Jaime Arguello INLS 613: Text Data Mining jarguell@email.unc.edu

(some material taken or adapted from slides by Hinrich Schutze)

## Clustering objective

- Grouping documents or instances into subsets or clusters
- Documents in the same cluster should be similar
- Documents in different clusters should be dissimilar
- A common form of unsupervised learning
- Unsupervised = no human-produced labels
- The goal is to discover structure from the data

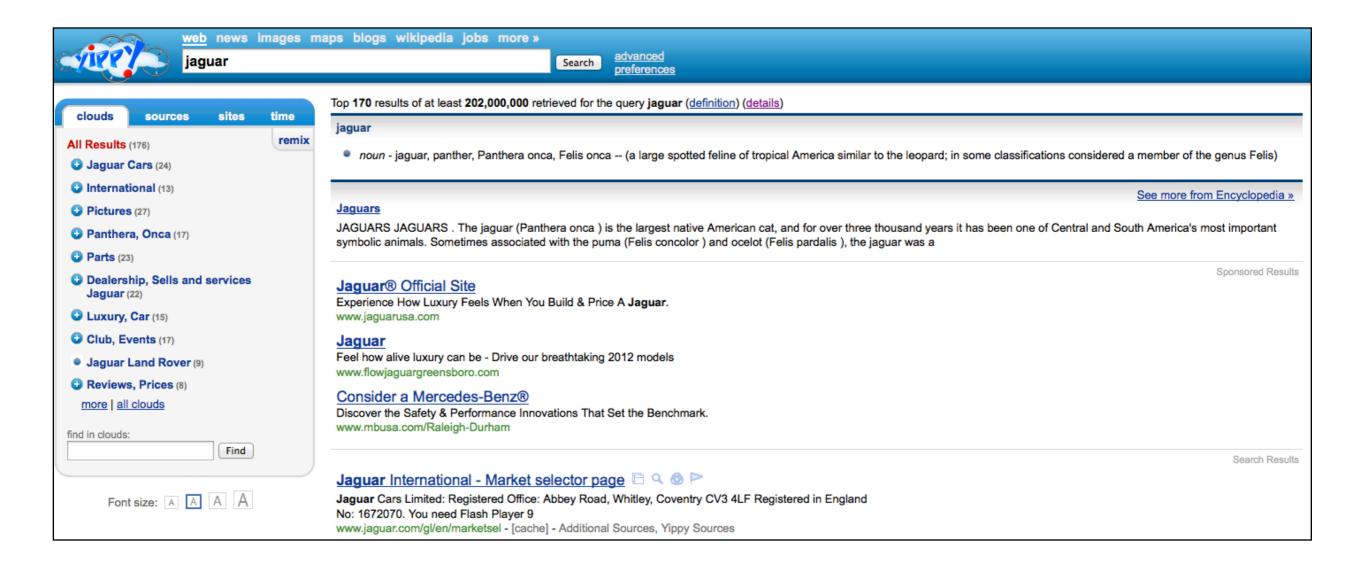
# Clustering vs. Classification

- Classification:
  - the input to the system is a set of labeled data
  - the algorithm learns a model for predicting the label on new examples
- Clustering:
  - the input to the system is a set of unlabeled data
  - the algorithm infers the labels from the data and assigns a label to each input instance

