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# **Chapter 18 Clustering**

**CS4811 – Artificial Intelligence**

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# Outline

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**Examples**

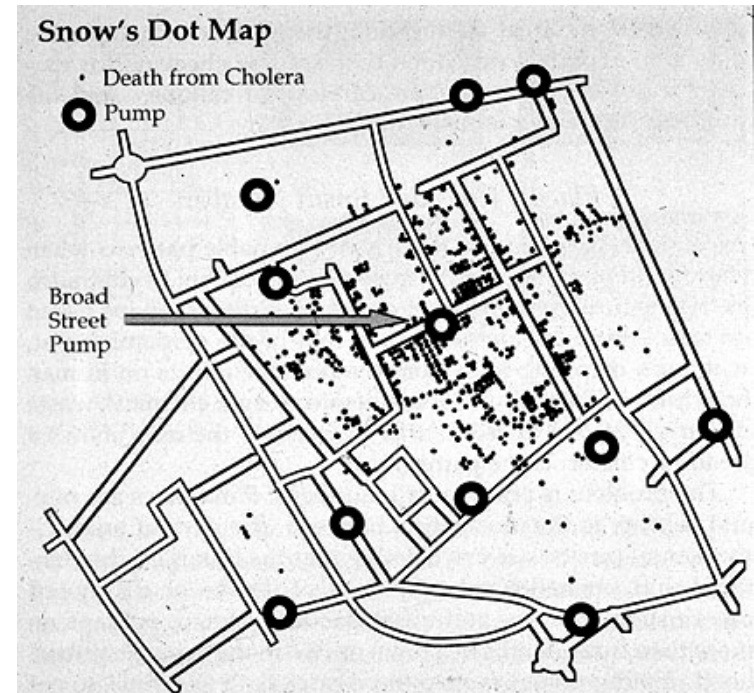
**Centroid approaches**

**Hierarchical approaches**

# Example: a cholera outbreak in London

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Many years ago, during a cholera outbreak in London, John Snow, a physician plotted the location of cases on a map. Properly visualized, the data indicated that cases clustered around certain intersections, where there were polluted wells, not only exposing the cause of cholera, but indicating what to do about the problem.



# Conceptual Clustering

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## *The clustering problem*

Given

- a collection of unclassified objects, and
- a means for measuring the similarity of objects (*distance metric*),

find

- classes (clusters) of objects such that some standard of quality is met (e.g., maximize the similarity of objects in the same class.)

Essentially, it is an approach to *discover* a useful summary of the data.

# Conceptual Clustering (cont'd)

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Ideally, we would like to represent clusters and their semantic explanations. In other words, we would like to define clusters

*extensionally* (i.e., by general rules) rather than *intensionally* (i.e., by enumeration).

For instance, compare

{ X | X teaches AI at MTU CS}, and

{ Laura Brown, Nilufer Onder}

# Curse of dimensionality

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- **While clustering looks intuitive in 2 dimensions, many applications involve 10 or 10,000 dimensions.**
- **High-dimensional spaces look different: the probability of random points being close drops quickly as the dimensionality grows.**

# Higher dimensional examples

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- **Observation that customers who buy diapers are more likely to buy beer than average allowed supermarkets to place beer and diapers nearby, knowing many customers would walk between them. Placing potato chips between increased the sales of all three items.**

SDSS DR4 Navigate Tool

http://cas.sdss.org/dr4/en/tools/chart/navi.asp

**DR4**  
SDSS  
|Home |Help |Chart |List |Exp|

Parameters

ra	18.87837 deg
dec	-0.86083 deg
opt	

**Get Image**

Drawing options

- Grid
- Label
- PhotoObjs
- SpecObjs
- Targets
- Outline
- BoundingBox
- Fields
- Masks
- Plates
- InvertImage

Selected object

ra	18.87684
dec	-0.86097
type	GALAXY
u	14.83
g	13.74
r	13.19
i	12.92
z	12.94

18.87837, -0.86083

Explore  
Recenter  
Add to notes  
Show notes

Done



# Sloan Digital Sky Survey

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- A cool tool to “map the universe.”
- Objects are represented by their radiation in 9 dimensions where each dimension represents radiation in one band of the spectrum.
- Clustered  $2 \times 10^9$  sky objects into similar objects, e.g., stars, galaxies, quasars, etc.
- The objective was to catalog and cluster the entire visible universe. Clustering sky objects by their radiation levels in different bands allowed astronomers to distinguish between galaxies, nearby stars, and many other kinds of celestial objects.

# Clustering CDs

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- **Intuition: music divides into categories and customers prefer a few categories**
- **But what are categories really?**
- **Represent a CD by the customers who bought it**
- **Similar CDs have similar sets of customers and vice versa**

# The space of CDs

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- Think of a space with one dimension for each customer
- Values in a dimension may be 0 or 1 only
- A CD's point in this space is  $(x_1, x_2, \dots, x_n)$ , where  $x_i = 1$  iff the  $i^{\text{th}}$  customer bought the CD
- Compare this with the correlated items matrix:  
rows = customers  
columns = CDs

# Clustering documents

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- Query “**salsa**” submitted to Google returns the following documents among others:
  - How to dance salsa
  - Salsa sauce
  - Salsa music
  - A marketing company called Salsa Labs
- It also presents the related searches:
  - Homemade salsa
  - Salsa artists
  - Canning salsa
  - Musica salsa
- The clusters are: dance, recipe, clubs, sauces, buy, Mexican, bands, natural, ...

# Clustering documents (cont'd)

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- Documents may be thought of as points in a high-dimensional space, where each dimension corresponds to one possible word.
- Clusters of documents in this space often correspond to groups of documents on the same topic, i.e., documents with similar sets of words may be about the same topic.
- Represent a document by a vector  $(x_1, x_2, \dots, x_n)$ , where  $x_i = 1$  iff the  $i^{\text{th}}$  word (in some order) appears in the document.
- Note that  $n$  can be infinite.

# Analyzing protein sequences

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- **Objects are sequences of {C, A, T, G}.**
- **Distance between sequences is “edit distance,” the minimum number of inserts and deletes to turn one into the other.**
- **Note that there is a “distance,” but no convenient space of points.**

# Measuring distance

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- To discuss, whether a set of points is close enough to be considered a cluster, we need a *distance measure*  $D(x,y)$  that tells how far points  $x$  and  $y$  are.
- The axioms for a distance measure  $D$  are:
  1.  $D(x,x) = 0$                       A point is distance 0 from itself
  2.  $D(x,y) = D(y,x)$                       Distance is symmetric
  3.  $D(x,y) \leq D(x,z) + D(z,y)$                       The triangle inequality
  4.  $D(x,y) \geq 0$                       Distance is positive

# K-dimensional Euclidean space

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The distance between any two points, say  $a = [a_1, a_2, \dots, a_k]$  and  $b = [b_1, b_2, \dots, b_k]$  is given in some manner such as:

1. Common distance (“L<sub>2</sub> norm”) :

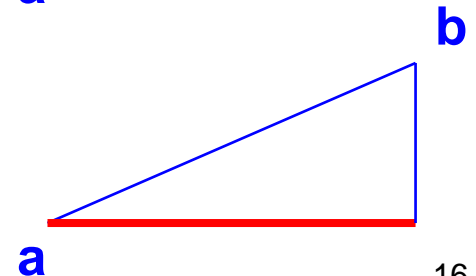
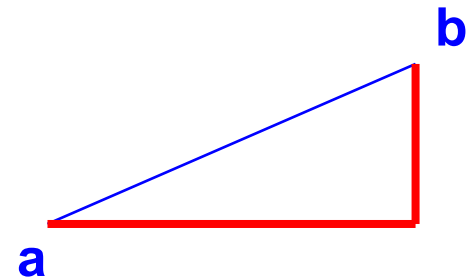
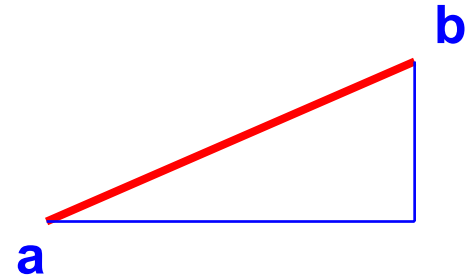
$$\sqrt{\sum_{i=1}^k (a_i - b_i)^2}$$

2. Manhattan distance (“L<sub>1</sub> norm”):

$$\sum_{i=1}^k |a_i - b_i|$$

3. Max of dimensions (“L<sub>∞</sub> norm”):

$$\max_{i=1}^k |a_i - b_i|$$





# Non-Euclidean spaces

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Here are some examples where a distance measure without a Euclidean space makes sense.

