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Clustering

(for classification)

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Clustering



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Today's Topic: Clustering

- **Document clustering**
 - Motivations
 - Document representations
 - Success criteria
- **Clustering algorithms**
 - Partitional
 - Hierarchical

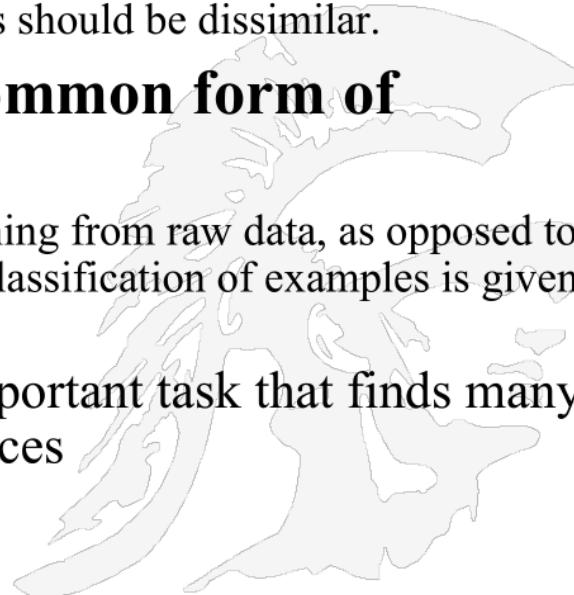


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What is Clustering?

- **Clustering: the process of grouping a set of objects into classes of similar objects**
 - Documents within a cluster should be similar.
 - Documents from different clusters should be dissimilar.
- **Clustering is the most common form of *unsupervised learning***
 - Unsupervised learning = learning from raw data, as opposed to supervised learning where a classification of examples is given *a priori*
 - Clustering is a common and important task that finds many applications in IR and other places



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Related Searches are a Form of Clustering

The image displays three screenshots of web browsers showing search results for the query "cars".

- Google:** Shows a list of news articles and reviews. Below the results, there is a section titled "Searches related to cars" which lists terms like "autotrader", "carmax", "cars for sale", "cars 2 full movie", "used cars", "cars 2", and "cars 2006". An arrow points from this section to the "Related searches" section in the Bing screenshot.
- Yahoo:** Shows a list of ads and search results. A sidebar on the left lists categories such as Web, News, Local, Answers, and More. Another sidebar on the right lists "See more ads for:" followed by "cars", "all electric cars", "used cars sale", "hybrid cars", and "rental cars". An arrow points from the "Ads related to cars" section in the Yahoo screenshot to the "Related searches" section in the Bing screenshot.
- Bing:** Shows a list of local results for "cars near los angeles california 90272" and a section titled "Related searches" which includes links to "Cars Games", "Cars Coloring Pages", "Car Pictures", "New Cars", "Hot Cars", "Classic Cars", and "Images of Cool Cars".

Google related searches
Yahoo does some clustering via alternate queries
Bing does a little better

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USC Viterbi School of Engineering yippy.com Search Engine

- Yippy (formerly Clusty) is a metasearch engine developed by Vivísimo which emphasizes clusters of results.

The figure consists of three side-by-side screenshots of a web browser displaying the Yippy search engine. The left screenshot shows the initial search screen with a search bar containing 'cars'. The middle screenshot shows the results page for 'cars', where various search categories like 'Sale', 'Reviews', and 'Dealers' are listed on the left, and specific search results are shown on the right. The right screenshot shows a more detailed view of the results, with multiple levels of clustering, such as 'car dealers' under 'Dealers' and 'trucks' and 'ebay' under 'Dealers'.

© 2009-2015 Yippy, Inc. All Rights Reserved. Ticker Symbol (OTC PINK:YIPI)

initial screen with query "cars"

clustered results appear on the left column: e.g.
sale
reviews
dealers
rentals

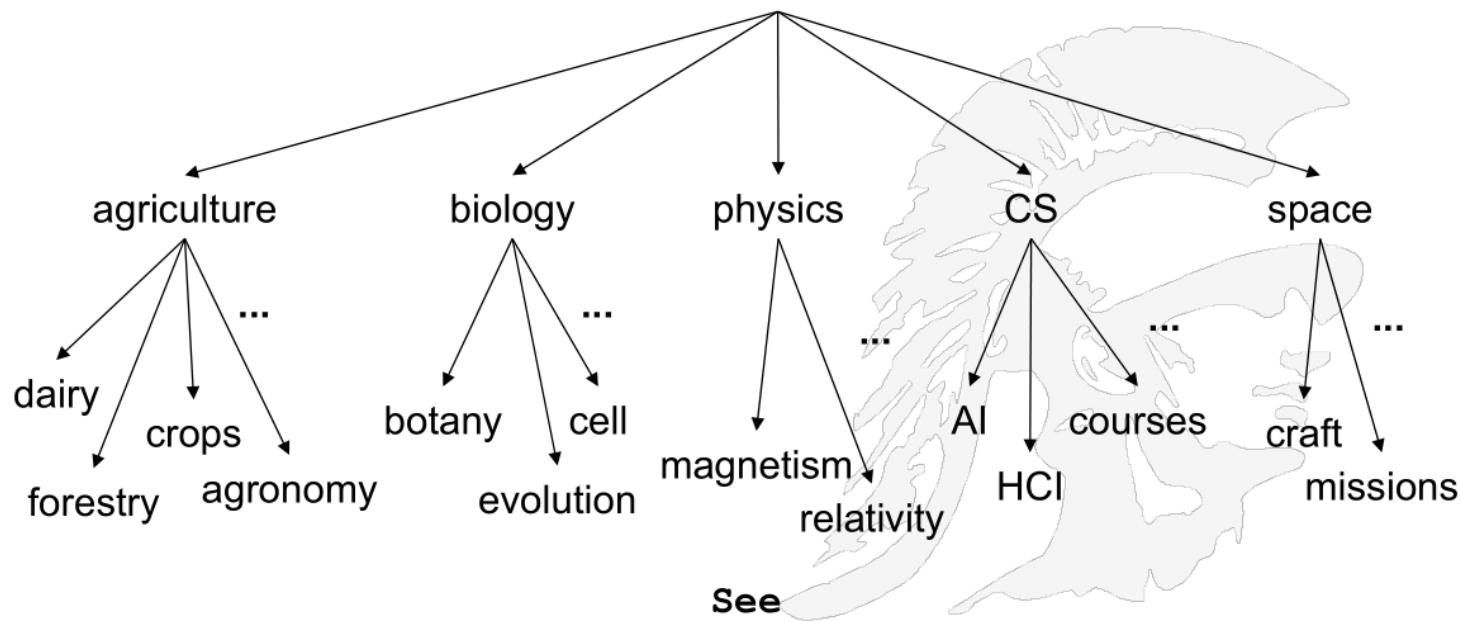
multiple level clusters:
car dealers
trucks
ebay

