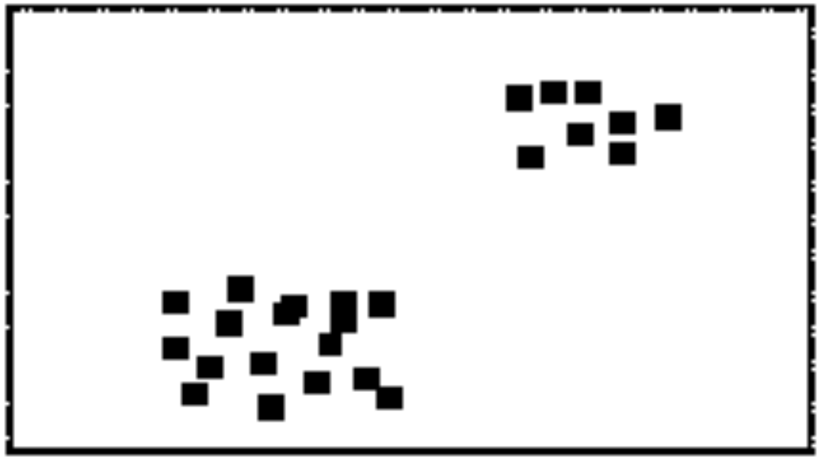
Data regions and empty regions

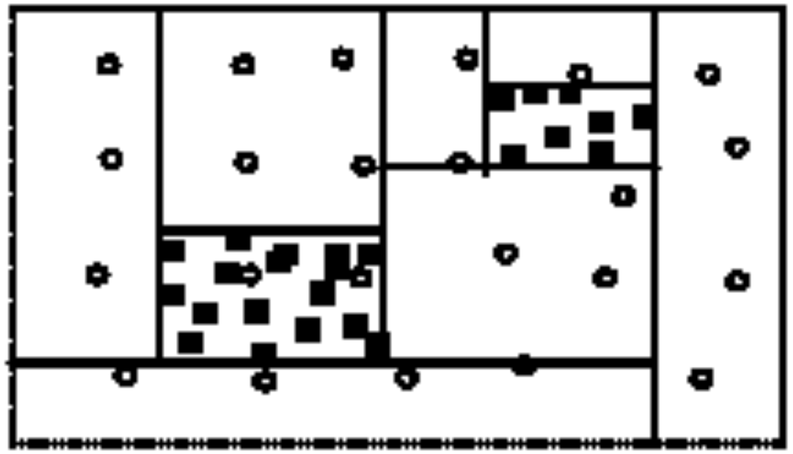
- Given a data space, separate
  - data regions (clusters) and
  - empty regions (holes, with few or no data points).
- Use a supervised learning technique, i.e., decision tree induction, to separate the two types of regions.
- Due to the use of a supervised learning method for an unsupervised learning task,
  - an interesting connection is made between the two types of learning paradigms.

Supervised learning for unsupervised learning

- Decision tree algorithm is not directly applicable.
  - it needs at least two classes of data.
  - A clustering data set has no class label for each data point.
- The problem can be dealt with by a simple idea.
  - Regard each point in the data set to have a class label *Y*.
  - Assume that the data space is uniformly distributed with another type of points, called **non-existing points**. We give them the class, *N*.
- With the *N* points added, the problem of partitioning the data space into data and empty regions becomes a supervised classification problem.

An example


(A): The original data space


(B). Partitioning with added N points

- A decision tree method is used for partitioning in (B).

Can it done without adding *N* points?

- Yes.
- Physically adding *N* points increases the size of the data and thus the running time.
- More importantly: it is unlikely that we can have points truly uniformly distributed in a high dimensional space as we would need an exponential number of points.
- Fortunately, no need to physically add any *N* points.
  - We can compute them when needed

Characteristics of the approach

- It provides representations of the resulting data and empty regions in terms of hyper-rectangles, or rules.
- It detects outliers automatically. Outliers are data points in an empty region.
- It may not use all attributes in the data just as in a normal decision tree for supervised learning.
  - It can automatically determine what attributes are useful. Subspace clustering …
- Drawback: data regions of irregular shapes are hard to handle since decision tree learning only generates hyper-rectangles (formed by axis-parallel hyper-planes), which are rules.