- **Web pages**: Roughly  $10^8$ -dimensional space where each dimension corresponds to one word. Rather use vectors to deal with only the words actually present in documents a and b.
- **Character strings**, such as DNA sequences: Rather use a metric based on the LCS---Lowest Common Subsequence.
- **Objects represented as sets of symbolic, rather than numeric, features**: Rather base similarity on the proportion of features that they have in common.

# Non-Euclidean spaces (cont'd)

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**object1 = {small, red, rubber, ball}**

**object2 = {small, blue, rubber, ball}**

**object3 = {large, black, wooden, ball}**

**similarity(object1, object2) = 3 / 4**

**similarity(object1, object3) =**  
**similarity(object2, object3) = 1/4**

**Note that it is possible to assign different weights to features.**

# Approaches to Clustering

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Broadly specified, there are two classes of clustering algorithms:

1. ***Centroid approaches***: We guess the ***centroid*** (central point) in each cluster, and assign points to the cluster of their nearest centroid.

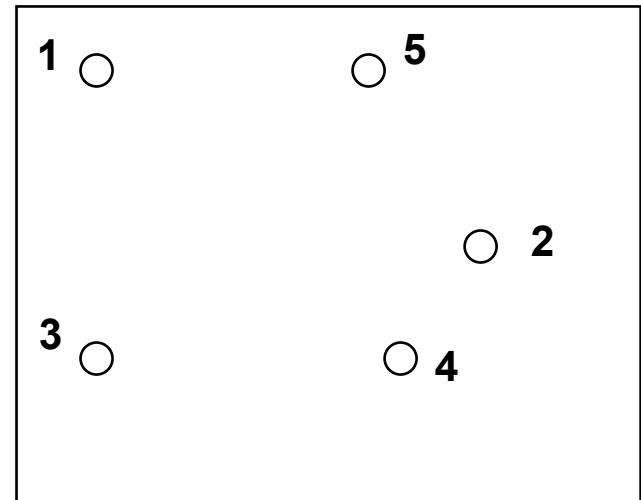
2. ***Hierarchical approaches***: We begin assuming that each point is a cluster by itself. We repeatedly merge nearby clusters, using some measure of how close two clusters are (e.g., distance between their centroids), or how good a cluster the resulting group would be (e.g., the average distance of points in the cluster from the resulting centroid.)

# The $k$ -means algorithm

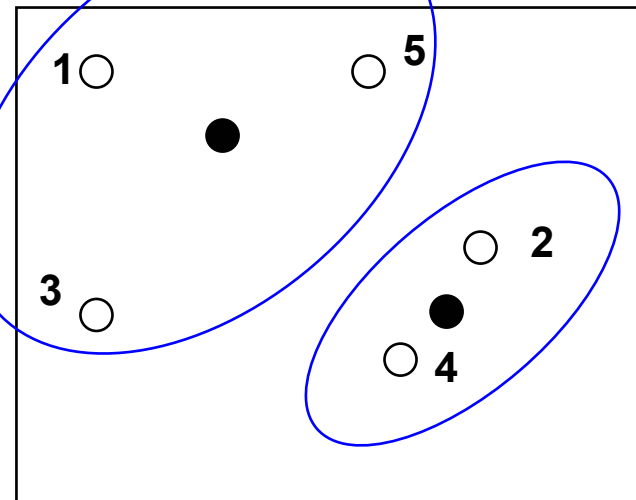
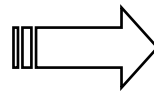
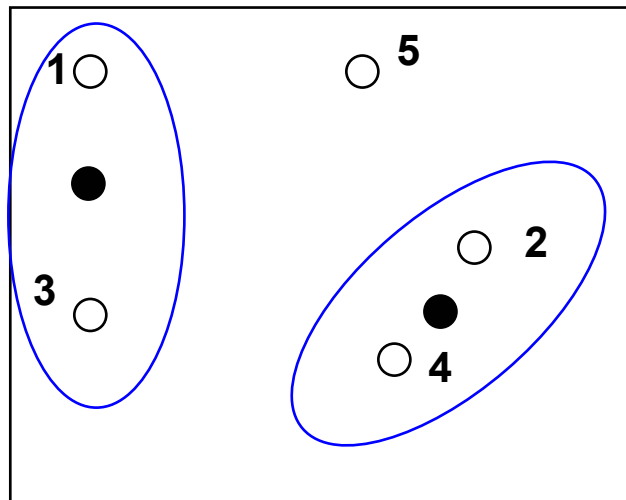
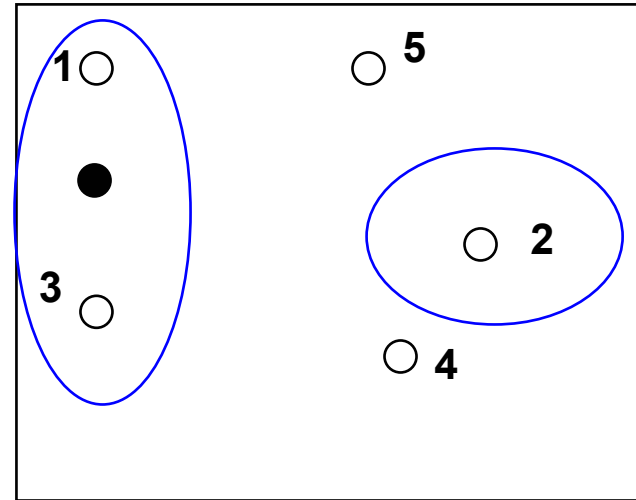
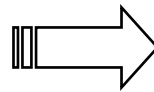
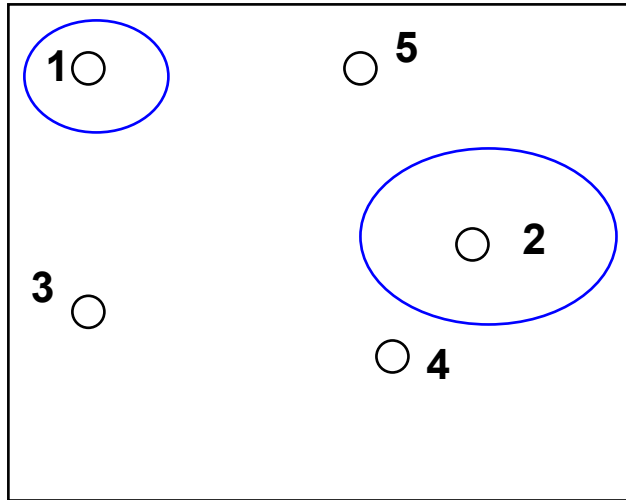
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- Pick  $k$  cluster centroids.
- Assign points to clusters by picking the closest centroid to the point in question. As points are assigned to clusters, the centroid of the cluster may migrate.

**Example:** Suppose that  $k = 2$  and we assign points 1, 2, 3, 4, 5, in that order. Outline circles represent points, filled circles represent centroids.