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Yahoo's Name Derives from Yet Another *Hierarchical Officious Oracle*

Yahoo! Hierarchy *isn't* clustering but *is* the kind of output you want from clustering – a taxonomy



<https://searchengineland.com/yahoo-directory-close-204370>

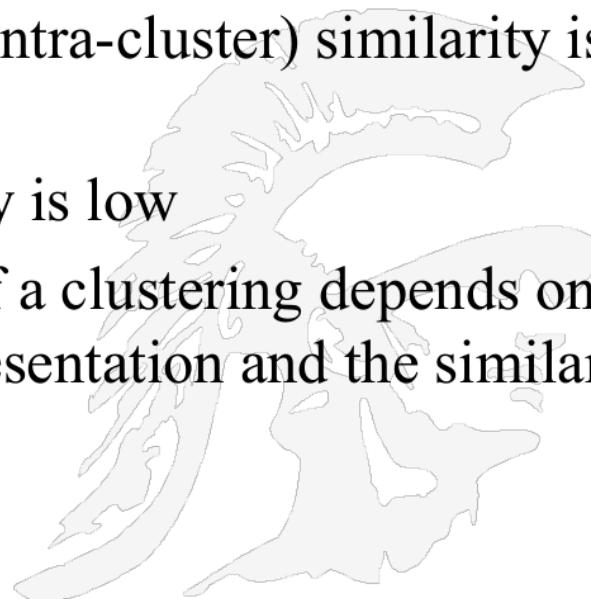
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What Is A Good Clustering?

- **Internal criterion:** A good clustering will produce high quality clusters in which:
 - the intra-class (that is, intra-cluster) similarity is high
 - the inter-class similarity is low
 - The measured quality of a clustering depends on both the document representation and the similarity measure used

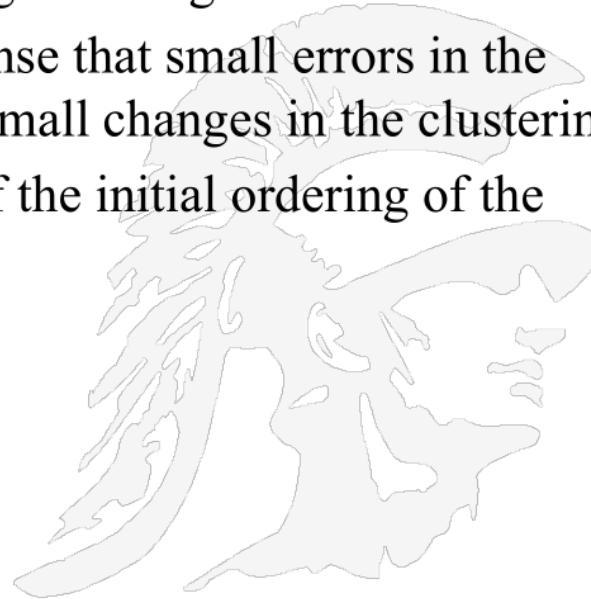


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Three Criteria of Adequacy for Clustering Methods

1. The method produces a clustering which is **unlikely to be altered drastically** when further objects are incorporated
 - i.e. it is stable even under significant growth
2. The method is **stable** in the sense that small errors in the description of objects lead to small changes in the clustering
3. The method is **independent** of the initial ordering of the objects

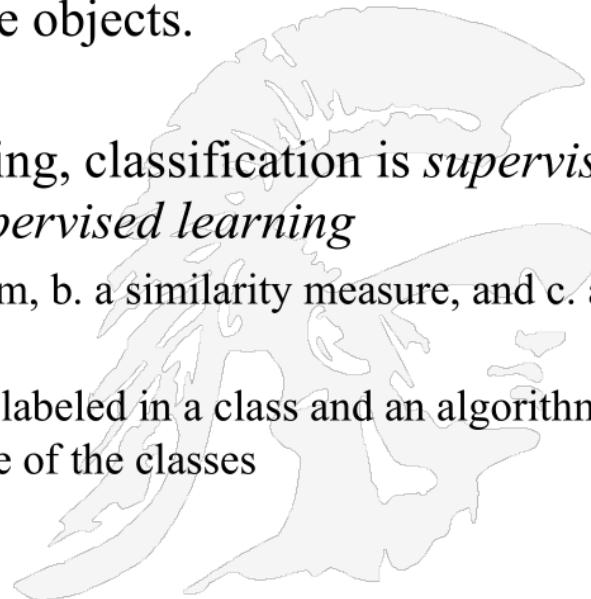


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Classification is Different from Clustering

- In general, in **classification** you have a set of predefined classes and want to know which class a new object belongs to.
- **Clustering** tries to group a set of objects and find whether there is *some* relationship between the objects.
 - Clustering *precedes* classification
- In the context of machine learning, classification is *supervised learning* and clustering is *unsupervised learning*
 - **Clustering** requires a. an algorithm, b. a similarity measure, and c. a number of clusters
 - **classification** has each document labeled in a class and an algorithm that assigns new documents to one of the classes