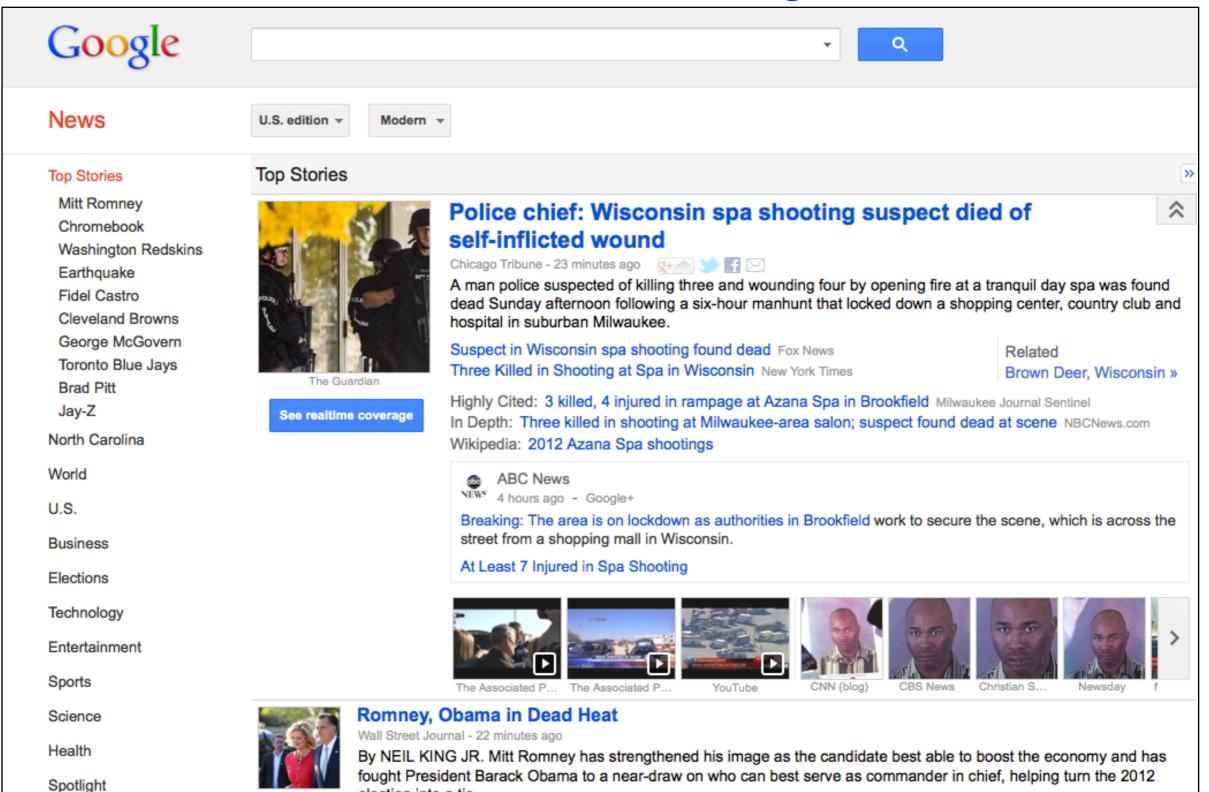
## Clustering applications

- Search engine results clustering: grouping search engine results by topic
  - the user can identify the relevant clusters and ignore the non-relevant ones
- Collection clustering: grouping documents by topic to support navigation and exploration
- Data analytics: grouping instances to identify popular trends (big clusters) and outliers (small clusters)

## Clustering Applications search engine results clustering



## Clustering Applications collection clustering



election into a tie ...

## Clustering Applications collection clustering

Google	▼ Q
News	U.S. edition - Modern -
Top Stories Mitt Romney Chromebook Washington Redskins Earthquake Muammar al-Gaddafi Fidel Castro Cleveland Browns George McGovern Brad Pitt Toronto Blue Jays News near you World	Image: Provide the second of the second
U.S. Business Elections Technology	SlashGear Written by   Oct 20, 2012 Written by   Chris Burns This piece of Samsung hardware is the most basic Chromebook you can buy right this minute, but it's not the low-quality piece of hardware the price suggests.   New Samsung Chromebook and Samsung Series 5 550 head-to-head
Entertainment Sports	ZDNet ZDNet ZDNet ZDNet
Science Health Spotlight	ZDNet Image: Source Control of the Chromebook. There's not much new or even innovative about this particular device, particularly from a UX standpoint it's the same Chrome OS we've seen before, except that it now runs

## Clustering objective

- Grouping documents or instances into subsets or clusters
- Documents within a the same cluster should be similar
- Documents from different clusters should be dissimilar