# The *k*-means algorithm example (cont'd)



# Issues

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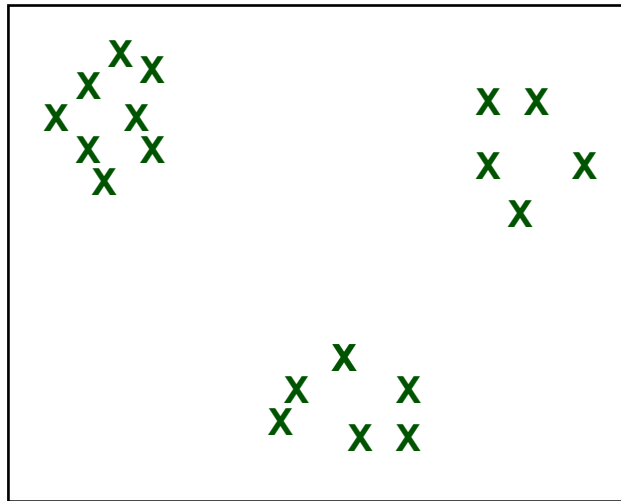
- **How to initialize the  $k$  centroids?**  
Pick points sufficiently far away from any other centroid, until there are  $k$ .
- **As computation progresses, one can decide to split one cluster and merge two, to keep the total at  $k$ . A test for whether to do so might be to ask whether doing so reduces the average distance from points to their centroids.**
- **Having located the centroids of  $k$  clusters, we can reassign all points, since some points that were assigned early may actually wind up closer to another centroid, as the centroids move about.**

# Issues (cont'd)

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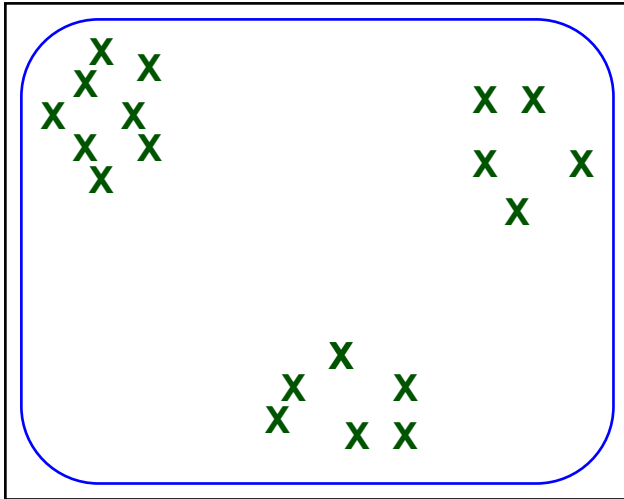
- How to determine  $k$ ?

One can try different values for  $k$  until the smallest  $k$  such that increasing  $k$  does not much decrease the average points of points to their centroids.

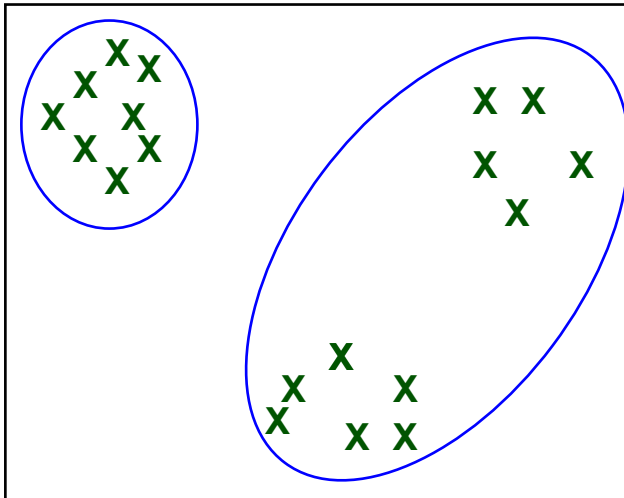


# Determining $k$

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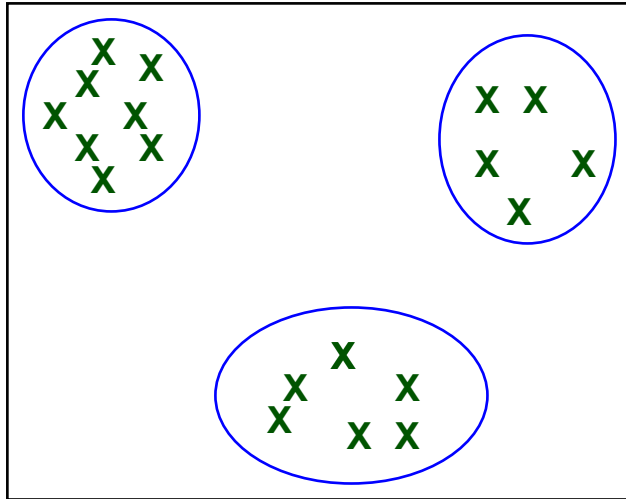
When  $k = 1$ , all the points are in one cluster, and the average distance to the centroid will be high.



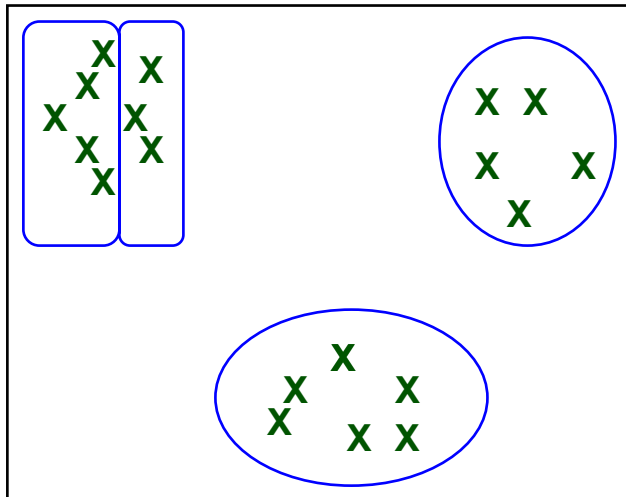
When  $k = 2$ , one of the clusters will be by itself and the other two will be forced into one cluster. The average distance of points to the centroid will shrink considerably.



# Determining $k$ (cont'd)



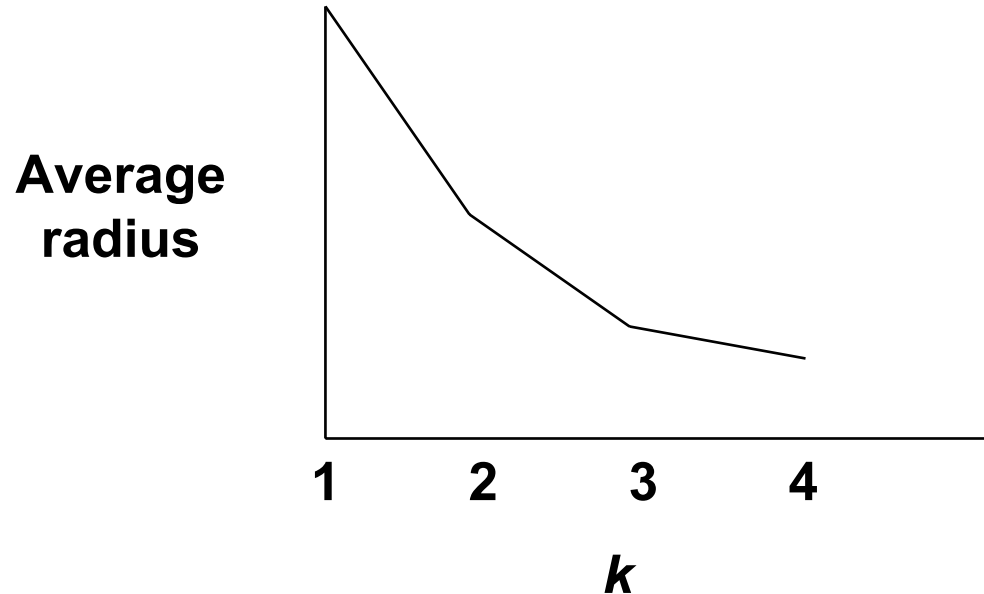
When  $k = 3$ , each of the apparent clusters should be a cluster by itself, and the average distance from the points to their centroids shrinks again.



When  $k = 4$ , then one of the true clusters will be artificially partitioned into two nearby clusters. The average distance to the centroids will drop a bit, but not much.