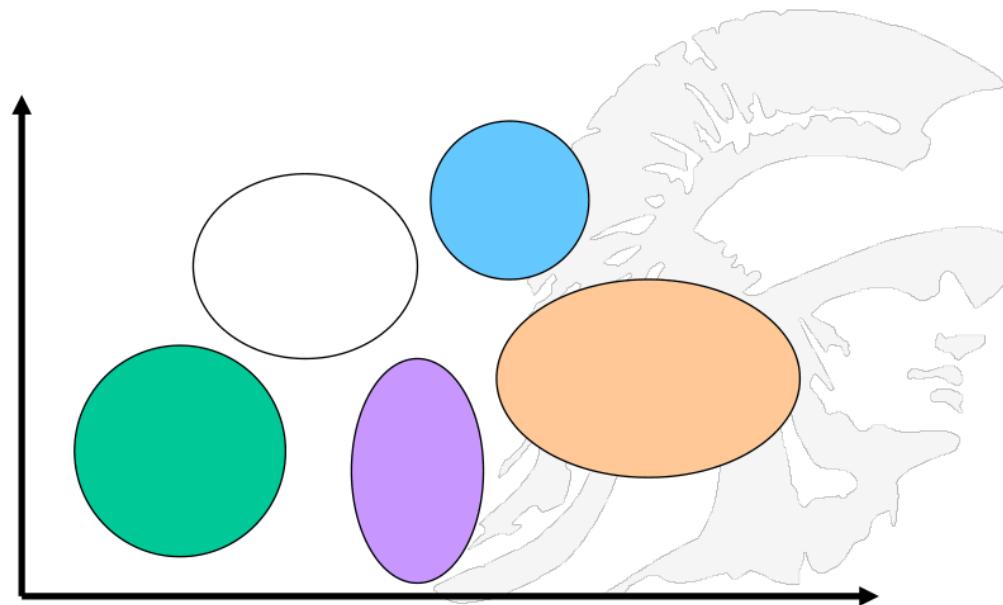


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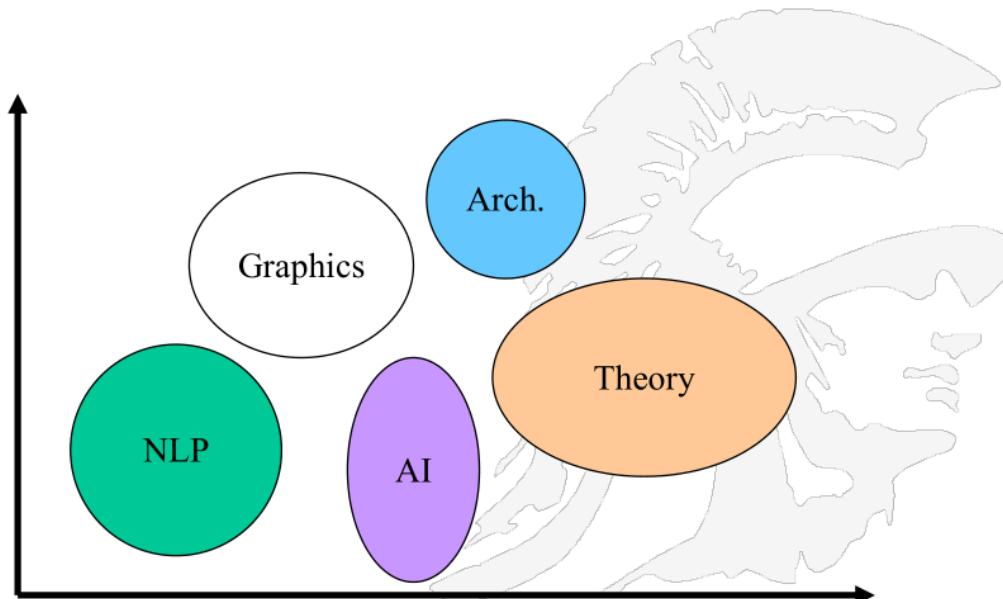
Begin with Clustering

- Step 1: Given a large set of computer science documents, first we cluster them using some algorithm (to be presented)

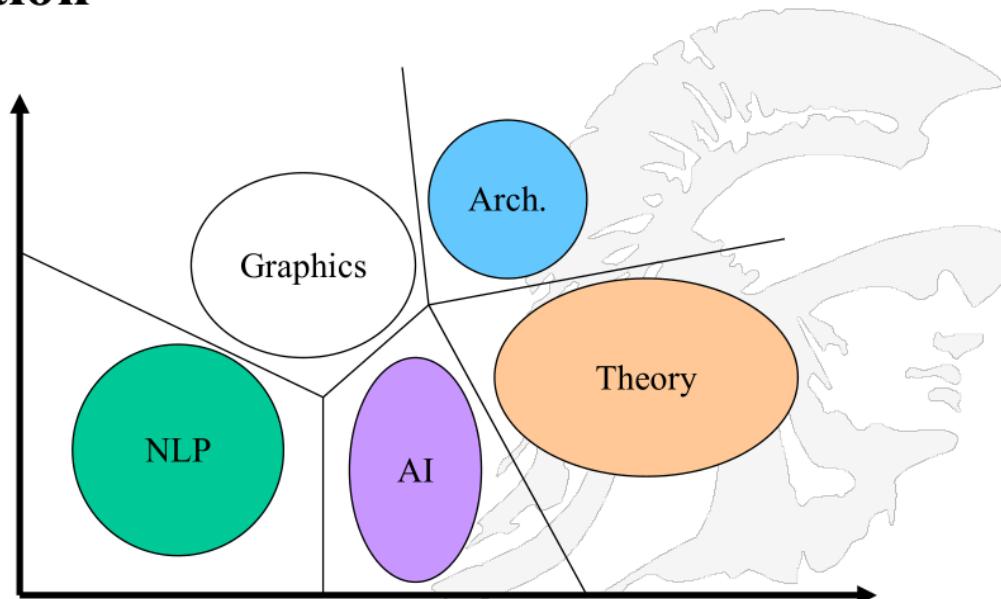




- Step 2: we label the clusters
 - choosing a popular name from each document cluster