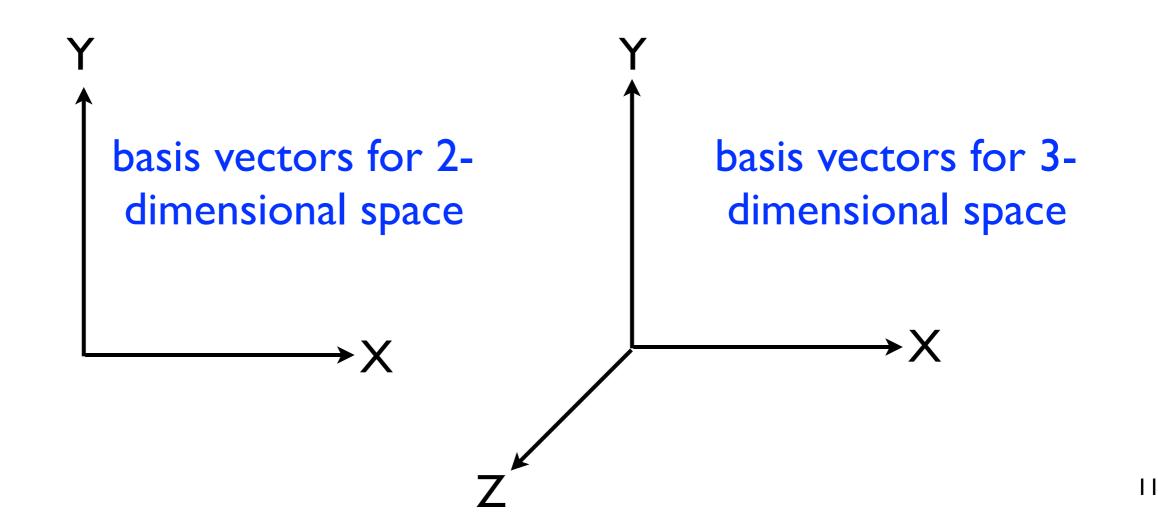


• What does it mean for documents to be "similar" or "dissimilar"?

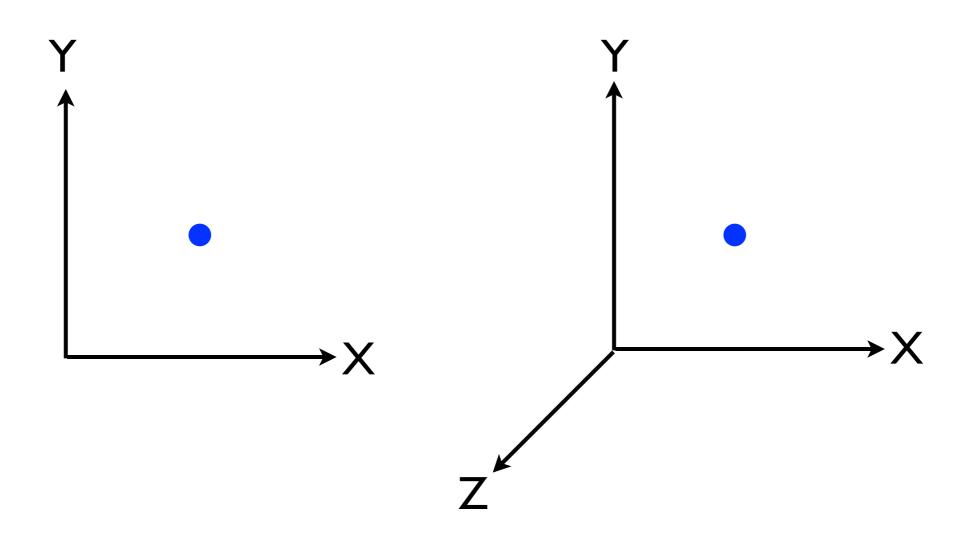
### Clustering basics

- What does it mean for documents to be similar or dissimilar?
- We need a computational way of modeling similarity
- One solution: model similarity using distance in a vector space representation of the collection or dataset
  - small distance = high similarity
  - long distance = low similarity