# Determining $k$ (cont'd)

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**This failure to drop further suggests that  $k = 3$  is right. This conclusion can be made even if the data is in so many dimensions that we cannot visualize the clusters.**

# The CLUSTER/2 algorithm

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- 1. Select  $k$  seeds from the set of observed objects. This may be done randomly or according to some selection function.**
- 2. For each seed, using that seed as a positive instance and all other seeds as negative instances, produce a maximally general definition that covers all of the positive and none of the negative instances (multiple classifications of non-seed objects are possible.)**

# The CLUSTER/2 algorithm (cont'd)

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- 3. Classify all objects in the sample according to these descriptions. Replace each maximally specific description that covers all objects in the category (to decrease the likelihood that classes overlap on unseen objects.)**
- 4. Adjust remaining overlapping definitions.**
- 5. Using a distance metric, select an element closest to the center of each class.**
- 6. Repeat steps 1-5 using the new central elements as seeds. Stop when clusters are satisfactory.**

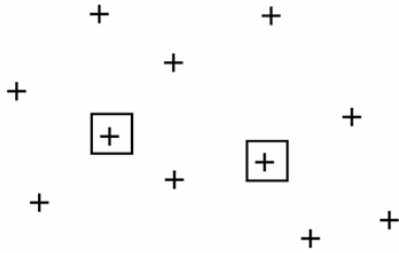
# The CLUSTER/2 algorithm (cont'd)

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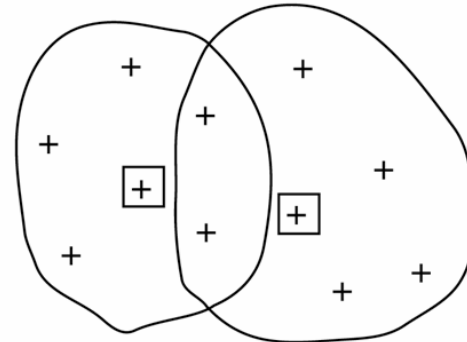
**7. If clusters are unsatisfactory and no improvement occurs over several iterations, select the new seeds closest to the edge of the cluster.**

# The steps of a CLUSTER/2 run

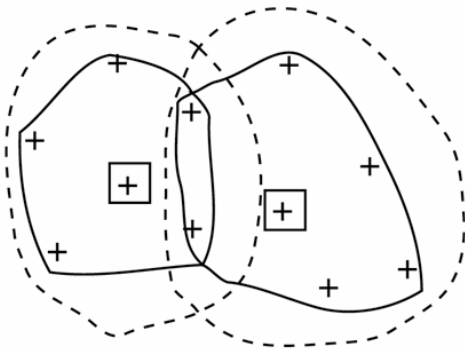
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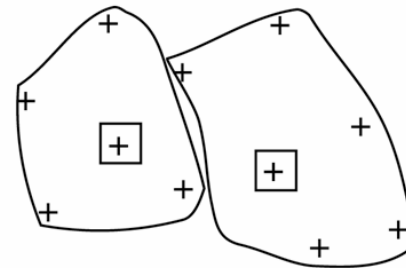
After selecting seeds (step 1).



After generating general descriptions (steps 2 and 3). Note that the categories overlap.



After specializing concept descriptions (step 4). There are still intersecting elements.



After eliminating duplicate elements (step 5).

# Document clustering

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**Automatically group related documents into clusters given some measure of similarity. For example,**

- **medical documents**
- **legal documents**
- **financial documents**
- **web search results**

# Hierarchical Agglomerative Clustering (HAC)

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- **Given  $n$  documents, create a  $n \times n$  doc-doc similarity matrix.**
- **Each document starts as a cluster of size one.**
- **do until there is only one cluster**
  - **Combine the two clusters with the greatest similarity (if  $X$  and  $Y$  are the closest pair of clusters, then we create  $X-Y$  as the parent of  $X$  and  $Y$ . Hence the name “hierarchical”.)**
  - **Update the doc-doc matrix.**



# Example

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Consider A, B, C, D, E as documents with the following similarities:

	A	B	C	D	E
A	-	2	7	9	4
B	2	-	9	11	14
C	7	9	-	4	8
D	9	11	4	-	2
E	4	14	8	2	-

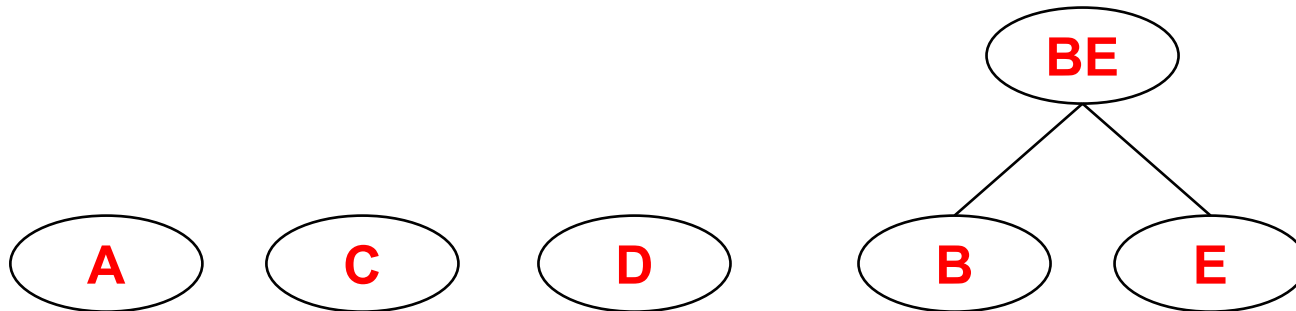
The pair with the highest similarity is:

**B-E = 14**

# Example

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So let's cluster B and E. We now have the following structure:



# Example

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Update the doc-doc matrix:

	A	BE	C	D
A	-	2	7	9
BE	2	-	8	2
C	7	8	-	4
D	9	2	4	-

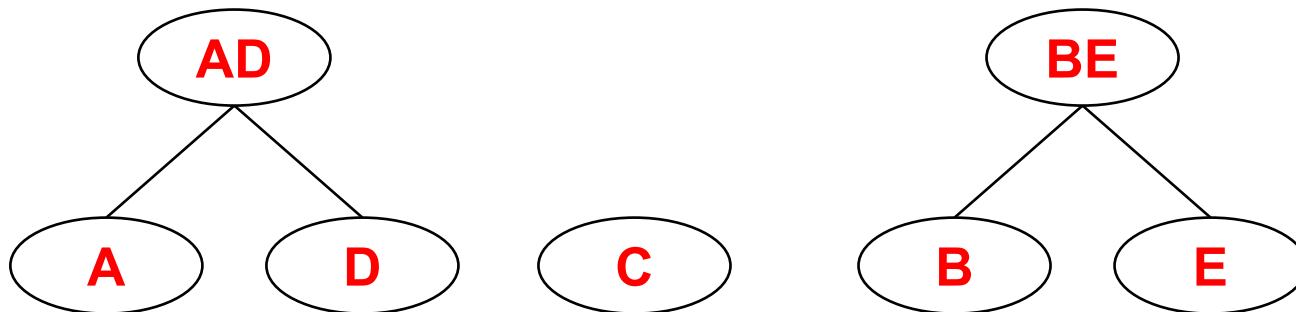
To compute (A, BE):  
take the minimum of  
(A,B)=2 and  
(A,E)=4.

This is called  
*complete linkage*.

# Example

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Highest link is A-D. So let's cluster A and D. We now have the following structure:



# Example

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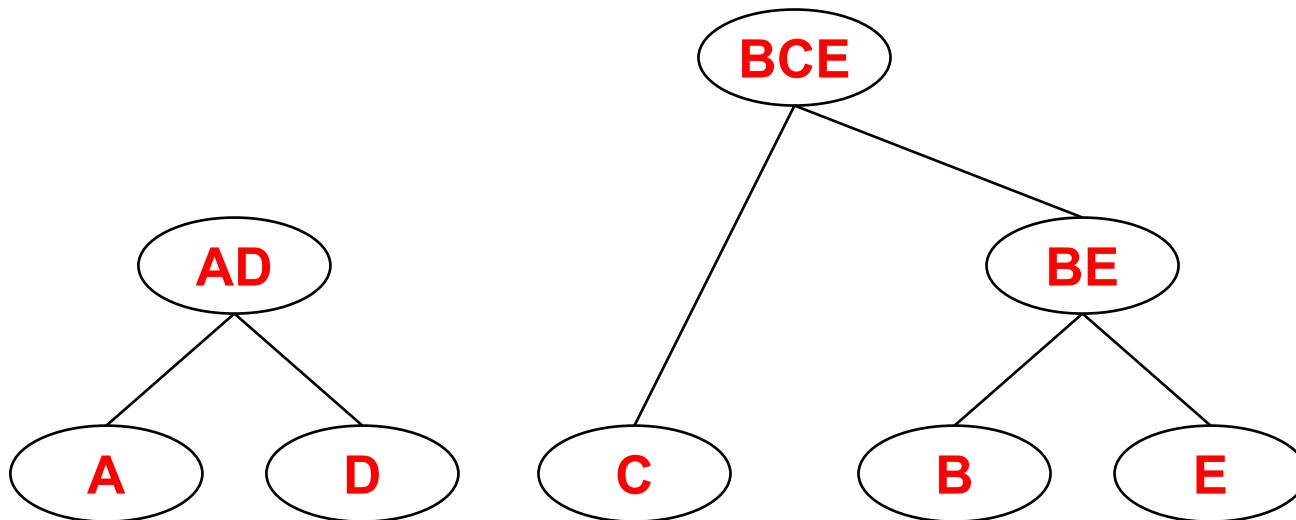
Update the doc-doc matrix:

	AD	BE	C
AD	-	2	4
BE	2	-	8
C	4	8	-

# Example

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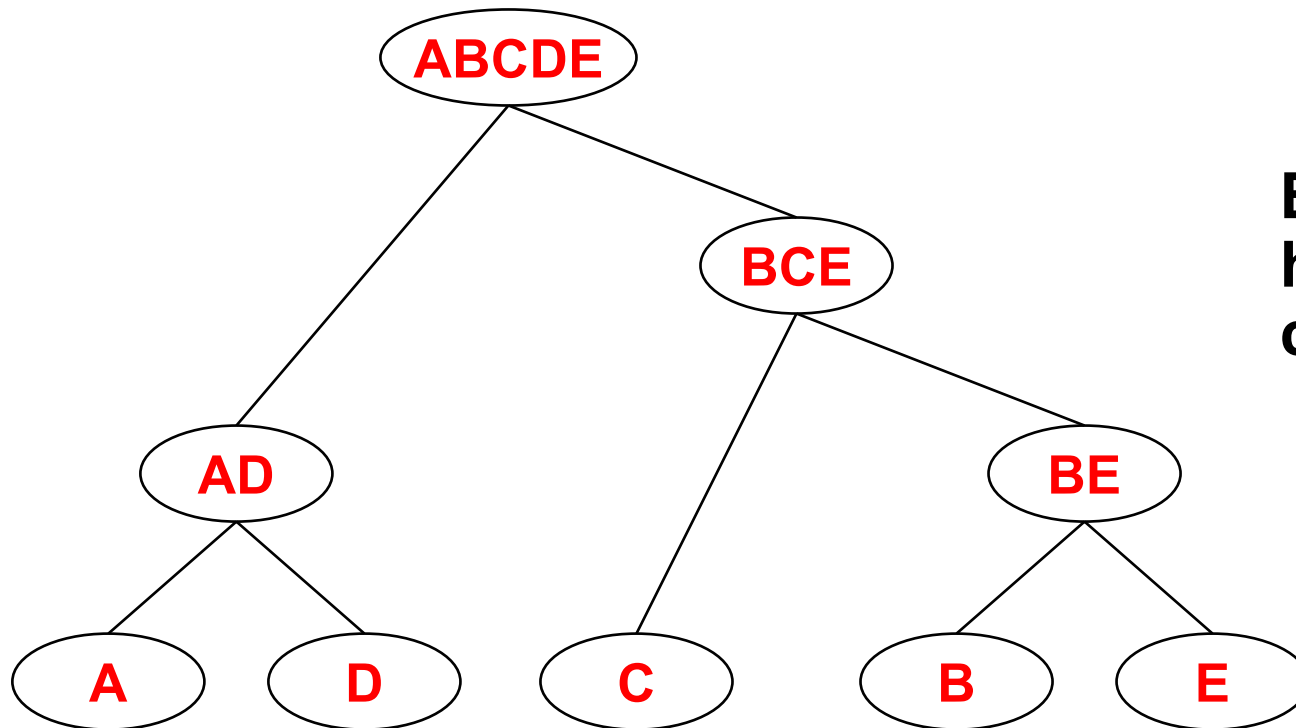
- Highest link is BE-C. So let's cluster BE and C. We now have the following structure:



# Example

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- At this point, there are only two nodes that have not been clustered. So we cluster AD and BCE. We now have the following structure:



**Everything  
has been  
clustered.**

# Time complexity analysis

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**Hierarchical agglomerative clustering (HAC) requires:**

- **$O(n^2)$  to compute the doc-doc similarity matrix**
- **One node is added during each round of clustering so there are now  $O(n)$  clustering steps**
- **For each clustering step we must re-compute the doc-doc matrix. This requires  $O(n)$  time.**
- **So we have:  $n^2 + (n)(n) = O(n^2)$  – so it's expensive!**
- **For 500,000 documents  $n^2$  is 250,000,000,000!!**



# One pass clustering

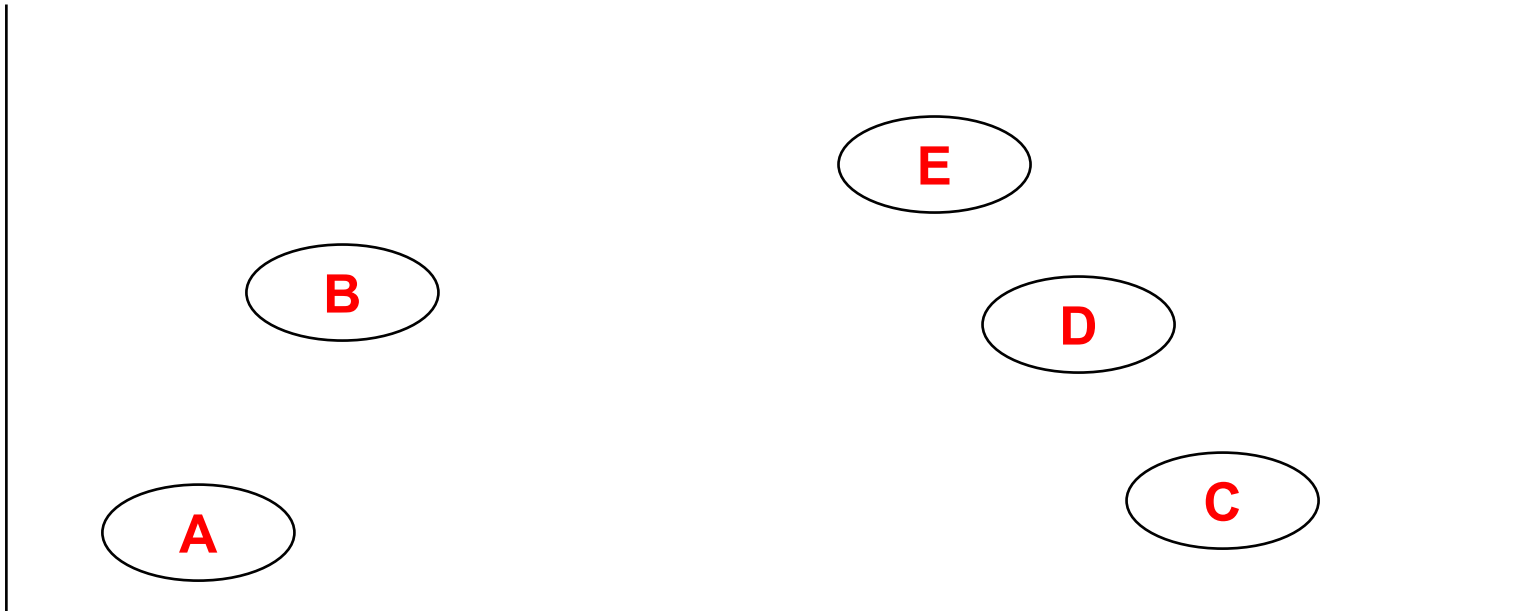
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- **Choose a document and declare it to be in a cluster of size 1.**
- **Now compute the distance from this cluster to all the remaining nodes.**
- **Add “closest” node to the cluster. If no node is really close (within some threshold), start a new cluster between the two closest nodes.**

