Clustering

Today's Topic: Clustering

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

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

What is NOT Clustering

- 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

Applications of Clustering 3 Scenarios

1. A telephone company needs to establish its network by putting its towers in a particular region it has acquired. The location of putting these towers can be found by using a clustering algorithm so that all its users receive optimum signal strength

2. The Miami DEA wants to make its law enforcement more stringent and hence have decided to make their patrol vans stationed across the area so that the areas of high crime rates are in the vicinity to the patrol vans

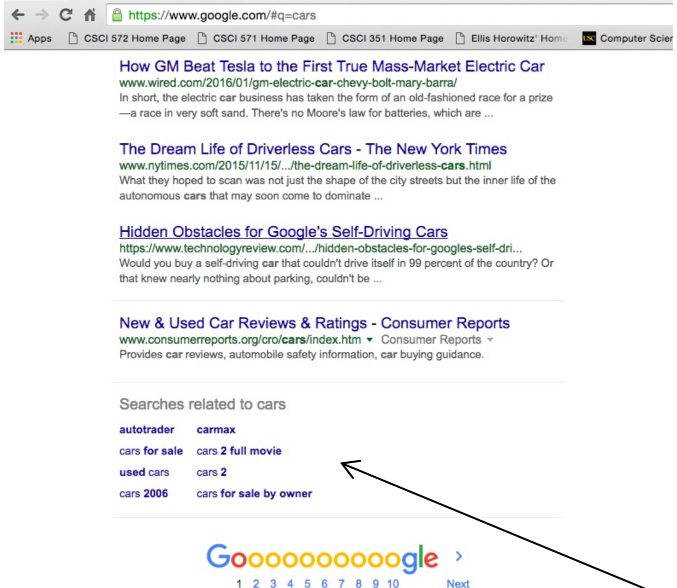
3. A hospital care chain wants to open a series of Emergency-Care wards, keeping in mind the factor of maximum accident prone areas in a region

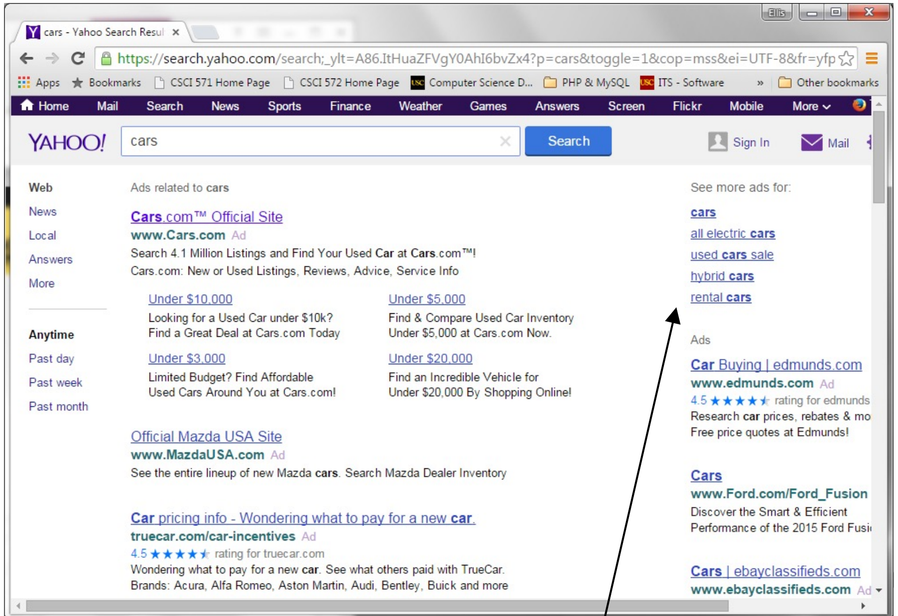
Why Search Engines Cluster Documents

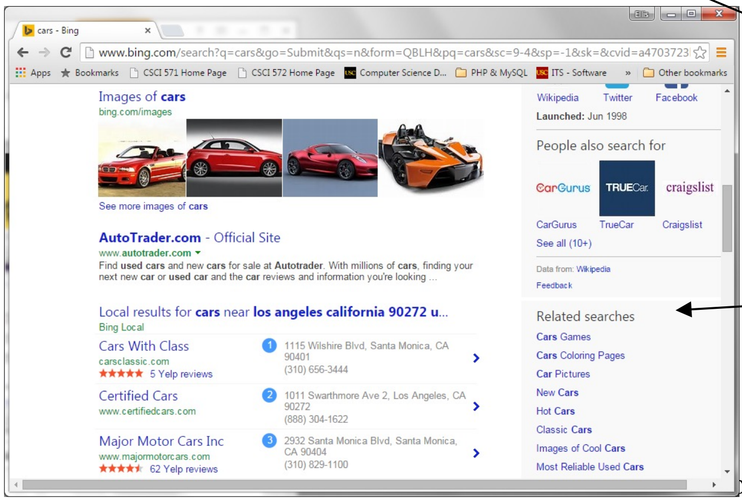
1. **For improving recall in search applications**
   – Better search results; similar documents are grouped
2. **For speeding up vector space retrieval**
   – Faster search if clustering occurs a priori
3. **Cleaner user interface**
4. **Automatic thesaurus generation by clustering related terms**

- ***Cluster hypothesis*** **- Documents with similar text are related**
- **Ergo, to improve search recall:**
  – In theory we could cluster docs in our corpus a priori so
  when a query matches a doc *D*, we also return other docs in the cluster containing *D*
  – ***This strategy doesn't work for search engines***

Related Searches are a Form of Clustering







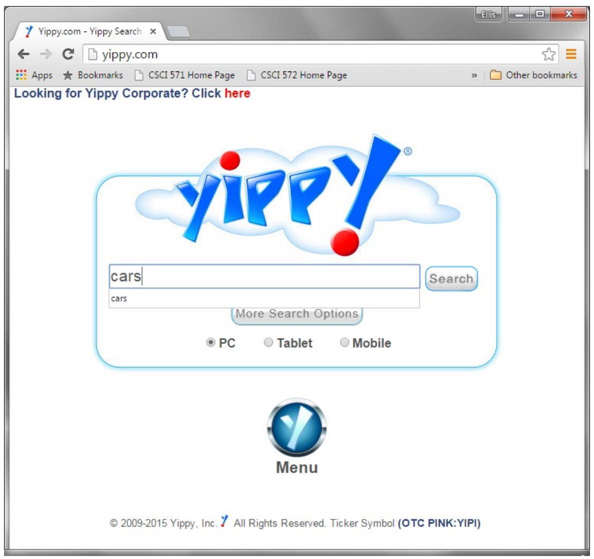
Google related searches

Yahoo does some clustering via alternate queries

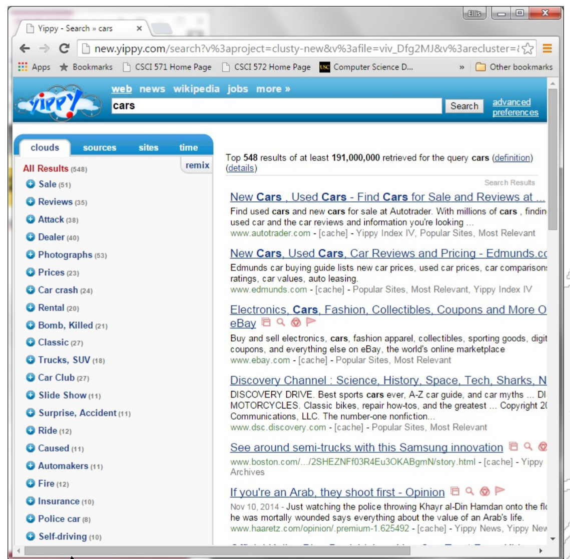
Bing does a little better

yippy.com Search Engine

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



initial screen
with query "cars"