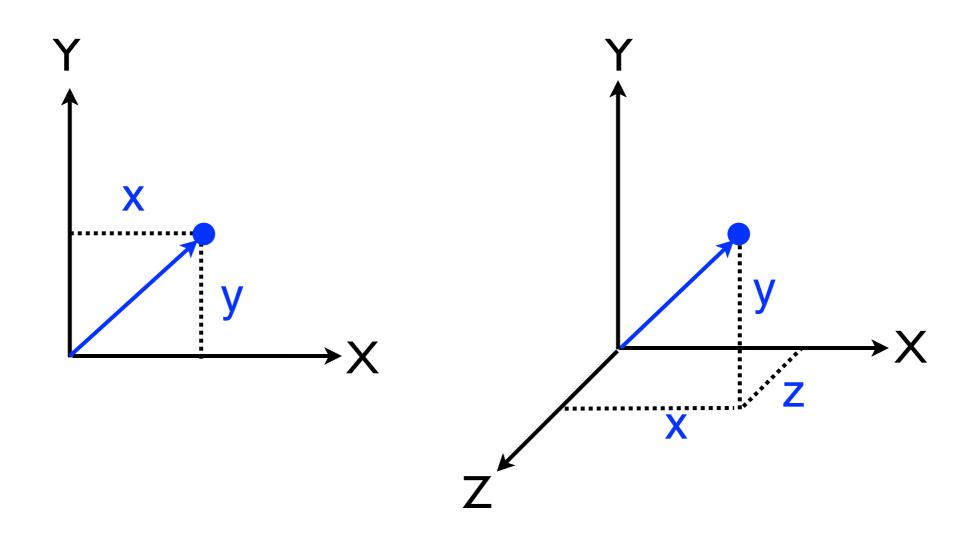
- A vector space is defined by a set of <u>linearly independent</u> basis vectors
- The basis vectors correspond to the dimensions or directions of the vector space



• A vector is a point in a vector space



- A 2-dimensional vector can be written as [x,y]
- A 3-dimensional vector can be written as [x,y,z]



w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
1	0	1	0	1	0	0	1	1	0
0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
									:
1	1	0	1	1	0	0	1	0	1

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
1	0	1	0	1	0	0	1	1	0
0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
1	1	0	1	1	0	0	1	0	1

 We can represent this document as a vector in a 10dimensional vector space

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10	
1	0	1	0	1	0	0	1	1	0	
0	1	0	1	1	0	1	1	0	0	
0	1	0	1	1	0	1	0	0	0	
0	0	1	0	1	1	0	1	1	1	ľ
1	1	0	1	1	0	0	1	0	1	

- This representation assumes binary term-weights.
- Are there other term-weighting schemes?



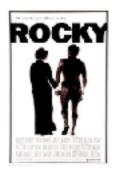
# TF, IDF, or TF.IDF?

adrain adrian all already also an and apartment apollo as aspiring at balboa become better big boxer boxing but by can career champion chance Creed current debt doesn earns every exhibition extra far fight for gazzo gets girl go has he heavyweight her himself his if in is it keep later life living loan lovers make man match meat men mickey named nobody of paulie pet philadelphia **FOCKY** set she shot small somebody someone still store struggling supplies surprised that they think this through time title to trainer training up want when where who willing with woman works



# TF, IDF, or TF.IDF?

ability adrain adrian already apollo aspiring balboa beat befriended befriends better boxer boxes boxing canvas cash champion checks chooses collecting collector creed current deadbeats debt debts distance **doesn** downtown earns ease easily exhibition explains extra extremely factory far forgot gazzogear giving gotten heavyweight idea interested italian | ergens keep living loan lot lovers managers match meat mickey nobody odds packing paulie pennsylvania pet philadelphia pittance promoter prove publicity ready rocky sells shark sharp shop shy skills SOMebody spends stallion struggling stunt supplies supposed surprised thanksgiving think thrilled title touting trainer training triumph unknown ve viciousness visits want willing win won