# Example

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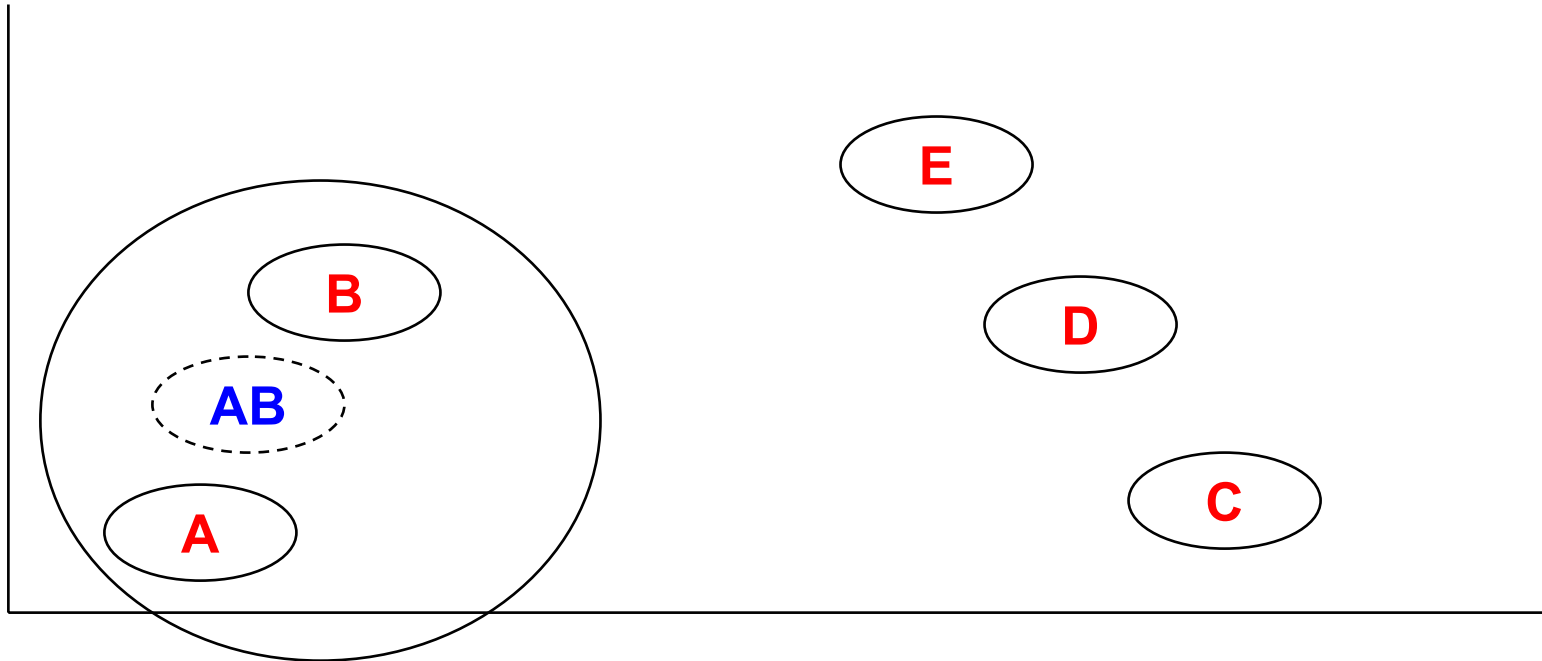
- Consider the following nodes



# Example

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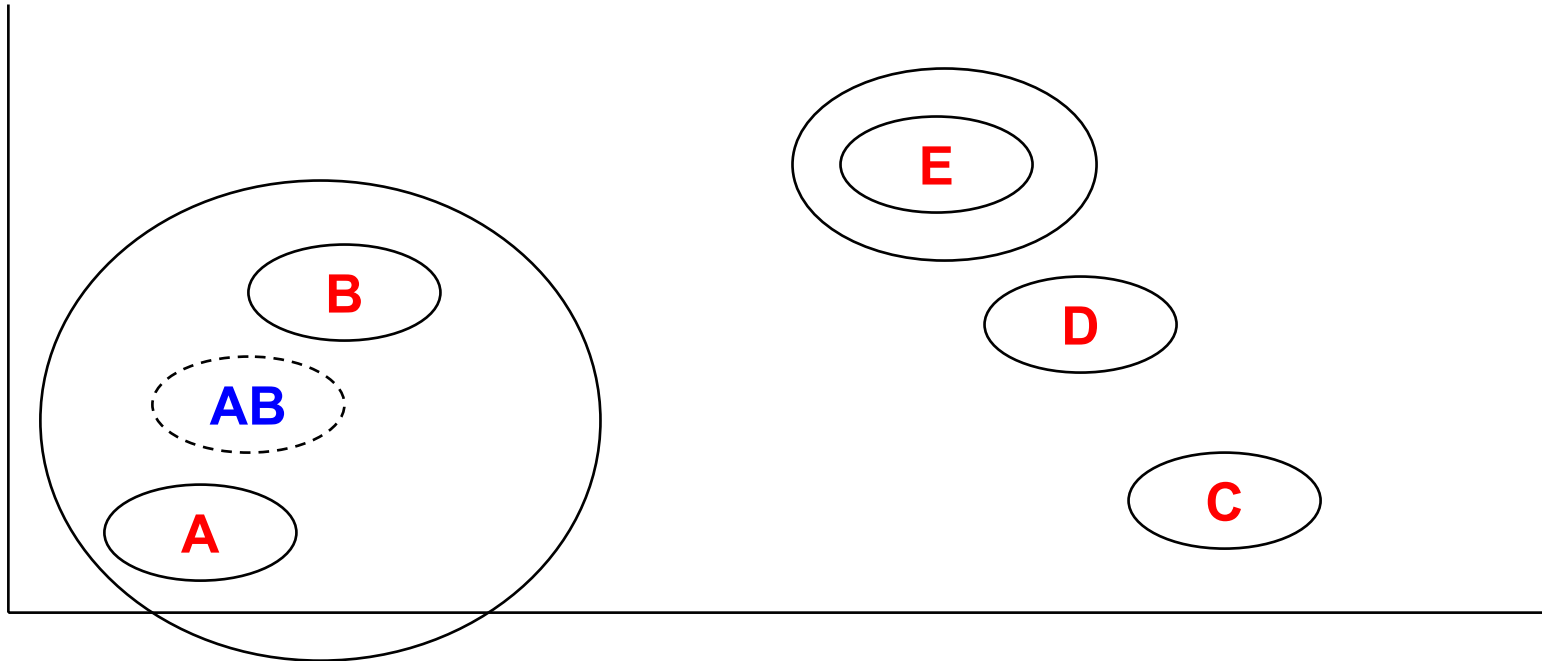
- Choose node A as the first cluster
- Now compute the distance between A and the others. B is the closest, so cluster A and B.
- Compute the centroid of the cluster just formed.



# Example

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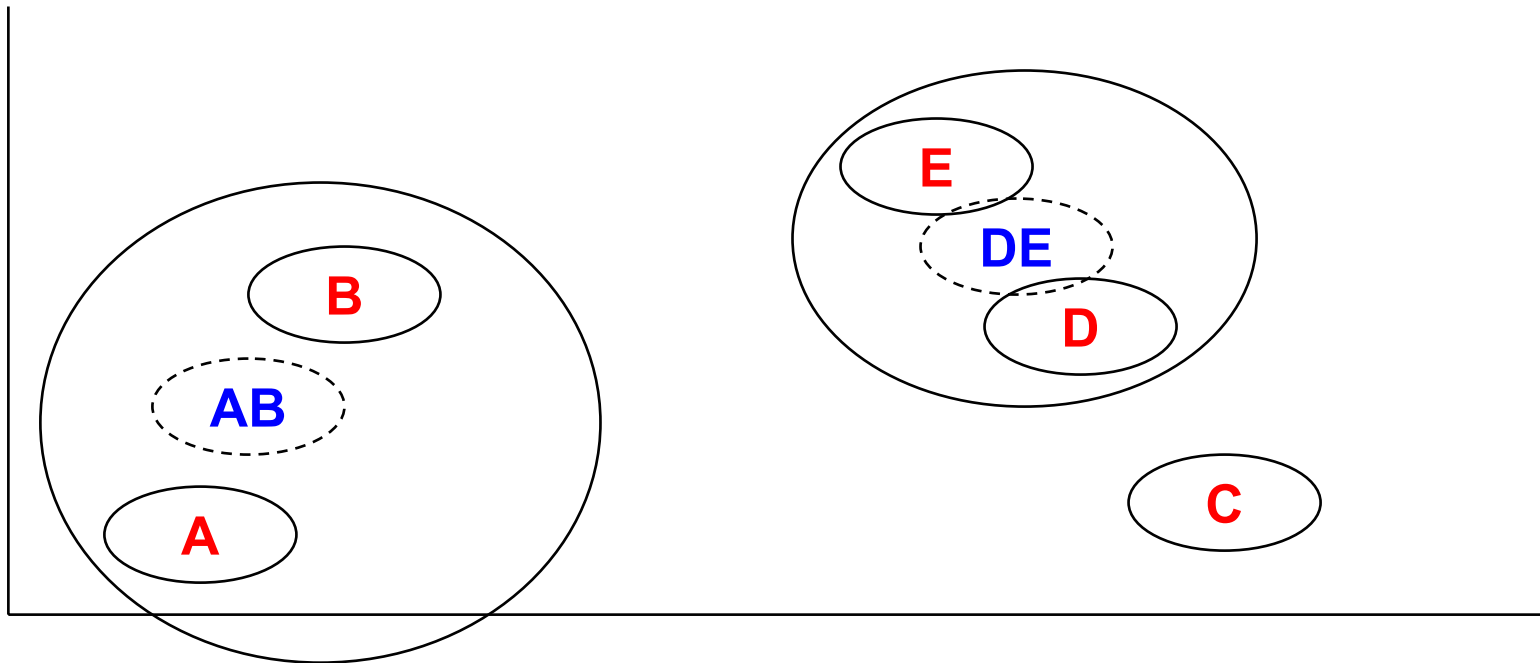
- Compute the distance between A-B and all the remaining clusters using the centroid of A-B.
- Let's assume all the others are too far from AB. Choose one of these non-clustered elements and place it in a cluster. Let's choose E.