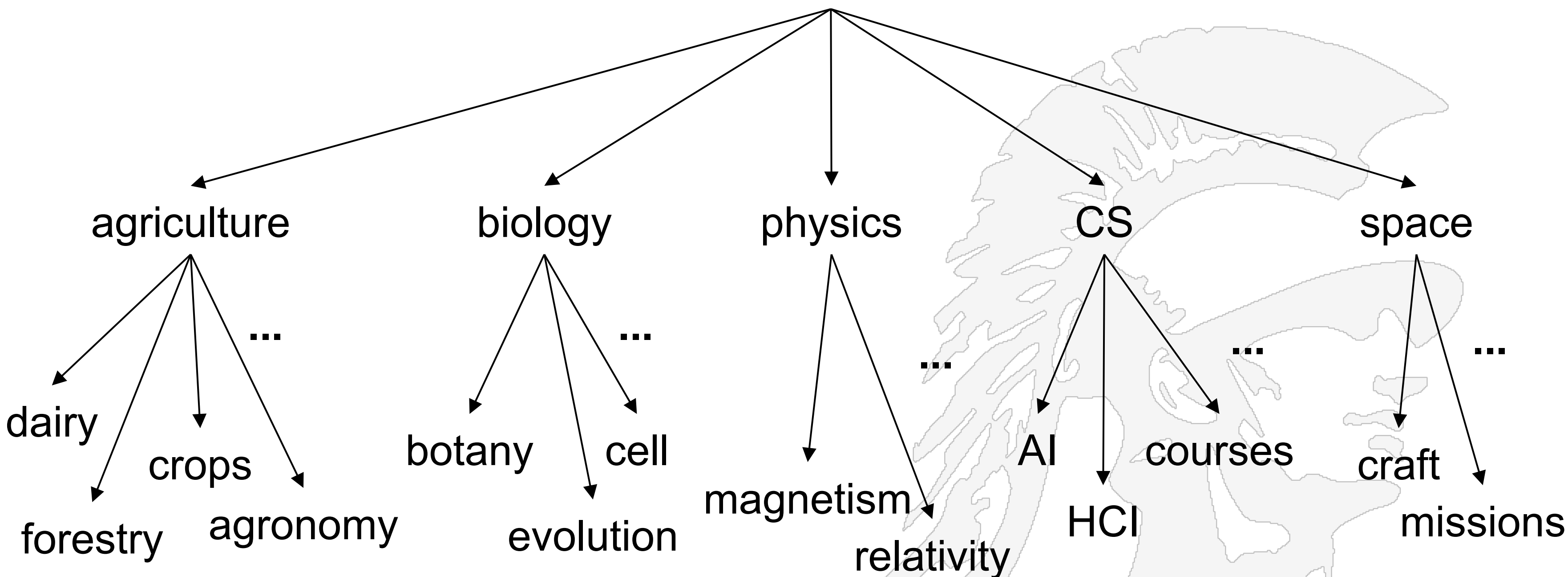


clustered results appear
on the left column: e.g.
sale
reviews
dealers
rentals

multiple level clusters:
car dealers
trucks
ebay

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

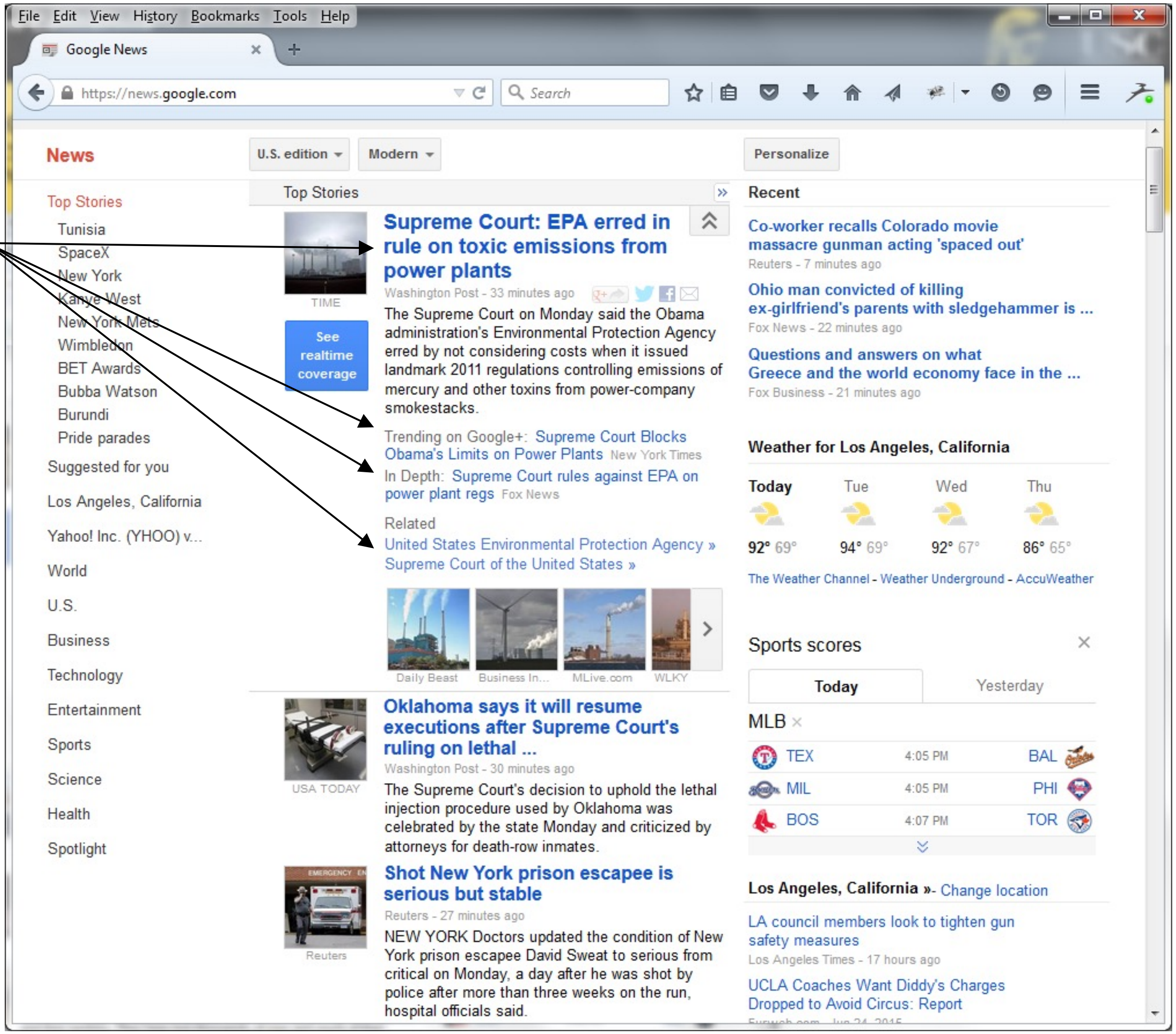
Yahoo! Hierarchy *isn't* clustering but *is* the kind of output you want from clustering – a taxonomy



See https://searchengineland.com/yahoo-directory-close-204370

Google News: Automatic Clustering Gives an Effective News Presentation Metaphor

recent Supreme court decisions clustered together



Typical newspaper clusters: World, US, Business, Technology, Sports, etc

These clusters must be constantly re-computed to make sure the latest news is included

Clustering Examples from Google RSS Feeds

Two examples of Google feeds
There is a main article, some text and beneath that related or clustered articles

Tesla's Model 3 Market Opportunity Is Bigger Than You Think
Motley Fool
Tesla's (NASDAQ:TSLA) forthcoming Model 3 will be unveiled next month, go into production in late 2017, cost about $35,000 before incentives, and ...

Tesla Signs Lease for 40K-SF Red Hook Dealership - Commercial Observer
Advertising enters the equation for **Tesla** Motors - Seeking Alpha
Tesla Motors Finally Gets Its Paws on **Tesla**.com - Inverse
Full Coverage

There's one new **Tesla** car that nobody is talking about
Businessinsider India
These two **Teslas** are all anyone has been talking about lately - especially Wall Street analysts who want to figure out which way **Tesla's** extremely ...