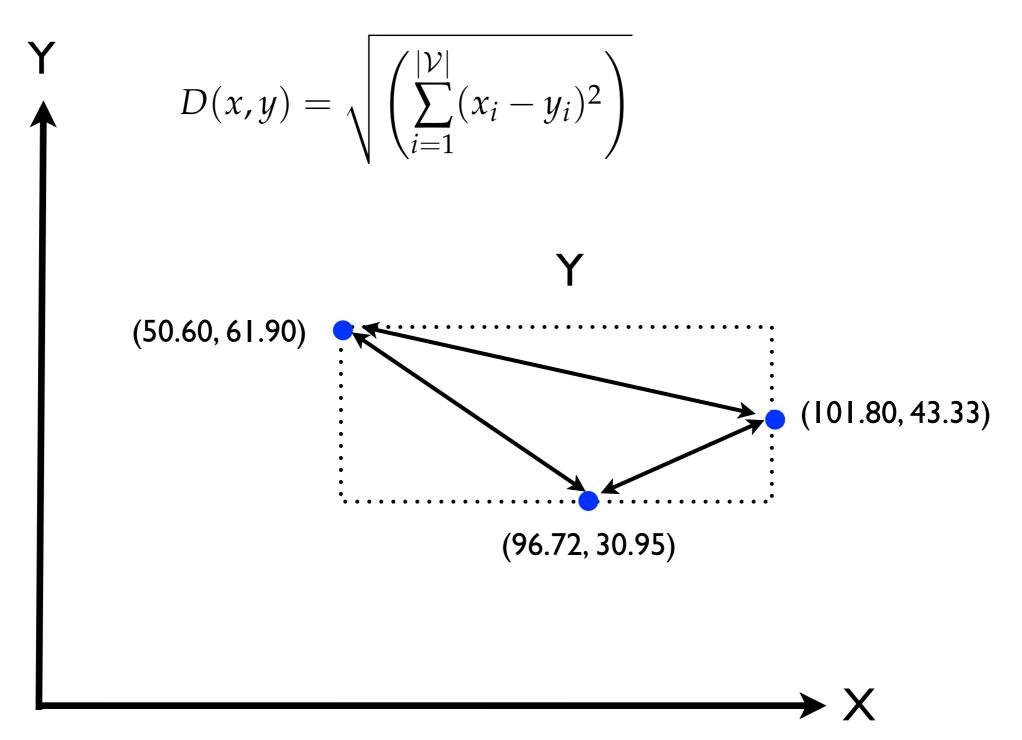


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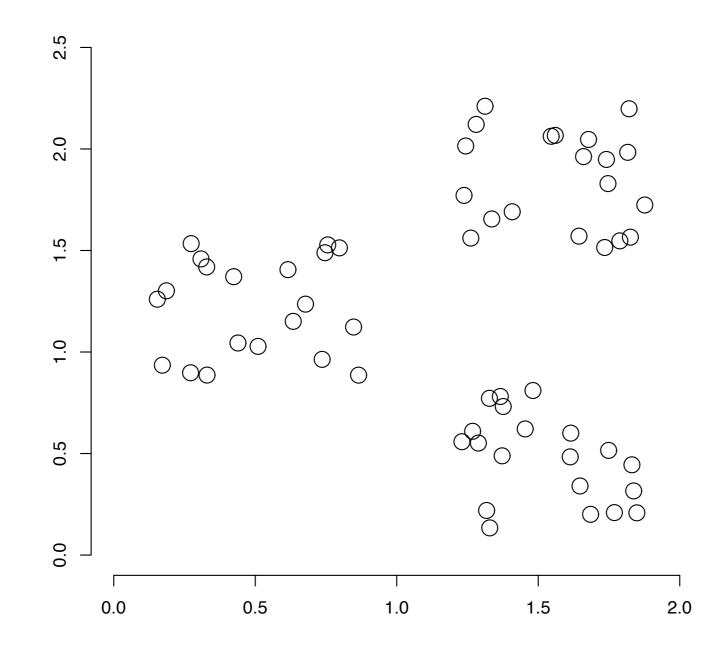
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• Similarity = Euclidean Distance:

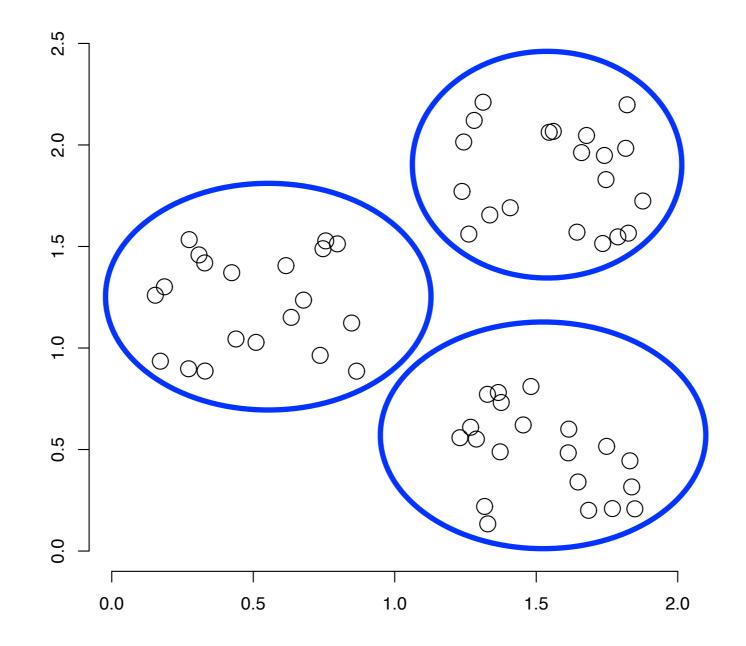
$$D(x,y) = \sqrt{\left(\sum_{i=1}^{|\mathcal{V}|} (x_i - y_i)^2\right)}$$



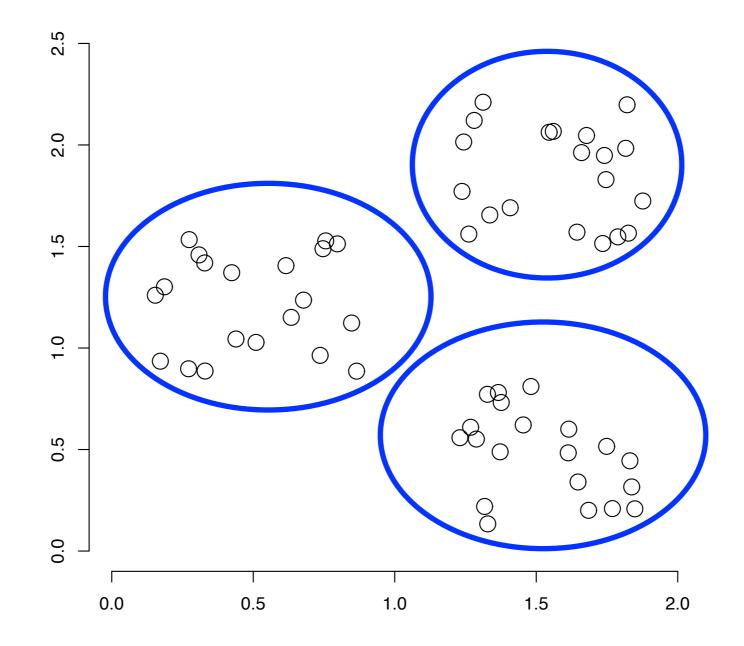
• What would we expect a clustering algorithm to do with this dataset?



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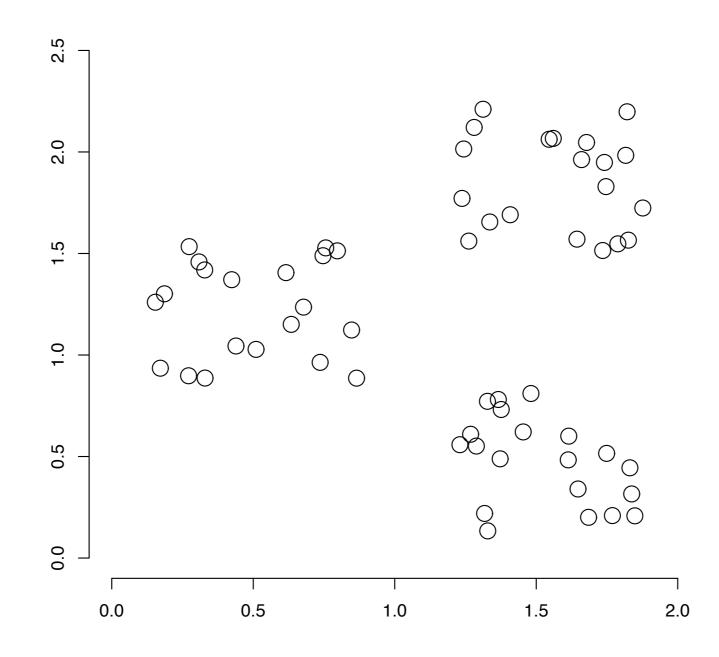