# Example

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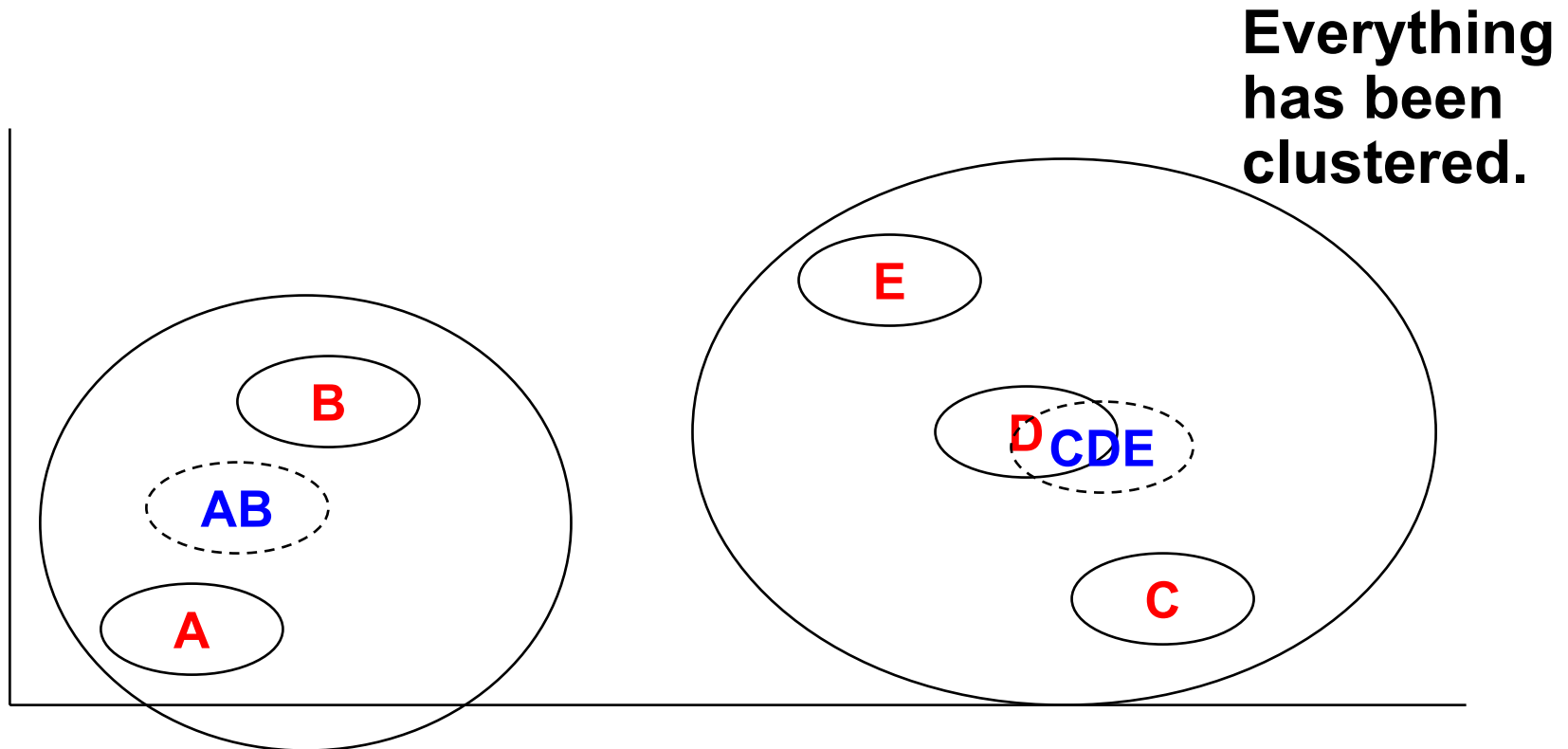
- Compute the distance from E to D and E to C.
- E to D is closer so we form a cluster of E and D.



# Example

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- Compute the distance from D-E to C.
- It is within the threshold so include C in this cluster.



# Time complexity analysis

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One pass requires:

- **n passes as we add node for each pass**
- **First pass requires n-1 comparisons**
- **Second pass requires n-2 comparisons**
- **Last pass needs 1**
- **So we have  $1 + 2 + 3 + \dots + (n-1) = (n-1)(n) / 2$**
- **$(n^2 - n) / 2 = O(n^2)$**
- **The constant is lower for one pass but we are still at  $n^2$  .**

# Remember k-means clustering

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- **Pick  $k$  points as the seeds of  $k$  clusters**
- **At the onset, there are  $k$  clusters of size one.**
- **do until all nodes are clustered**
  - **Pick a point and put it into the cluster whose centroid is closest.**
  - **Recompute the centroid of the modified cluster.**



# Time complexity analysis

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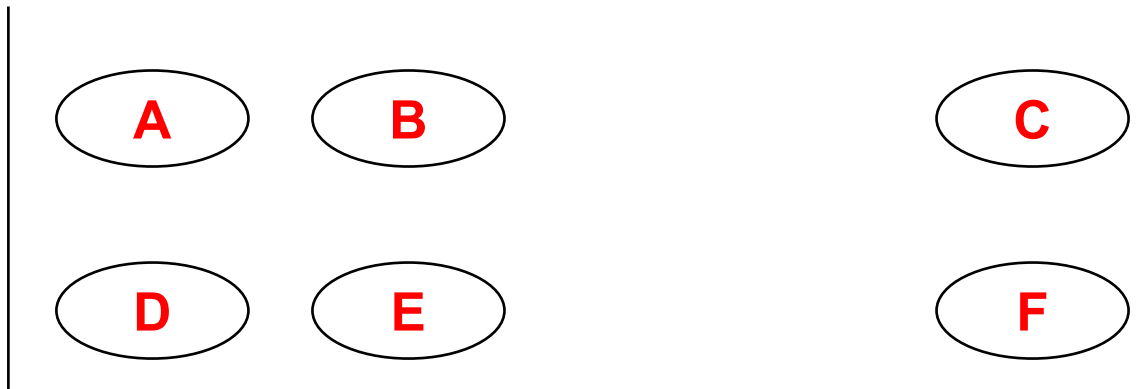
**K-means requires:**

- **Each node gets added to a cluster, so there are  $n$  clustering steps**
- **For each addition, we need to compare to  $k$  centroids**
- **We also need to recompute the centroid after adding the new node, this takes a constant amount of time (say  $c$ )**
- **The total time needed is  $(k + c) n = O(n)$**
- **So it is a linear algorithm!**

# But there are problems...

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- **K** needs to be known in advance or need trials to compute **k**
- Tends to go to local minima that are sensitive to the starting centroids:



If the seeds are B and E, the resulting clusters are {A,B,C} and {D,E,F}.

If the seeds are D and F, the resulting clusters are {A,B,D,E} and {C,F}.