VIDEO: **Tesla** Drag Race! Model S vs. Model X In STUNNING Showdown - AutoSpies.com
Tesla Model S & Model X Comparison (Price, Range, Acceleration) After Removal Of 85 kWh Version - InsideEVs
Tesla Will Begin Taking Preorders on Its Make-or-Break Vehicle - GreatNews
Full Coverage

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

Three Criteria of Adequacy for Clustering Methods

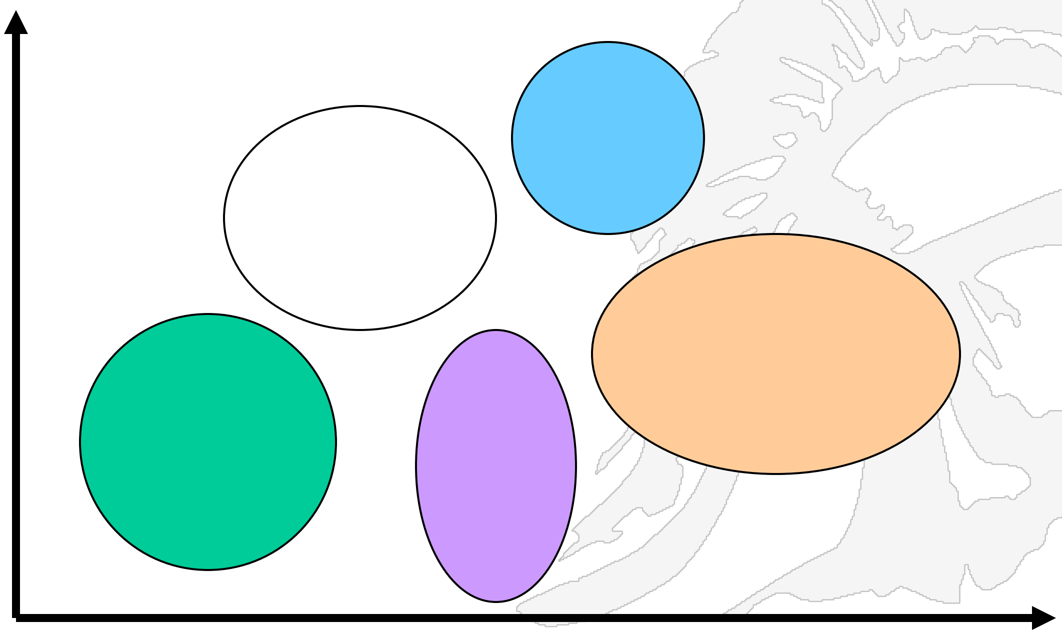
1. The method produces a clustering which is **unlikely to be altered drastically** when further objects are incorporated
   – i.e. it is stable even under significant growth
2. The method is **stable** in the sense that small errors in the description of objects lead to small changes in the clustering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