- Step 3: we compute boundaries for the clusters that can be used as new documents appear; i.e. classification

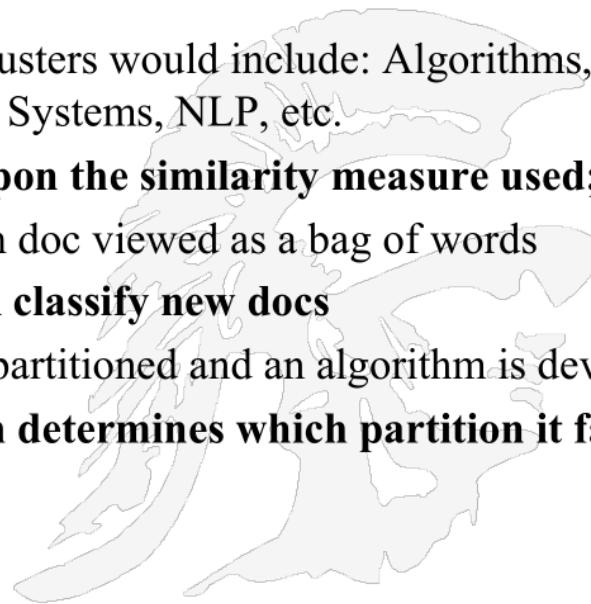


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Classification Requires Initial Clusters and Boundaries

- **Definition:** *Supervised Learning*, inferring a function from labeled training data
- 1. **The documents in each cluster define the “training” docs for each category**
 - E.g. in computer science named clusters would include: Algorithms, Theory, AI, Databases, Operating Systems, NLP, etc.
- 2. **Documents are in a cluster based upon the similarity measure used;**
 - generally a vector space with each doc viewed as a bag of words
- 3. **A classifier is an algorithm that will classify new docs**
 - Essentially, the decision space is partitioned and an algorithm is devised
- 4. **Given a new doc, the new algorithm determines which partition it falls into**



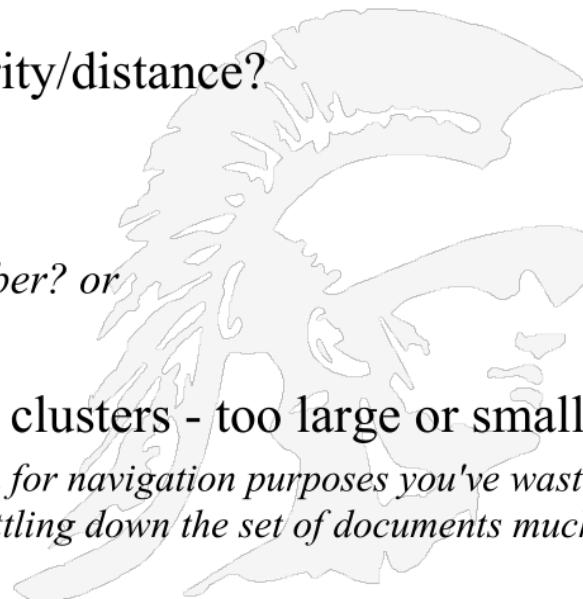
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Now Let's Return to the Earlier Problem: Clustering

- **Questions to consider when clustering**

- How do we represent the document?
 - *Usually as a vector space*
- How do we compute similarity/distance?
 - *Using cosine similarity*
- How many clusters?
 - *will it be a fixed a priori number? or*
 - *completely data driven?*
- Be careful to avoid “trivial” clusters - too large or small
 - *If a cluster is too large, then for navigation purposes you've wasted an extra user click without whittling down the set of documents much*

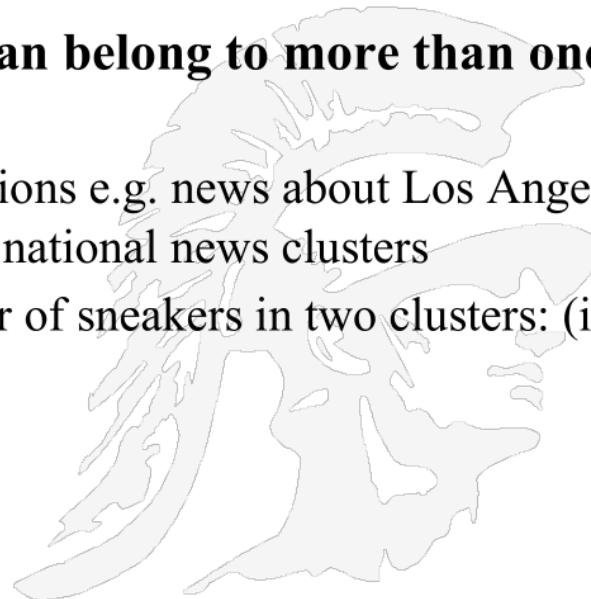


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Issue: Hard vs. Soft Clustering

- ***Hard clustering:*** Each document belongs to exactly one cluster
 - More common and easier to do
- ***Soft clustering:*** A document can belong to more than one cluster.
 - Makes sense for some applications e.g. news about Los Angeles might be included in local and national news clusters
 - E.g. you may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes



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What Definition of Similarity/Distance Will Be Used