• Propose an algorithm that might be able to do this!



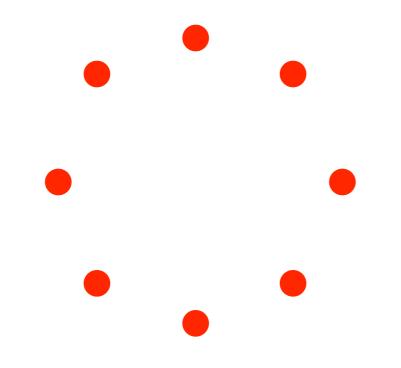
- Input: number of desired clusters K
- Output: assignment of documents to K clusters
- Algorithm:
  - randomly select K documents (seeds)
  - assign each remaining document to its nearest seed

• Could this work?

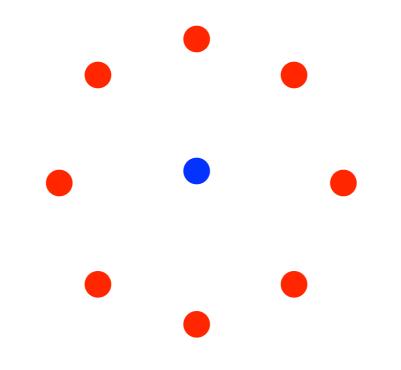


## **K-Means Clustering**

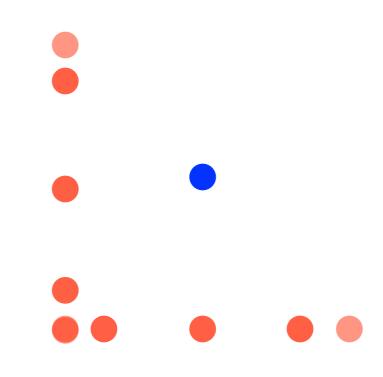
- The key to understanding K-means clustering is to understand the idea of a cluster centroid
- Given a cluster, you can think of its centroid as a point (or vector) that corresponds to its "center of mass"



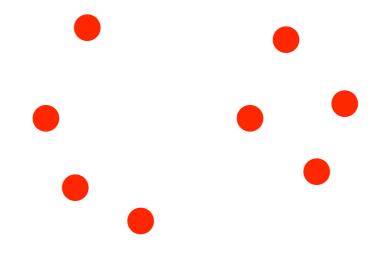
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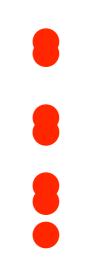
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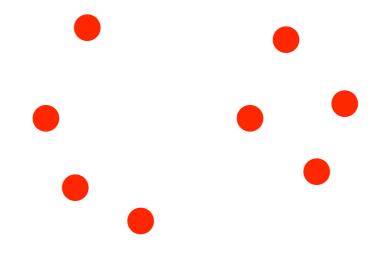
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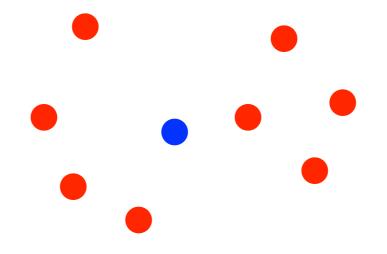
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	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
	1	0	1	0	1	0	0	1	1	0
docs	0	1	0	1	1	0	1	1	0	0
assigned to cluster 1	0	1	0	1	1	0	1	0	0	0
	0	0	1	0	1	1	0	1	1	1
	0	0	1	0	1	1	0	1	1	1
	1	1	0	1	1	0	0	1	0	1
cluster 1 centroid	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
	?	?	?	?	?	?	?	?	?	?