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

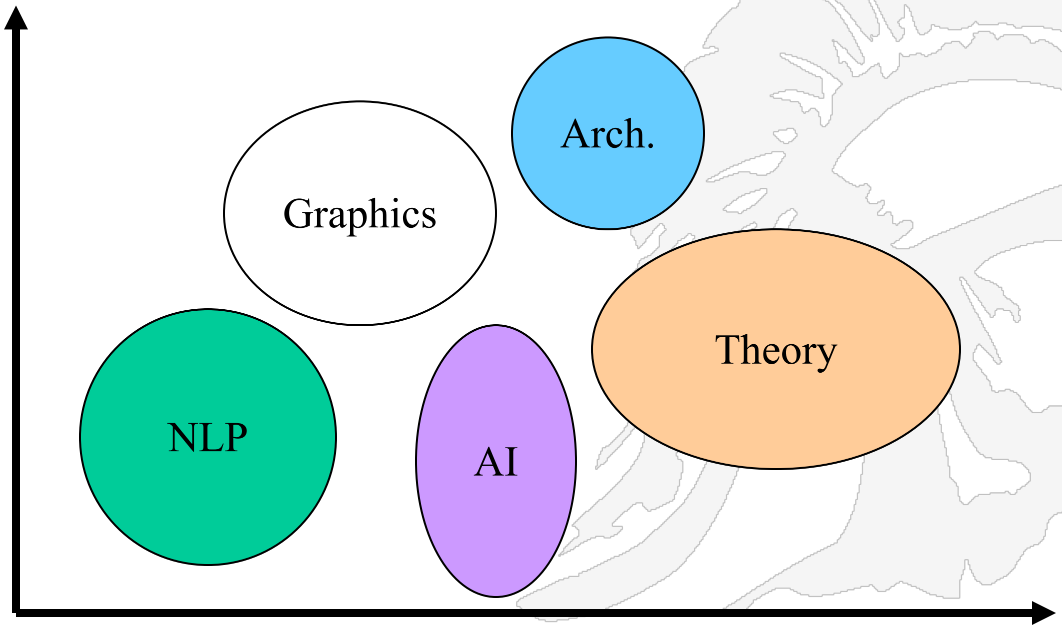
Begin with Clustering

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



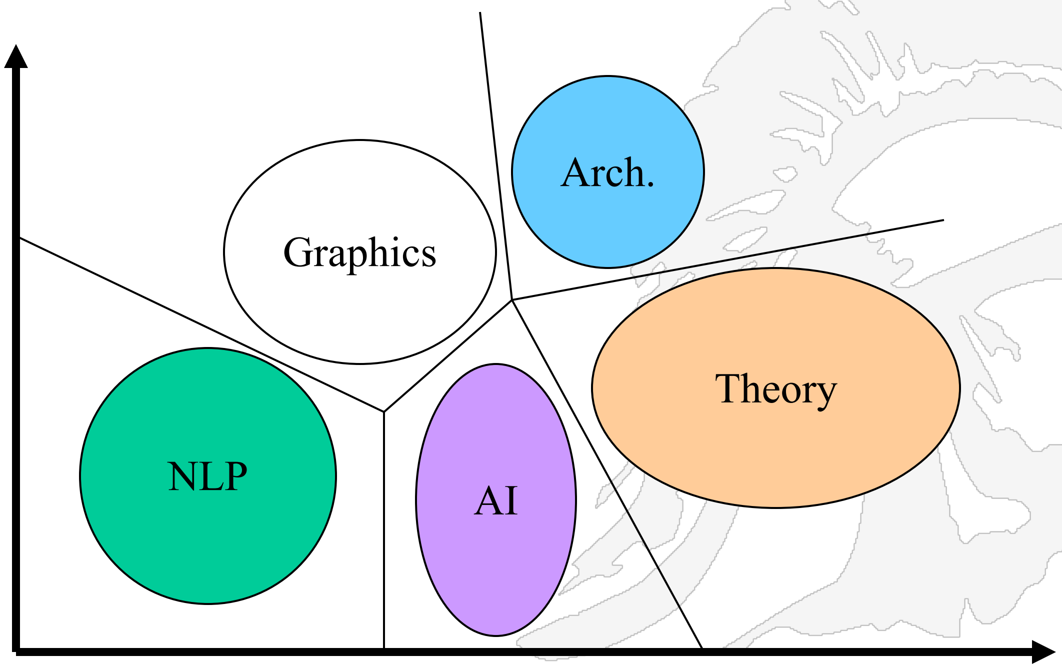
Then We Name the Clusters

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



Still Clustering: Determine Decision Boundaries

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



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**

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*

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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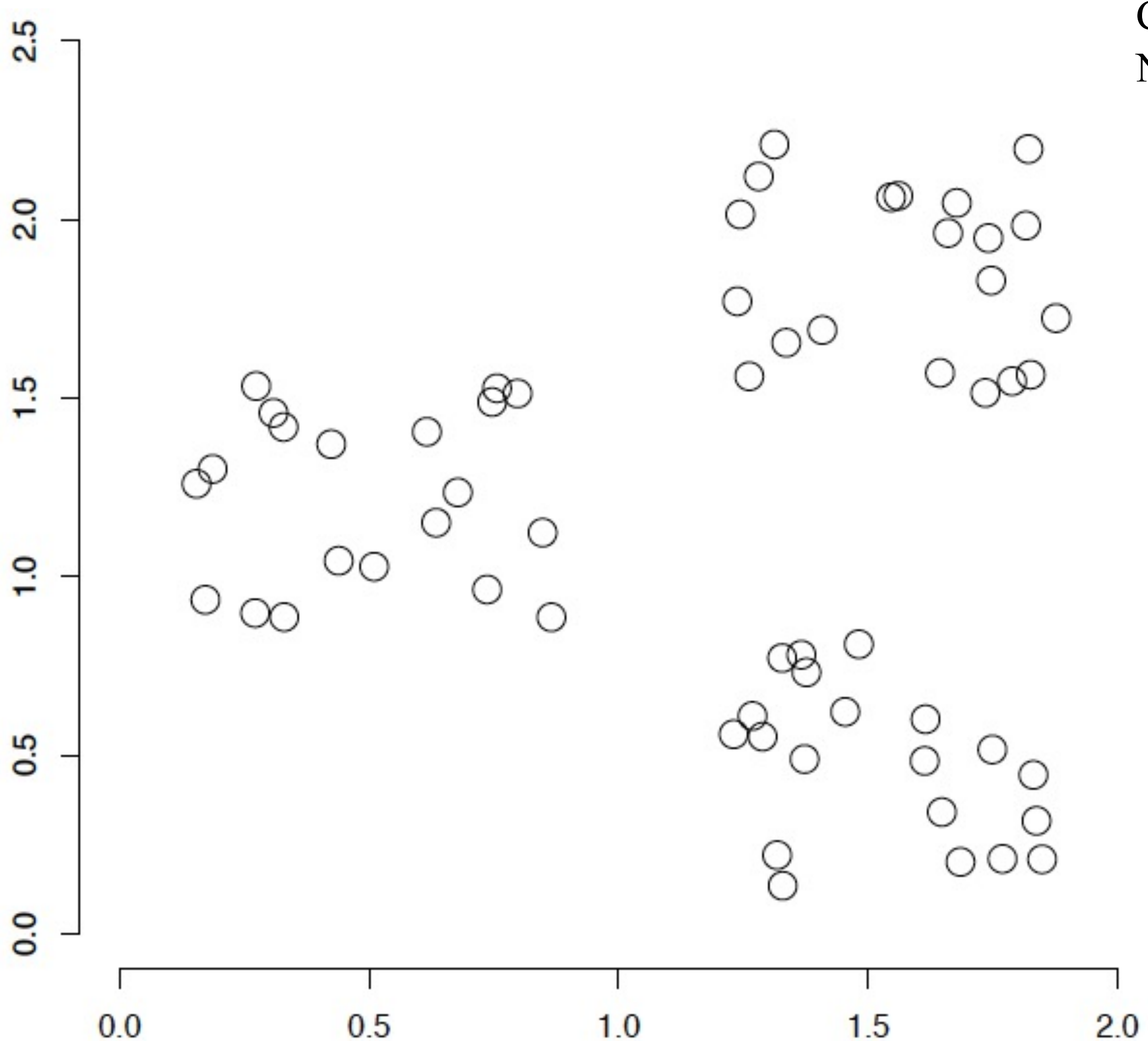
What Definition of Similarity/Distance Will Be Used

- **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)

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

  - **Most clustering implementations use cosine similarity**
  - **Euclidean distance is a close alternative that is also popular**

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**

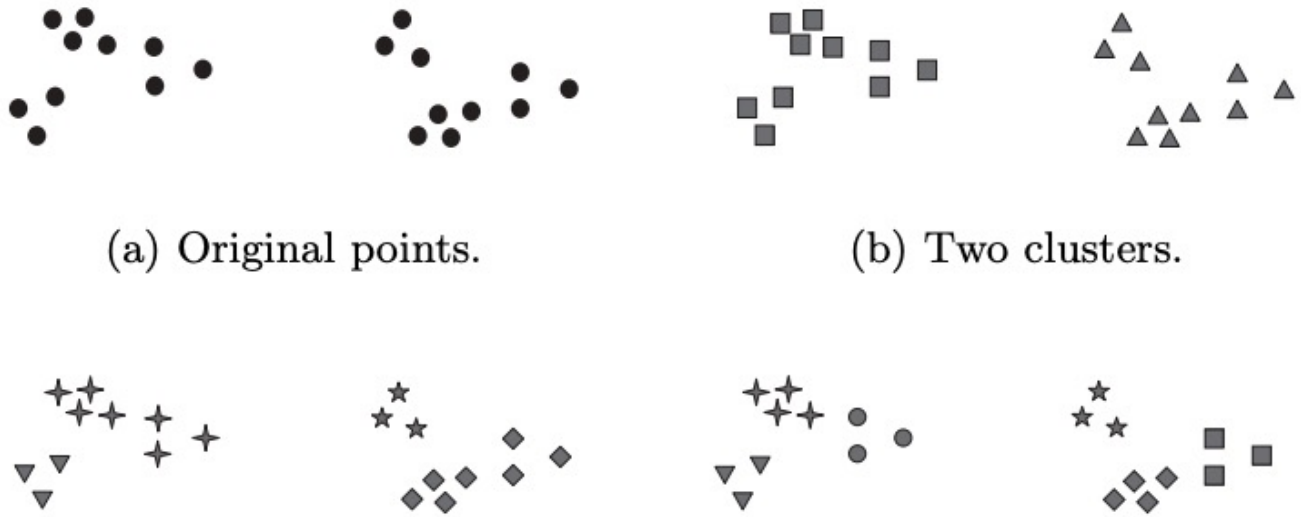
Clustering Algorithms

- **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)

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

"Optimal" K-Means Clustering

- The **optimal *k*-means clustering problem** calls for finding cluster centers that minimize the intra-class variance, i.e. the sum of squared distances from each data point being clustered to its cluster center;
- **The problem stated formally**:
  - Given a finite set S where each element is a vector of length d, find a subset T of size k that minimizes the sum of squares of the distances between elements in S and their closest element in T
- Finding an exact solution to the k-means problem for arbitrary input has been shown to be **NP-hard**
- **NP**-hardness (non-deterministic polynomial-time **hard**), in computational complexity theory, is a class of problems that are, informally, "at least as **hard** as the hardest problems in **NP**".
- finding a polynomial algorithm to solve any NP-hard problem would give polynomial algorithms for all the problems in NP, which is unlikely

K-Means Clustering Algorithm Mathematical Formulation

(*stated mathematically*)

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

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

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

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.

An Approximation Clustering 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**

K-Means Depends on Centroids

- **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.**

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:**

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

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

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

Some Adjustments to the Algorithm

- **How to pick the initial cluster means points**
  - **Try multiple runs**
    - Choose different random points as the cluster means and see which yields the best result
  - **Select the original set of means by methods other than random**
    - E.g., pick the most distant (from each other) points as cluster centers (this is called the *k-means*++ algorithm)
- **For termination conditions there are several possibilities, e.g.,**
  - After a fixed number of iterations
  - When the document partition is unchanged
  - When the centroid positions don't change

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Time Complexity

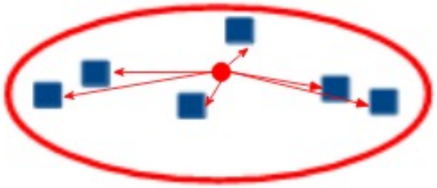
- **Computing distance between two vectors is O*(m)* where *m* is the dimensionality of the vectors**
- **Re-assigning *n* vectors to *k* clusters: *O(kn)* distance computations, or *O(knm)***
- **Computing centroids: Each vector gets added once to some centroid: *O(nm)***
- **Assume these two steps are each done once for *i* iterations: *O(iknm)***
- ***Note:***
- ***m is the size of the vector***
- ***n is the number of vectors (items)***
- ***k is the number of clusters***
- ***i depends upon convergence***

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

Additional Evaluation Metrics for K-means Clustering

- ***inertia*** evaluates how far the points are within a cluster, or specifically the sum of distances of all the points within a cluster from the centroid of that cluster



Intra cluster distance

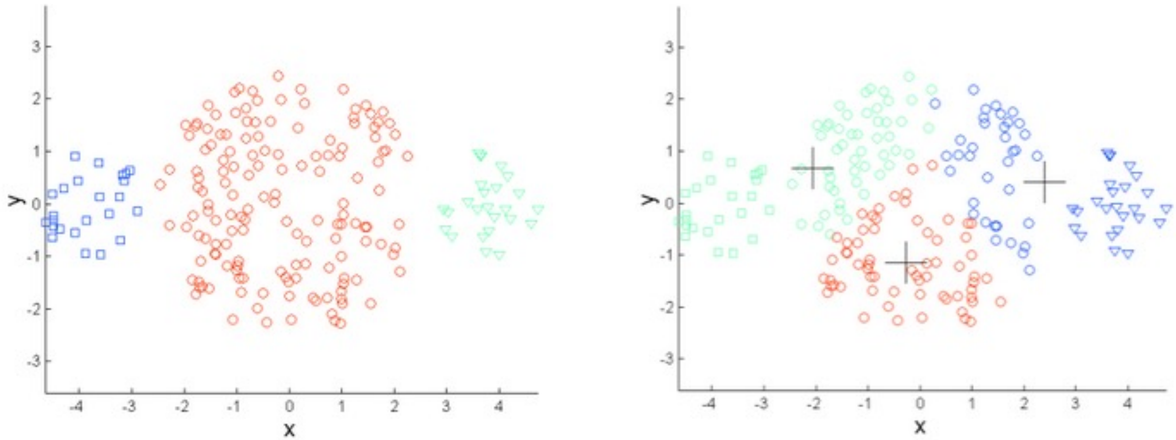
- ***Dunn Index*** takes into account the distance between two clusters. This distance between the centroids of two different clusters is known as **inter-cluster distance**. It is computed as the ratio of the minimum inter-cluster distance and the maximum of the intra-cluster distances

$$\text{Dunn Index} = \frac{\text{min(Inter cluster distance)}}{\text{max(Intra cluster distance)}}$$