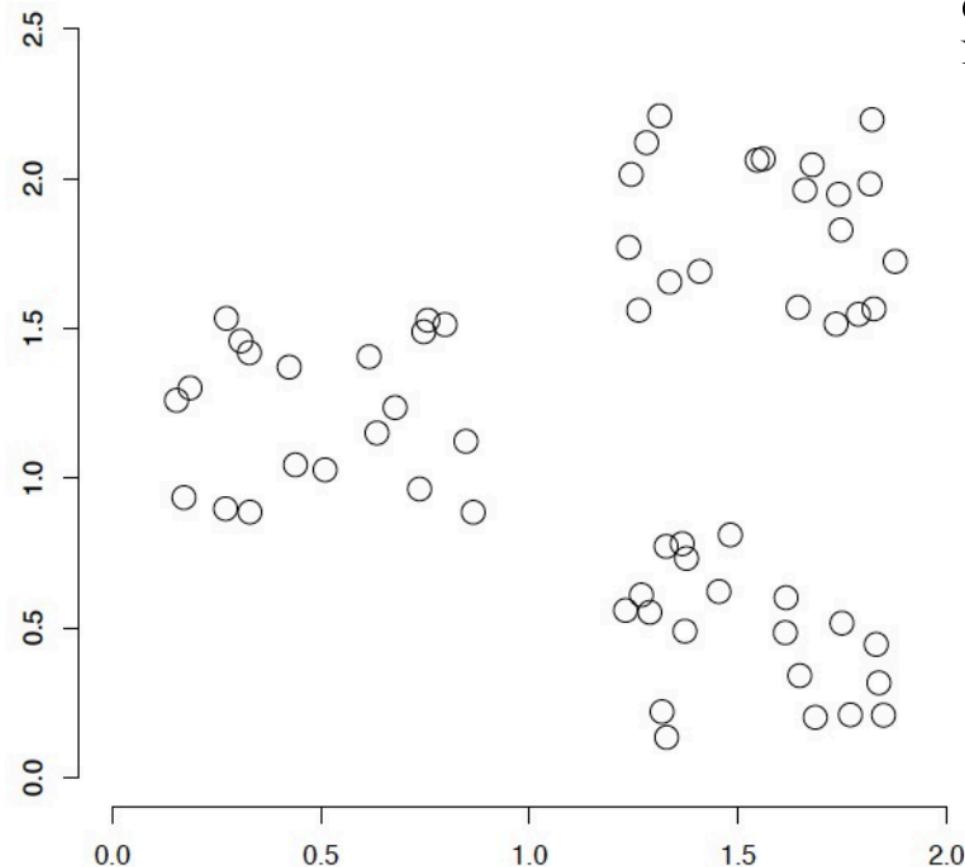
- Once again we will treat documents as vectors
 - Cosine similarity (seen before many times)
 - Cosine similarity is a measure of similarity between two vectors of an inner product space that measures the cosine of the angle between them. Range from 0 (dissimilar) to 1 (exactly similar)
 - Most clustering implementations use cosine similarity
 - Euclidean distance is a close alternative that is also popular

$$\text{similarity} = \cos(\theta) = \frac{A \cdot B}{\|A\|\|B\|} = \frac{\sum_{i=1}^n A_i \times B_i}{\sqrt{\sum_{i=1}^n (A_i)^2} \times \sqrt{\sum_{i=1}^n (B_i)^2}}$$

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A Data Set with Clear Cluster Structure



Circles represent documents as N-vectors

- How would you design an algorithm for finding the three clusters in this case?

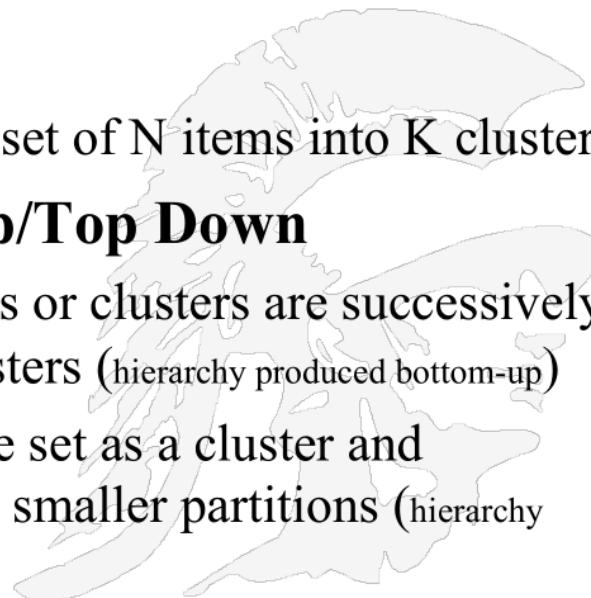
- Hint: use a distance measure

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Clustering Algorithms

- **Two general methodologies**
 - Partitioning Based Algorithms
 - Hierarchical Algorithms
- **Partitioning Based**
 - Choose K and then divide a set of N items into K clusters
- **Hierarchical – Bottom Up/Top Down**
 - **agglomerative**: pairs of items or clusters are successively linked to produce larger clusters (hierarchy produced bottom-up)
 - **divisive**: start with the whole set as a cluster and successively divide sets into smaller partitions (hierarchy produced top-down)

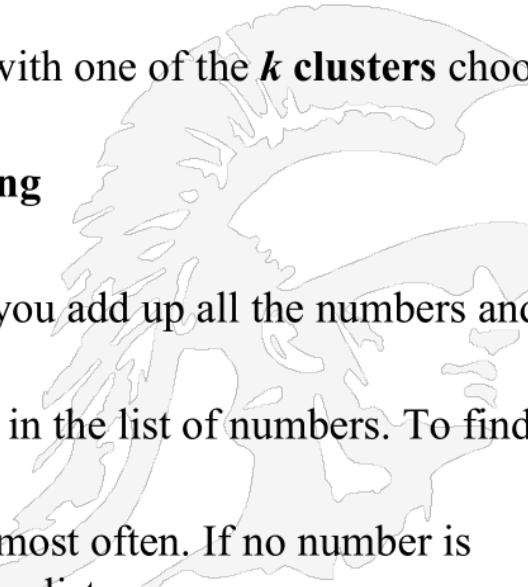


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A Partitioning Algorithm K-Means Clustering Algorithm

- **Clustering algorithm strategy**
 - Choose k random data items out of the n items; call these items the *means*; they designate the prototype or name of the cluster
 - **Refine it iteratively**
 - Associate each of the $n-k$ items with one of the **k clusters** choosing the **cluster** that it is nearest to;
 - **This is called K -means clustering**
- **Recall**
 - The "**mean**" is the "average" where you add up all the numbers and then divide by the number of numbers.
 - The "**median**" is the "middle" value in the list of numbers. To find the median, you may have to sort
 - The "**mode**" is the value that occurs most often. If no number is repeated, then there is no mode for the list



Different Ways of Clustering the Same Set of Points



(a) Original points.