Building the Tree

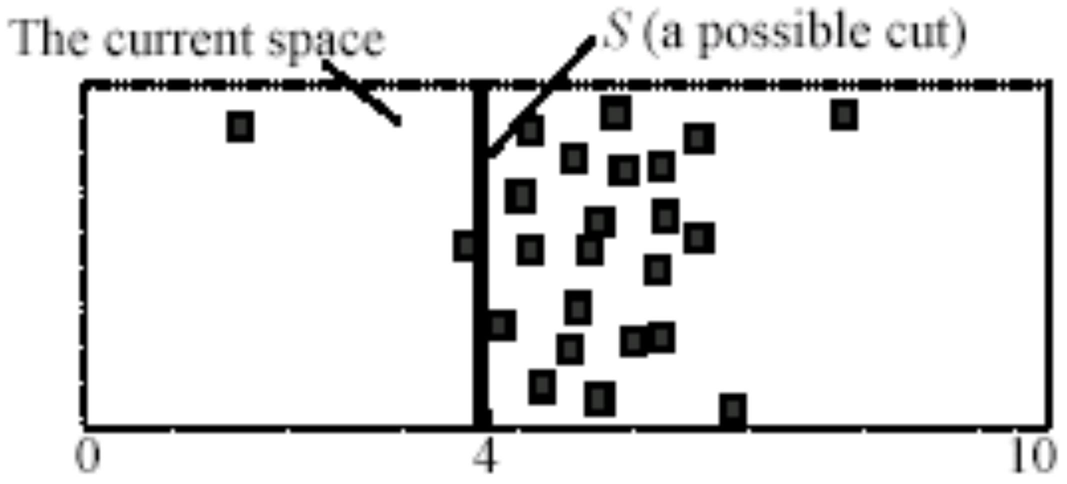
- The main computation in decision tree building is to evaluate entropy (for information gain):

$$entropy(D) = -\sum_{j=1}^{|C|} \Pr(c_j)\log_2 \Pr(c_j)$$

- Can it be evaluated without adding *N* points? Yes.
- Pr(c_j) is the probability of class c_j in data set *D*, and |*C*| is the number of classes, *Y* and *N* (2 classes).
  - To compute Pr(c_j), we only need the number of *Y* (data) points and the number of *N* (non-existing) points.
  - We already have *Y* (or data) points, and we can compute the number of *N* points on the fly. Simple: as we assume that the *N* points are uniformly distributed in the space.