- *The larger the min(inter-cluster distance) the farther apart are the clusters; the smaller the max(intra-cluster distance) the more compact are the clusters*

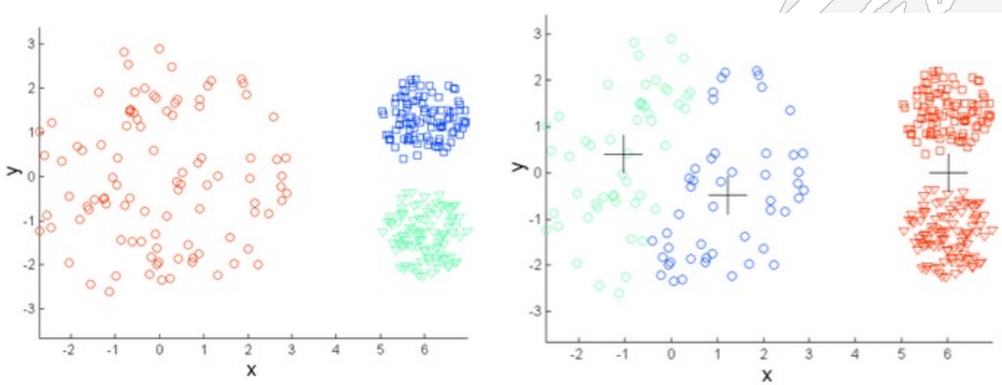
Difficulties with K-Means Clustering

When cluster sizes are very different in size, points in the larger section can be mis-clustered



Original Points K-means (k = 3)

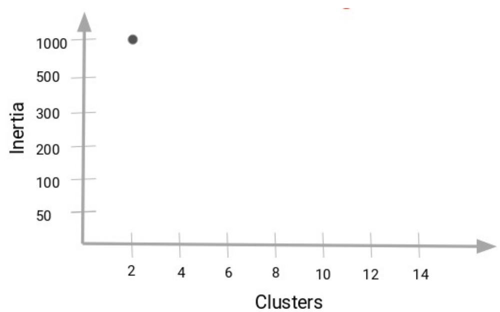
When the densities of the original points are different the more spreadout points can be mis-clustered



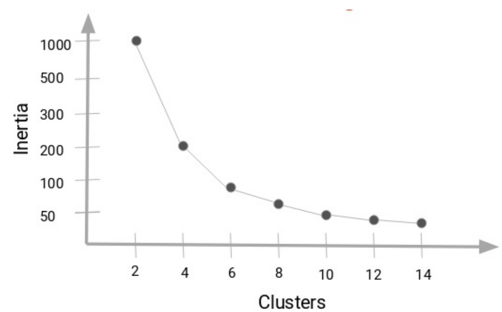
Original Points K-means (k = 3)

How to Choose the Right Number of Clusters

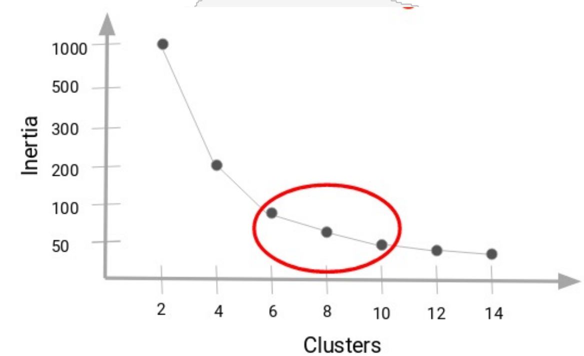
- **Plot a graph, also known as an elbow curve, where the x-axis will represent the number of clusters and the y-axis will be an evaluation metric.**
- **Let's say we use inertia**



Train your model on 2 clusters
Compute and plot the inertia



Train the model on successively higher clusters



Any number of clusters between 6 and 10 will work

the cluster value where this decrease in inertia value becomes constant can be chosen as the right cluster value for your data.

Evaluating K-Means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
  - can show that m_i corresponds to the center (mean) of the cluster
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Limitations of K-Means

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- K-means has problems when the data contains outliers

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

Agglomerative Clustering Algorithm - a Bottom Up Approach

- **Basic Agglomerative Clustering Algorithm**
  1. Compute the distance matrix between the input data points (i.e. the distance between all pairs of points)
  2. Let each data point be a cluster unto itself
  3. Repeat
  4. Merge the two closest clusters
  5. Update the distance matrix
  6. Until only a single cluster remains

- **Key operation is the computation of the distance between two clusters**
  – Different definitions of the distance between clusters lead to somewhat different algorithms

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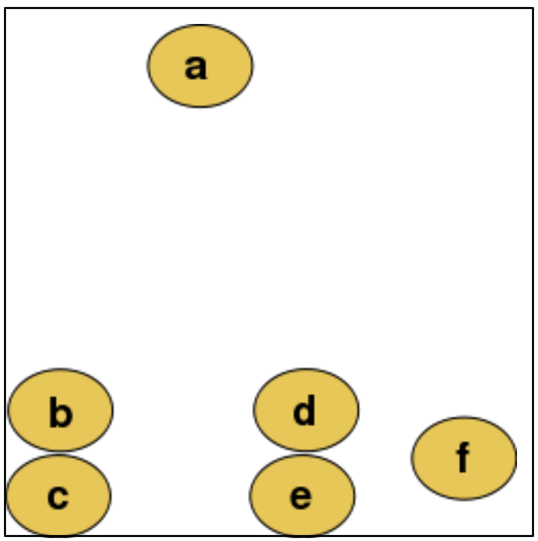
How Can We Compute the Distance Between Two Clusters

- 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**

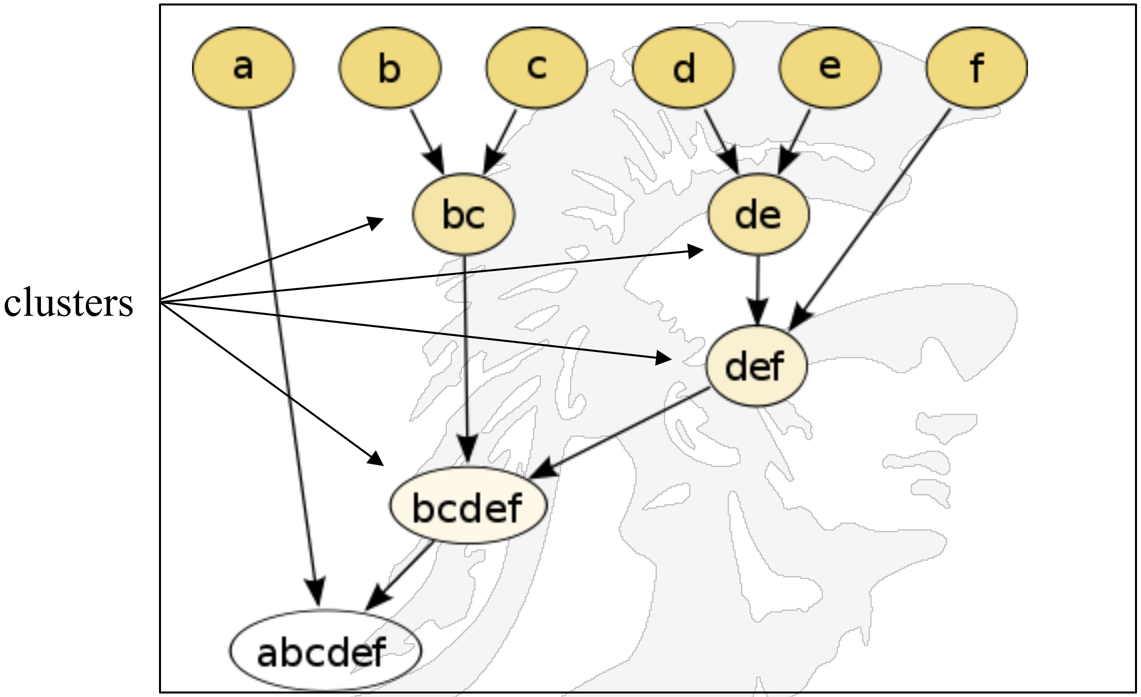
1. **Center of Gravity**
   – Compute the distance between the two centroids of the cluster
2. **Average Link**
   – Compute the average distance between all pairs of points across the two clusters
3. **Single Link**
   – Compute the distance between the two closest points in the two clusters, i.e. the most cosine similar
4. **Complete Link**
   – Compute the distance between the furthest points in the two clusters, i.e. the least cosine similar