(b) Two clusters.



(c) Four clusters.



(d) Six clusters.

K-means clustering critically depends upon the value of k



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K-Means Clustering Algorithm Mathematical Formulation

(stated mathematically)

Given an initial set of k means $m_1^{(1)}, \dots, m_k^{(1)}$, the algorithm proceeds by alternating between two steps:

[1]

Assignment step: Assign each observation to the cluster whose mean yields the least within-cluster sum of squares. Since the sum of squares is the squared Euclidean distance, this is intuitively the "nearest" mean

$$S_i^{(t)} = \{x_p : \|x_p - m_i^{(t)}\|^2 \leq \|x_p - m_j^{(t)}\|^2 \forall j, 1 \leq j \leq k\},$$

where each x_p is assigned to exactly one $S^{(t)}$, even if it could be assigned to two or more of them.

Update step: Calculate the new means to be the **centroids** of the observations in the new clusters.

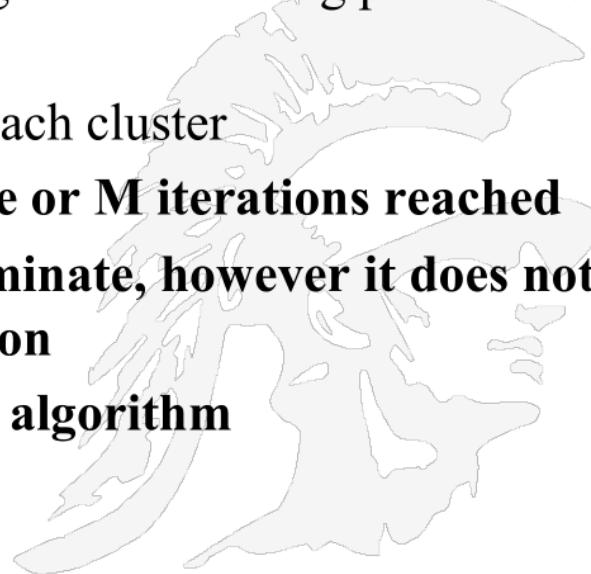
$$m_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{x_j \in S_i^{(t)}} x_j$$

- The algorithm has converged when the assignments no longer change.
- The algorithm will converge to a (local) optimum.
- There is no guarantee that the global optimum is found using this algorithm.





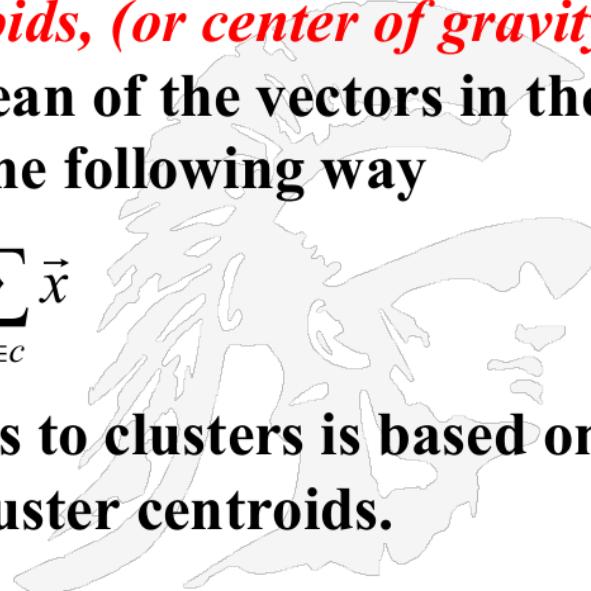
- 1. Select K points as initial centroids**
- 2. repeat**
 - form K clusters by assigning each remaining point to its closest centroid
 - re-compute the centroid of each cluster
- 3. until centroids do not change or M iterations reached**
 - the algorithm will always terminate, however it does not always find the optimal solution
 - this is an example of a greedy algorithm





- Assumes instances are real-valued vectors
 - Let \vec{x} represent the vectors in a cluster c
- Then we define the *centroids, (or center of gravity)*, of the cluster to be the mean of the vectors in the cluster; we write this in the following way

$$\vec{\mu}(c) = \frac{1}{|c|} \sum_{\vec{x} \in c} \vec{x}$$



- Reassignment of instances to clusters is based on distance to the current cluster centroids.

Here is a demo of k-means clustering; this is a copy where you can modify the code (eg. alter the number of clusters, data points, etc.).

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There are Several Possible Distance Metrics

- Euclidean distance (L_2 norm):

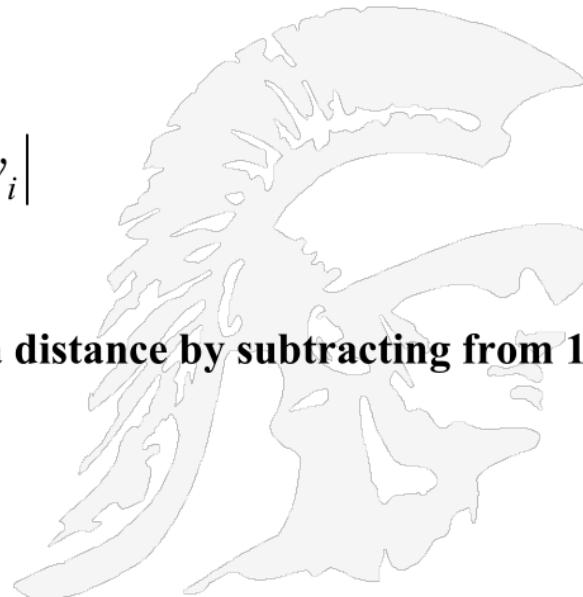
$$L_2(\vec{x}, \vec{y}) = \sqrt{\sum_{i=1}^m (x_i - y_i)^2}$$