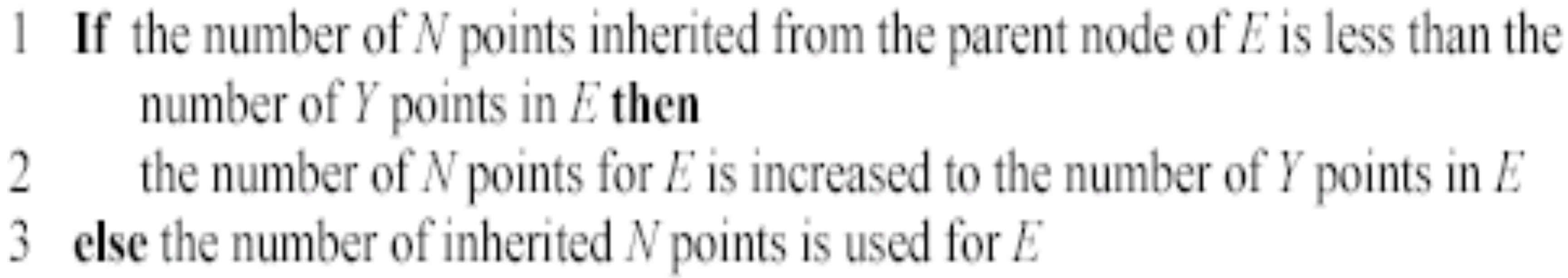
An example

- The space has 25 data (*Y*) points and 25 *N* points. Assume the system is evaluating a possible cut *S*.
  - # *N* points on the left of *S* is 25 * 4/10 = 10. The number of *Y* points is 3.
  - Likewise, # *N* points on the right of *S* is 15 (= 25 - 10).The number of *Y* points is 22.
- With these numbers, entropy can be computed.



How many *N* points to add?

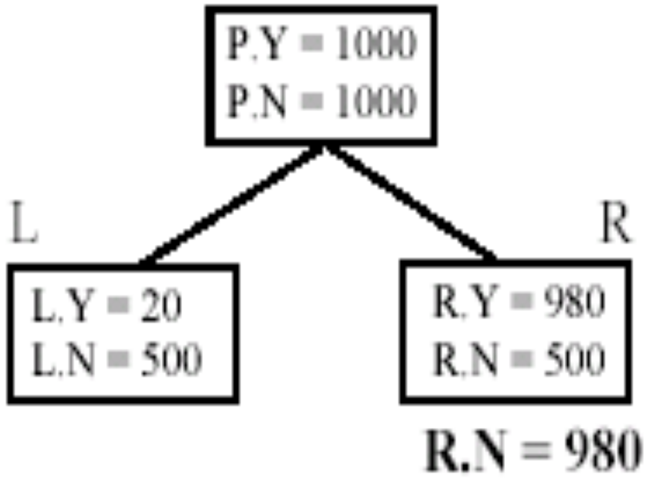
- We add a different number of *N* points at each different node.
  - The number of *N* points for the current node *E* is determined by the following rule (note that at the root node, the number of inherited *N* points is 0):



```
1  If the number of $N$ points inherited from the parent node of $E$ is less than the
      number of $Y$ points in $E$ then
2     the number of $N$ points for $E$ is increased to the number of $Y$ points in $E$
3  else the number of inherited $N$ points is used for $E$
```

An example

Example 17: Fig. 20 gives an example. The (parent) node *P* has two children nodes *L* and *R*. Assume *P* has 1000 *Y* points and thus 1000 *N* points, stored in *P.Y* and *P.N* respectively. Assume after splitting, *L* has 20 *Y* points and 500 *N* points, and *R* has 980 *Y* points and 500 *N* points. According to the above rule, for subsequent partitioning, we increase the number of *N* points at *R* to 980. The number of *N* points at *L* is unchanged.



How many *N* points to add? (cont…)

- Basically, for a *Y* node (which has more data points), we increase *N* points so that

  #Y = #N

- The number of *N* points is not reduced if the current node is an *N* node (an *N* node has more *N* points than *Y* points).
  - A reduction may cause outlier *Y* points to form *Y* nodes (a *Y* node has an equal number of *Y* points as *N* points or more).
  - Then data regions and empty regions may not be separated well.

Building the decision tree

- Using the above ideas, a decision tree can be built to separate data regions and empty regions.
- The actual method is more sophisticated as a few other tricky issues need to be handled in
  - tree building and
  - tree pruning.

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Summary

- Clustering is has along history and still active
  - There are a huge number of clustering algorithms
  - More are still coming every year.
- We only introduced several main algorithms. There are many others, e.g.,
  - density based algorithm, sub-space clustering, scale-up methods, neural networks based methods, fuzzy clustering, co-clustering, etc.
- Clustering is hard to evaluate, but very useful in practice. This partially explains why there are still a large number of clustering algorithms being devised every year.
- Clustering is highly application dependent and to some extent subjective.