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



corresponding dendrogram

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

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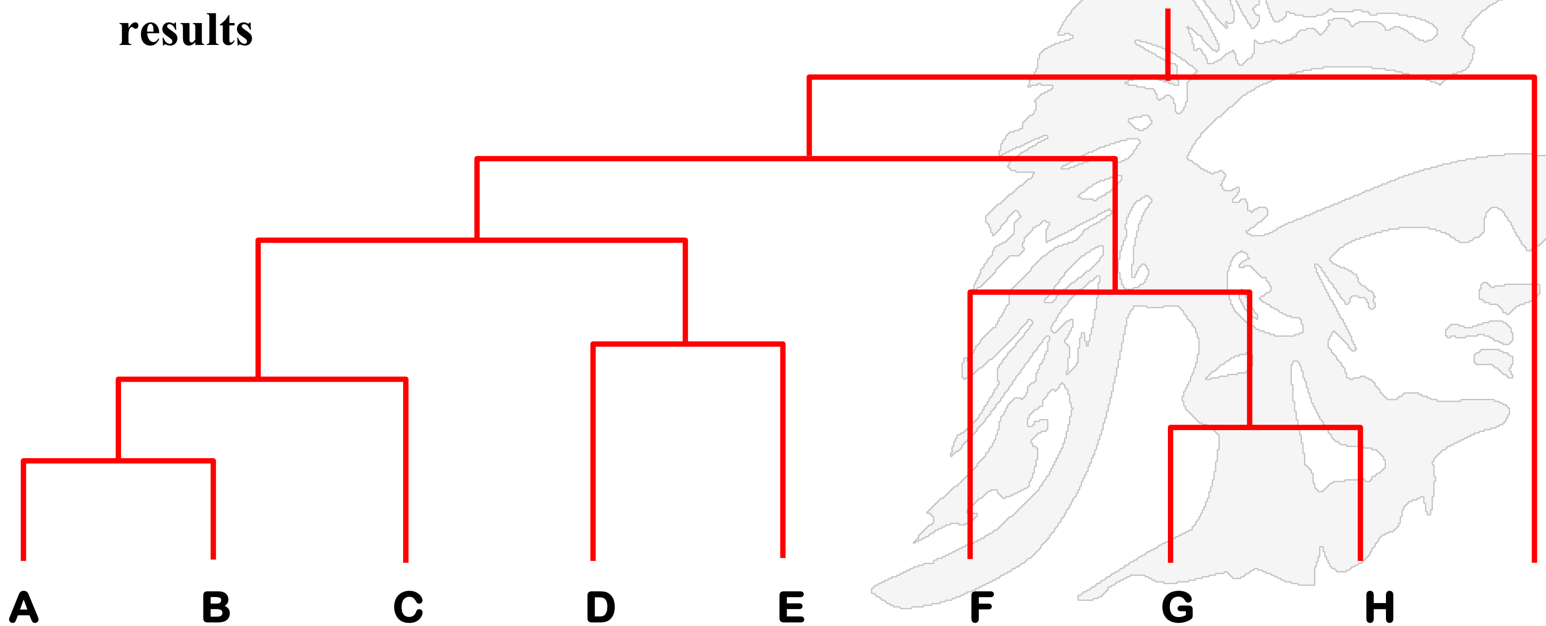
Hierarchical Agglomerative Clustering

- 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
  - Dendrograms 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

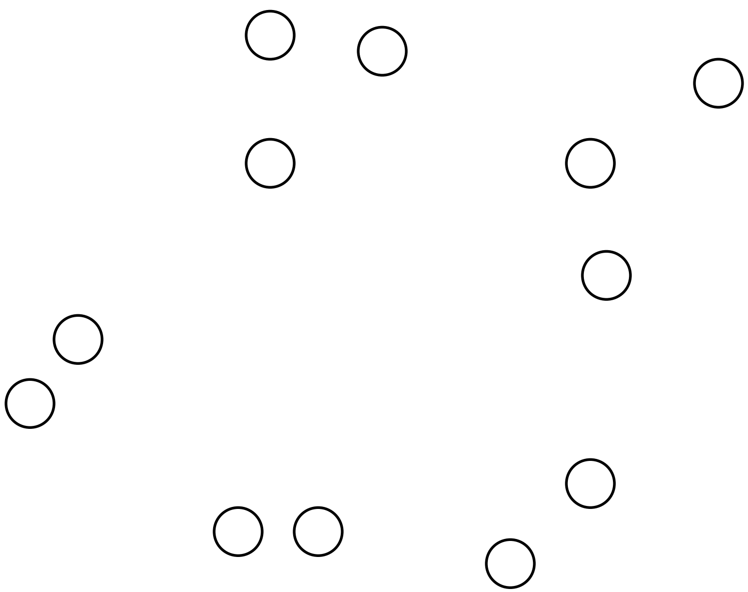


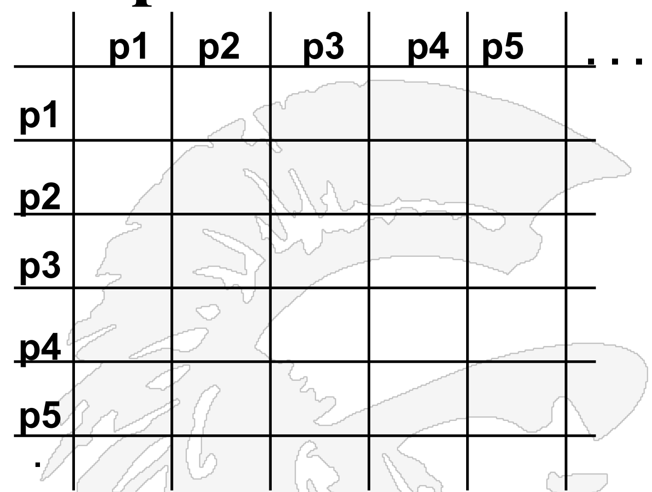
Hierarchical Agglomerative Clustering

- **Basic procedure**
  - **1.** Place each of N documents into a class of its own.
  - 2. Compute all pairwise document-document similarity coefficients
    - ***Total of N(N-1)/2 coefficients***
  - **3. Form a new cluster by combining the most similar pair of current clusters *i* and *j***
    - (use one of the methods described in a previous slide, e.g., complete link, etc.);
    - update similarity matrix by deleting the rows and columns corresponding to *i* and *j*;
    - calculate the entries in the row corresponding to the new cluster *i+j*.
  - **4. Repeat step 3 if the number of clusters left is great than 1.**