- L_1 norm:

$$L_1(\vec{x}, \vec{y}) = \sum_{i=1}^m |x_i - y_i|$$

- Cosine Similarity (transform to a distance by subtracting from 1):

$$1 - \frac{\vec{x} \cdot \vec{y}}{|\vec{x}| \cdot |\vec{y}|}$$

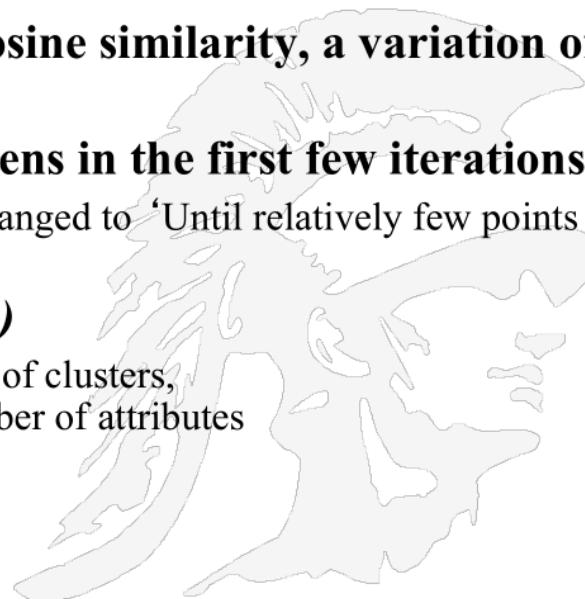


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K-means Clustering – Summary Details

- **Initial centroids are often chosen randomly**
 - Clusters produced vary from one run to another
- **The centroid is (typically) the mean of the points in the cluster**
- **'Closeness' is measured by cosine similarity, a variation of Euclidean distance**
- **Most of the convergence happens in the first few iterations.**
 - Often the stopping condition is changed to 'Until relatively few points change clusters'
- **Complexity is $O(i * k * n * m)$**
 - n = number of points, k = number of clusters,
 i = number of iterations, m = number of attributes

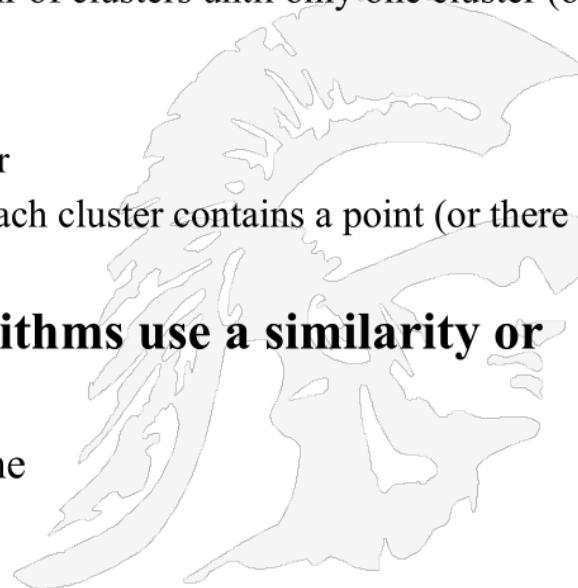


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Hierarchical Clustering Algorithms

- Two main types of hierarchical clustering
 - **Agglomerative:**
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left (bottom-up)
 - **Divisive:**
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each cluster contains a point (or there are k clusters), (top-down)
- Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time



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How Can We Compute the Distance Between Two Clusters

- As before, the **Centroid** of a cluster is the component-wise average of the vectors in a cluster, which is itself a vector
- Example, the Centroid of (1,2,3); (4,5,6); (7,2,6); is (4,3,5)
- **4 possible ways to compute the distance between two clusters**

1. Center of Gravity

- Compute the distance between the two centroids of the cluster

2. Average Link

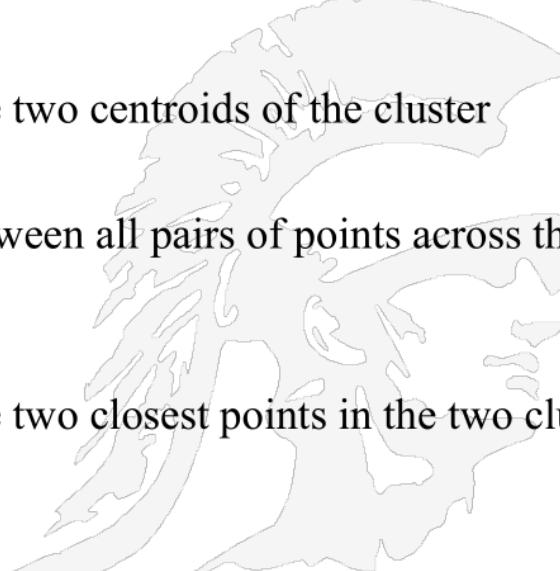
- Compute the average distance between all pairs of points across the two clusters

3. Single Link

- Compute the distance between the two closest points in the two clusters, i.e. the most cosine similar

4. Complete Link

- Compute the distance between the furthest points in the two clusters, i.e. the least cosine similar