# Two questions for you

---

- 1. Why did the computer go to the restaurant?**
- 2. What do you do when you have a slow algorithm that produces quality results, and a fast algorithm that cannot guarantee quality?**

# Two questions for you

---

- 1. Why did the computer go to the restaurant?**
- 2. What do you do when you have a slow algorithm that produces quality results, and a fast algorithm that cannot guarantee quality?**

**1. To get a byte.**

**2. Many things...**

**One option is to use the slow algorithm on a portion of the problem to obtain a better starting point for the fast algorithm.**

# Buckshot clustering

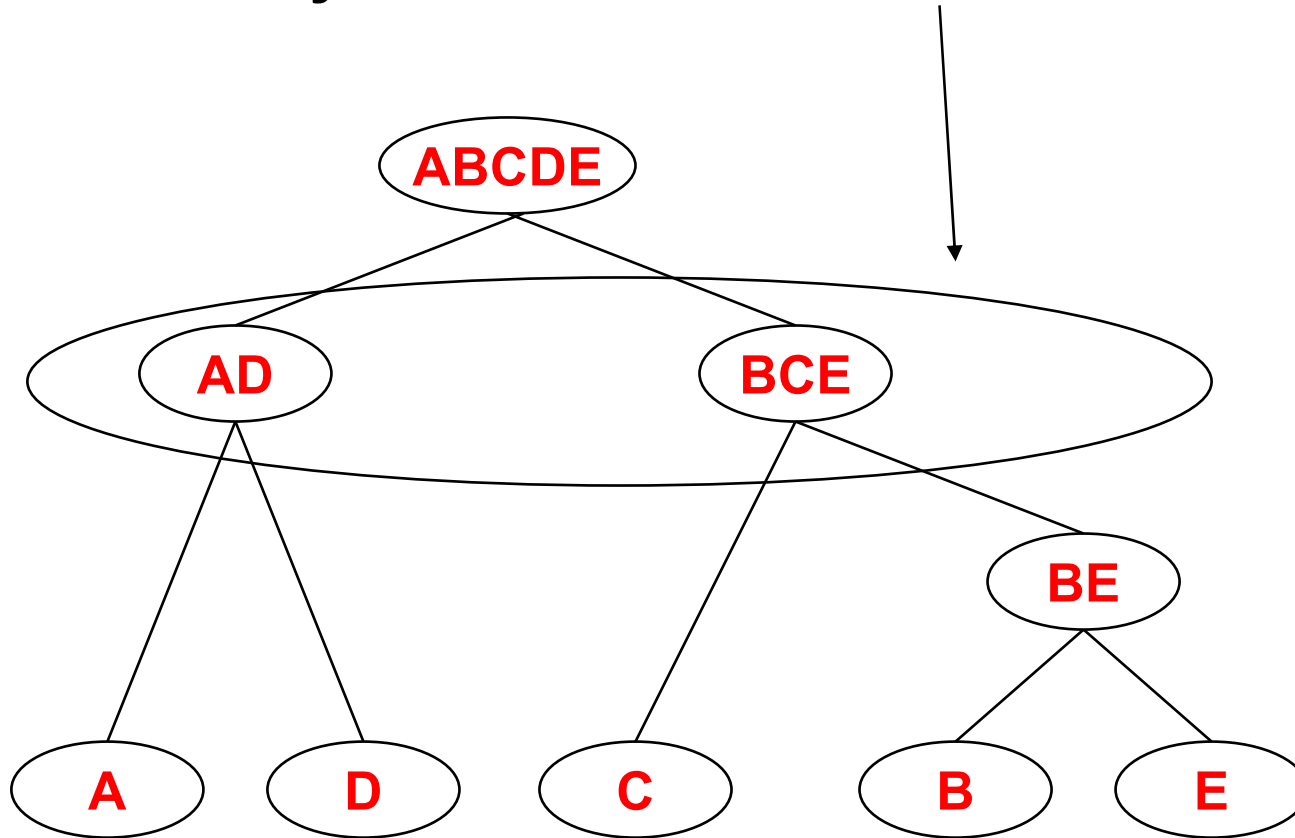
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- The goal is to reduce the run time by combining HAC and k-means clustering. It uses HAC to bootstrap k-means.
- Select  $d$  documents where  $d$  is  $\text{SQRT}(n)$ .
- Cluster these  $d$  documents using HAC, this will take  $O(n)$  time.
- Use the results of HAC as initial seeds for k-means.
- The overall algorithm is  $O(n)$  and avoids problems of bad seed selection.

# Getting the k clusters

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Cut where you have k clusters



# Effect of document order

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- **With hierarchical clustering we get the same clusters every time.**
- **With one pass clustering, we get different clusters based on the order we process the documents.**
- **With k-means clustering, we get different clusters based on the selected seeds.**

# Computing the distance (time)

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- **In our time complexity analysis we finessed the time required to compute the distance between two nodes**
- **Sometimes this is an expensive task depending on the analysis required**



# Computing the distance (methods)

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- **To compute the intra-cluster distance:**  
(Sum/min/max/avg) the (absolute/squared) distance between
  - All pairs of points in the cluster, or
  - Between the centroid and all points in the cluster
- **To compute the inter-cluster distance for HAC:**
  - Single linkage: distance between closest neighbors
  - Complete linkage: distance between farthest neighbors
  - Group-average: average distance between all pairs of neighbors
  - Centroid-distance: distance between centroids (most commonly used)

# More on document clustering

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- **Applications**

- **Structuring search results**
- **Suggesting related pages**
- **Automatic directory construction / update**
- **Finding near identical pages**
  - Finding mirror pages (e.g., for propagating updates)
  - Eliminate near-duplicates from results page
  - Plagiarism detection
  - Lost and found (find identical pages at different URLs at different times)

- **Problems**

- **Polysemy, e.g., “bat,” “Washington,” “Banks”**
- **Multiple aspects of a single topic**
- **Ultimately amounts to general problem of information structuring**

# Clustering vs. classification

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- ***Clustering*** is when the clusters are not known
- If the system of clusters is known, and the problem is to place a new item into the proper cluster, this is ***classification***

# How many possible clusterings?

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If we have  $n$  points and would like to cluster them into  $k$  clusters, then there are  $k$  clusters the first point can go to, there are  $k$  clusters for each of the remaining points. So the total number of possible clusterings is  $k^n$ .

Brute force enumeration will not work. That is why we have iterative optimization algorithms that start with a clustering and iteratively improve it.

Finally, note that noise (outliers) is a problem for clustering too. One can use statistical techniques to identify outliers.

# Cluster structure

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- **Hierarchical vs. flat**
- **Overlap**
  - Disjoint partitioning, e.g., partition congressmen by state
  - Multiple dimensions of partitioning, each disjoint, e.g., partition congressmen by state; by party; by House/Senate
  - Arbitrary overlap, e.g., partition bills by congressmen who voted for them
- **Exhaustive vs. non-exhaustive**
- **Outliers: what to do?**
- **How many clusters? How large?**

# Measuring the quality of the clusters

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**A good clustering is one where**

- (intra-cluster distance) the sum of distances between objects in the same cluster are minimized**
- (inter-cluster distance) while the distances between different clusters are maximized**

**The objective is to minimize:  $F(\text{intra}, \text{inter})$**

# Related communities

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- **machine learning**
- **data mining**
- **statistics**
- **visualization**
- **databases**

# Sources for the slides

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- David Grossman's clustering slides:  
<http://ir.iit.edu/~dagr/IRcourse/Notes/08Clustering.pdf>
- Subbarao Kambhampati's clustering slides:  
<http://rakaposhi.eas.asu.edu/cse494/notes/f02-clustering.ppt>
- Jeffrey Ullman's clustering slides:  
[www-db.stanford.edu/~ullman/cs345-notes.html](http://www-db.stanford.edu/~ullman/cs345-notes.html)
- Ernest Davis' clustering slides:  
[www.cs.nyu.edu/courses/fall02/G22.3033-008/index.htm](http://www.cs.nyu.edu/courses/fall02/G22.3033-008/index.htm)
- John Snow's cholera map is from  
[http://krygier.owu.edu/krygier\\_html/geog\\_222/geog\\_222\\_lo/geog\\_222\\_lo01.html](http://krygier.owu.edu/krygier_html/geog_222/geog_222_lo/geog_222_lo01.html)