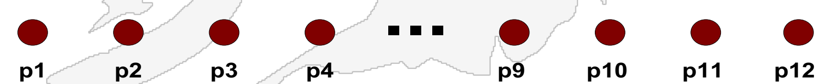
Example of HAC Input/ Initial setting

- Start with clusters of individual points and a distance/proximity matrix



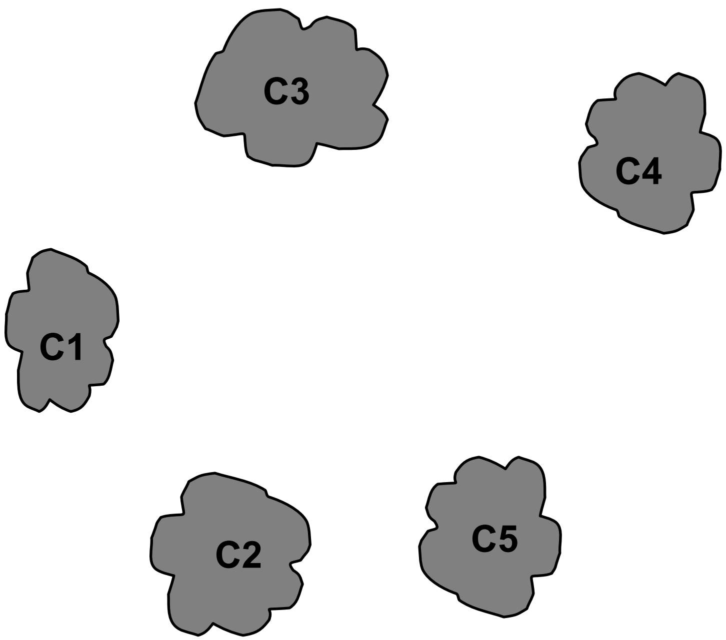


Distance/Proximity Matrix



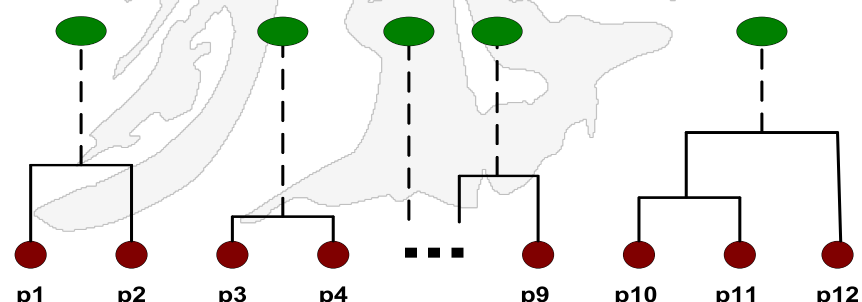
Intermediate State

- After some merging steps, we have some clusters



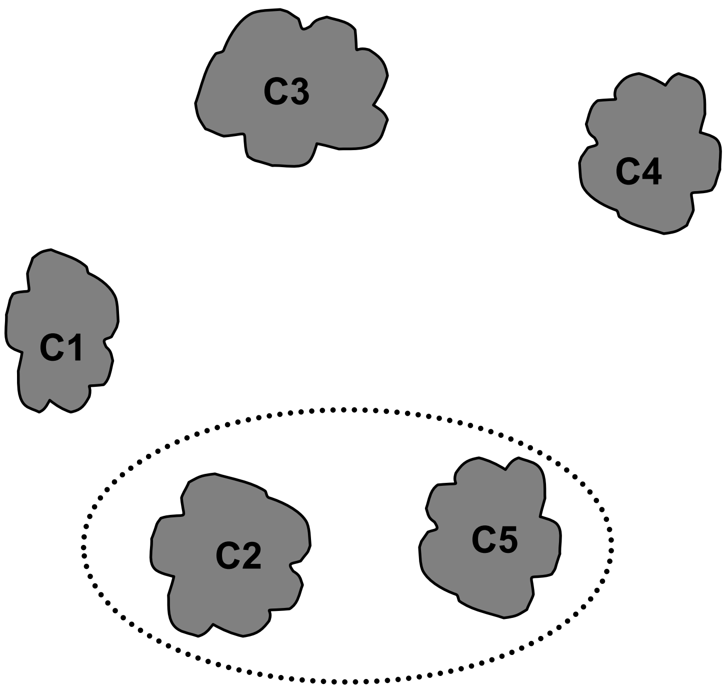
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

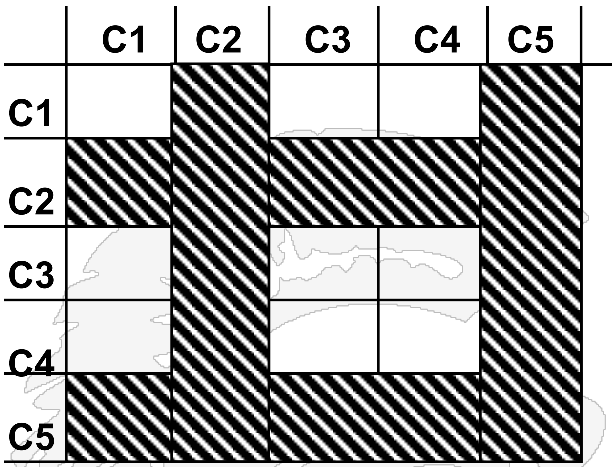
Distance/Proximity Matrix (above)
Dendrogram (below)



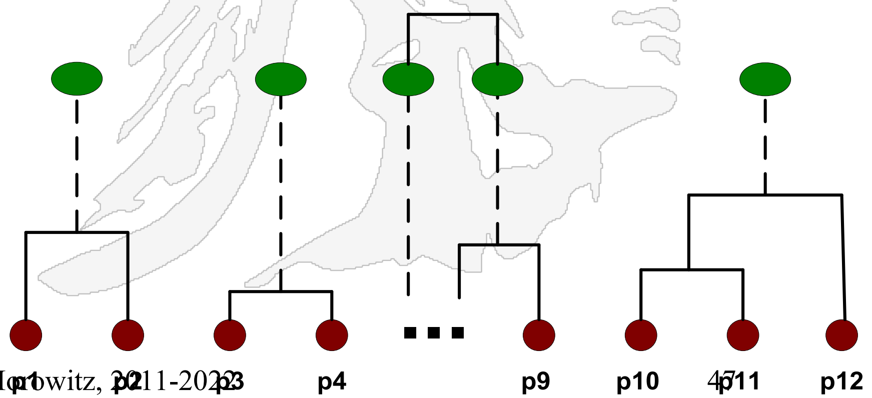
Intermediate State

- **Merge the two closest clusters (C2 and C5) and update the distance matrix.**

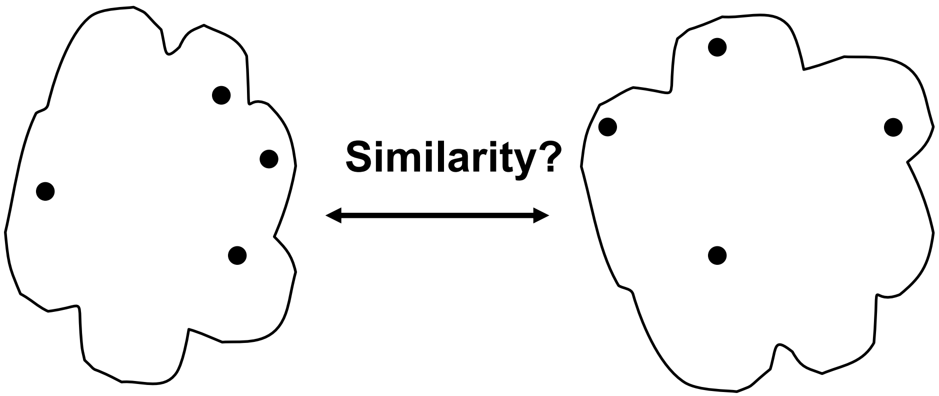




Distance/Proximity Matrix



How to Define Inter-Cluster Similarity



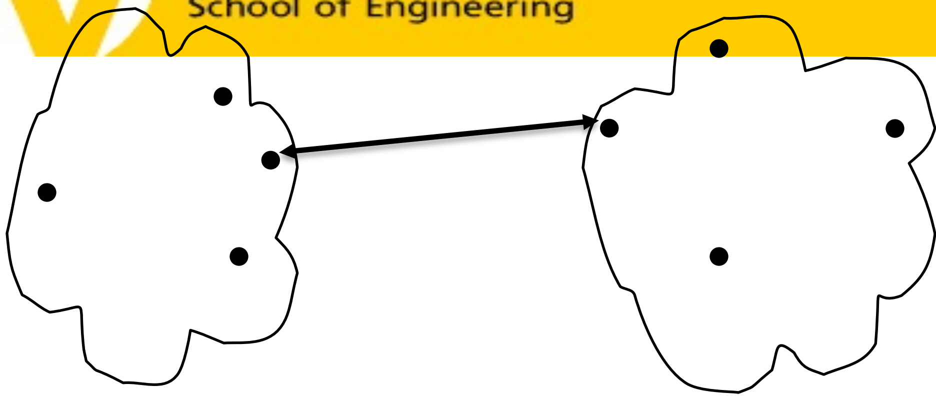
- MIN
- MAX
- Group Average
- Distance Between Centroids