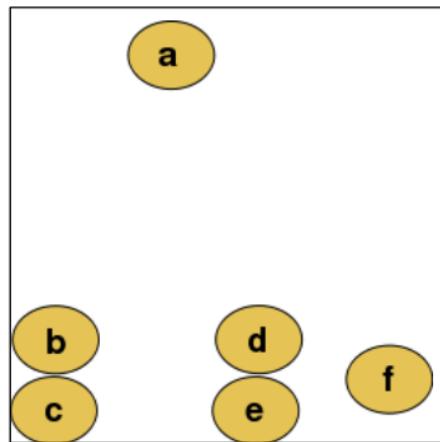


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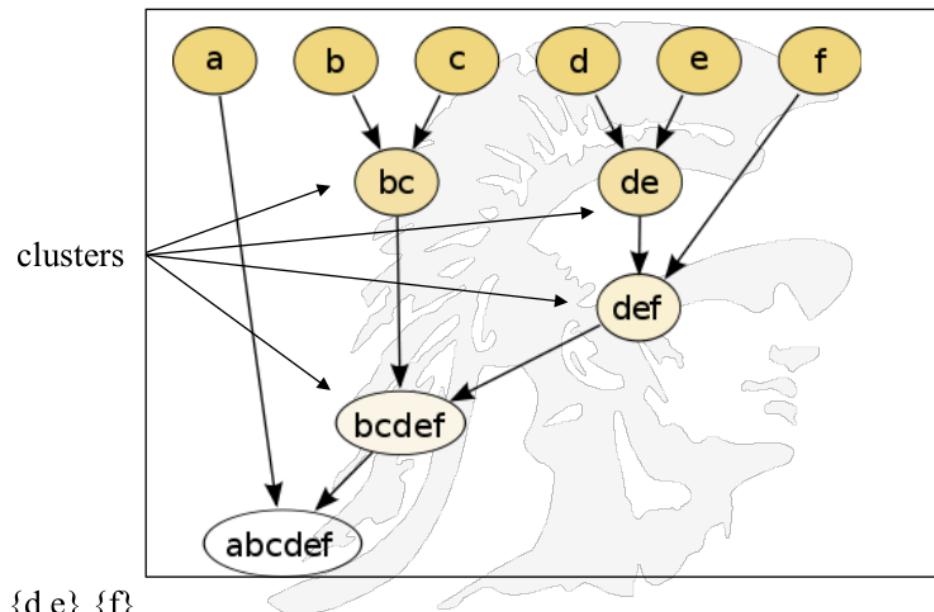
A Dendrogram is Used to Display Clusters

- A **dendrogram** is a tree diagram frequently used to illustrate the arrangement of the clusters produced by hierarchical clustering



original input

second row clusters are: {a}, {b c}, {d e} {f}
third row clusters are: {a}, {b c} {d e f}



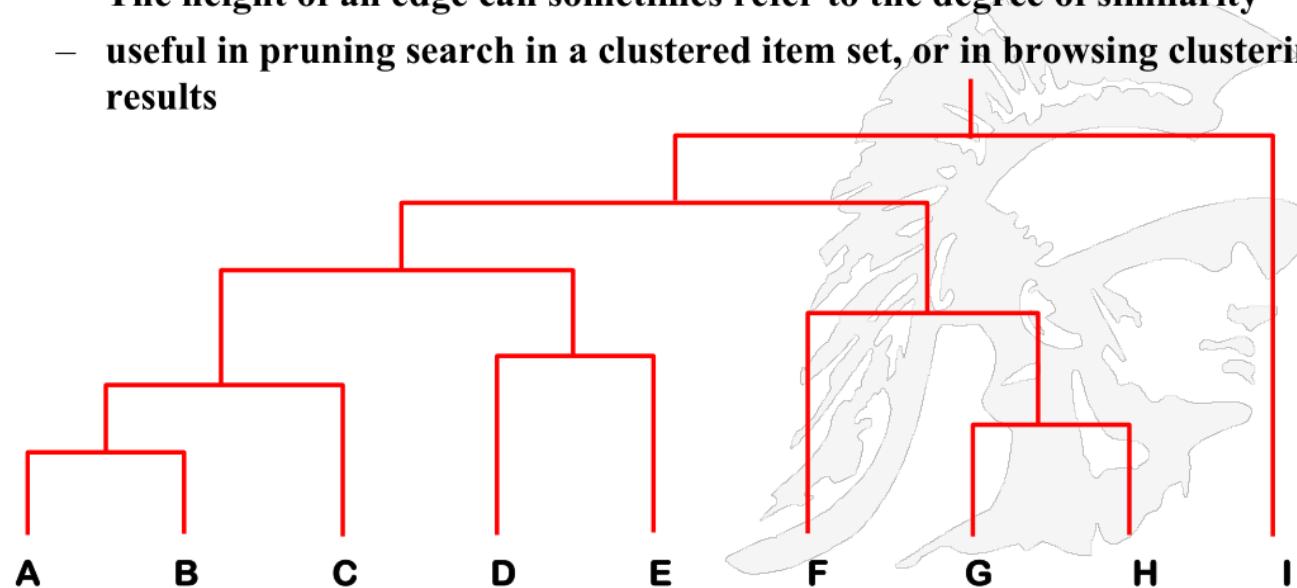
corresponding dendrogram

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Hierarchical Agglomerative Clustering

- HAC starts with unclustered data and performs successive pairwise joins among items (or previous clusters) to form larger ones
 - this results in a hierarchy of clusters which can be viewed as a **dendrogram**
 - Dendograms are usually drawn as shown below
 - The height of an edge can sometimes refer to the degree of similarity
 - useful in pruning search in a clustered item set, or in browsing clustering results



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Divisive Clustering Algorithm

1. Start at the top with all documents in one cluster.
 2. The cluster is split using a partitioning clustering algorithm.
 - Use the k-means clustering algorithm, which is linear in computing time whereas HAC (hierarchical agglomerative clustering) algorithms are quadratic
 3. Apply the procedure recursively until each document is in its own singleton cluster
- Studies show that the divisive algorithms produce more accurate hierarchies than bottom up
 - Bottom-up methods make clustering decisions based on local patterns without initially taking into account the global distribution. These early decisions cannot be undone.
 - Top-down clustering benefits from complete information about the global distribution when making top-level partitioning decisions.