Look back at slide 38

	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

How to Define Inter-Cluster Similarity

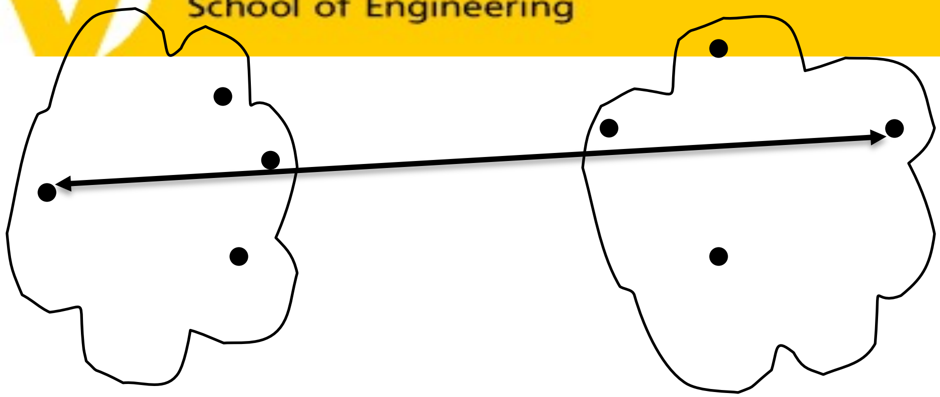


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

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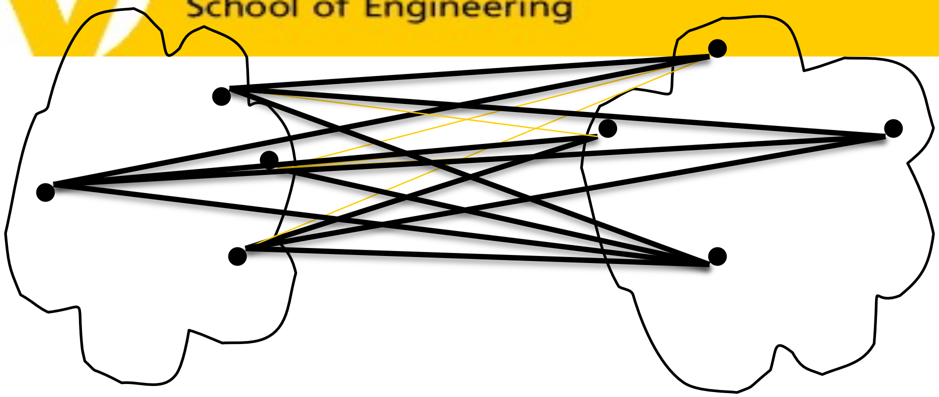
How to Define Inter-Cluster Similarity

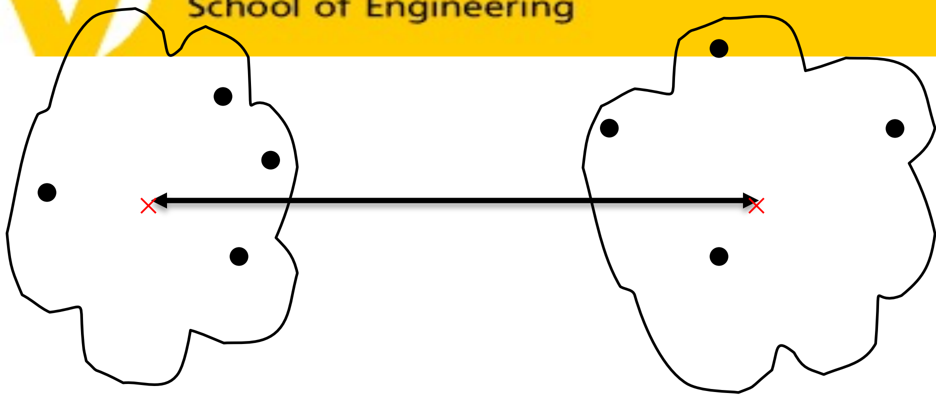


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

How to Define Inter-Cluster Similarity



	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

General Hierarchical Agglomerative Clustering Algorithm and Complexity

1. Compute similarity between all pairs of documents
2. Do N – 1 times
   1. Find closest pair of documents/clusters to merge
   1. Update similarity of all documents/clusters to new cluster

$O(N^2)$

Naïve: $O(N^2)$ Priority Queue: O(N) Single link: O(N)

Naïve: O(N) Priority Queue: O(N log N) Single link: O(N)

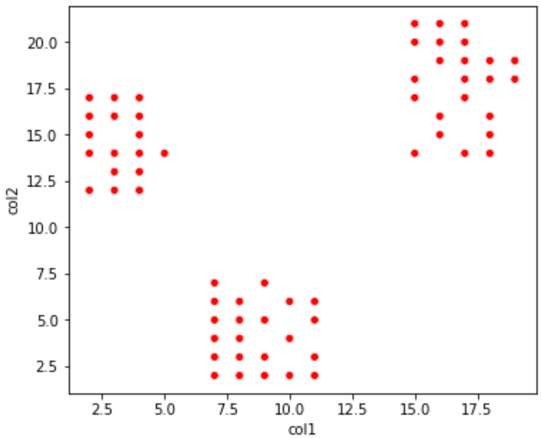
Divisive Clustering Algorithm

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

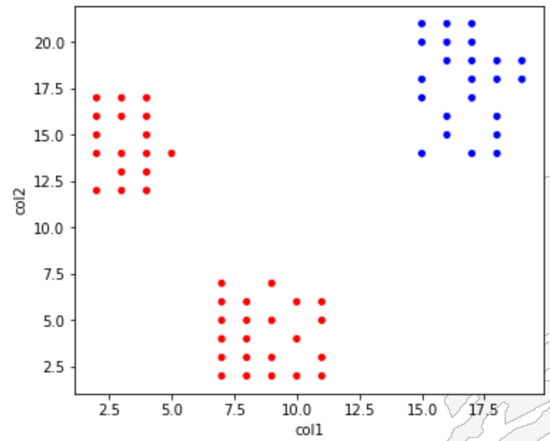
- Studies show that the divisive algorithms produce more accurate hierarchies than bottom up
  - Bottom-up methods make clustering decisions based on local patterns without initially taking into account the global distribution. These early decisions cannot be undone.
  - Top-down clustering benefits from complete information about the global distribution when making top-level partitioning decisions.

Divisive Clustering Example

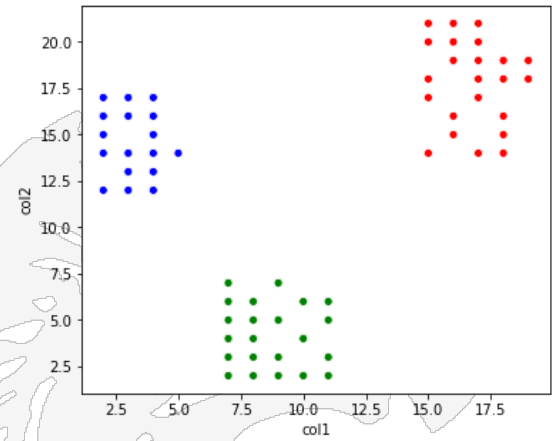
1. Initially, all points in the dataset belong to one single cluster.
2. Partition the cluster into two least similar cluster
3. Proceed recursively to form new clusters until the desired number of clusters is obtained.



All points in one cluster



Two clusters (blue/red)



Three clusters (blue/red/green)

- **At this point the sum of inertia within each of the three clusters is smaller than the previous two examples of two clusters and one cluster**
- **subsequent splitting will only divide points within the existing three clusters**

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How to Label Clusters Two Approaches

1. **Show titles of typical documents**
   – Titles are easy to scan
   – Authors create them for quick scanning!
   – But you can only show a few titles which may not fully represent cluster
2. **Show words/phrases prominent in cluster**
   – Use distinguishing words/phrases
   – But harder to scan

- **Common heuristics - list 5-10 most frequent terms in the centroid vector**
  – Drop stop-words;