## K-means Clustering cluster centroid

	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
docs assigned to cluster 1	1	0	1	0	1	0	0	1	1	0
	0	1	0	1	1	0	1	1	0	0
	0	1	0	1	1	0	1	0	0	0
	0	0	1	0	1	1	0	1	1	1
	0	0	1	0	1	1	0	1	1	1
	1	1	0	1	1	0	0	1	0	1
cluster 1 centroid (average!)	w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
	0.33	0.5	0.5	0.5	1	0.33	0.33	0.83	0.5	0.5

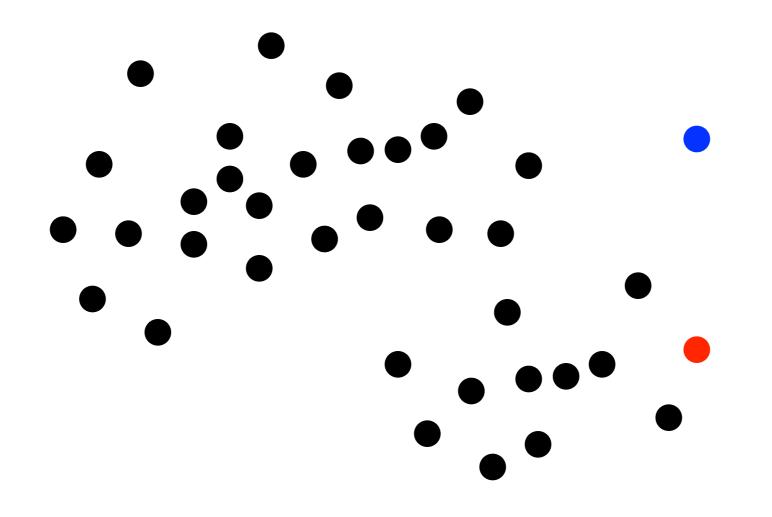
#### K-means Clustering cluster centroid

• For each dimension *i* , set:

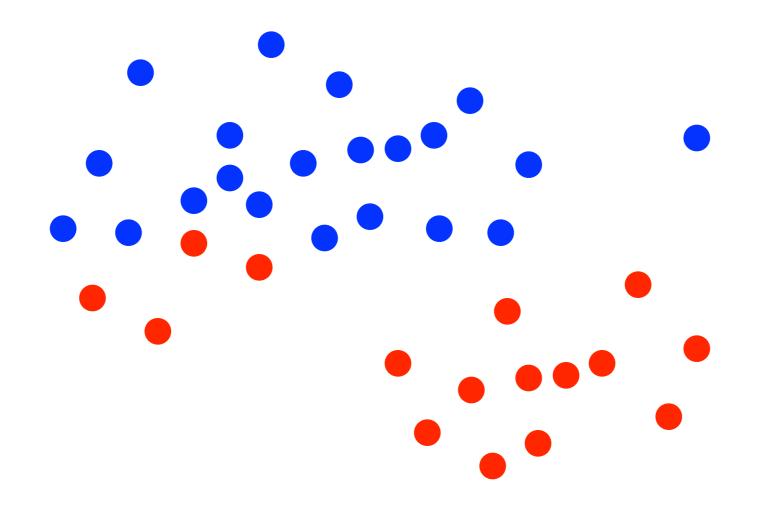
$$c_i = \frac{1}{|C|} \sum_{d \in C} d_i$$

- Input: number of desired clusters K
- Output: assignment of documents to K clusters
- Algorithm:
  - Step 1: randomly select K documents (seeds)
  - Step 2: assign each document to its nearest seed
  - Step 3: compute all K cluster centroids
  - Step 4: re-assign each document to its nearest centroid
  - Step 5: re-compute all K cluster centroids
  - Step 6: repeat steps 4 and 5 until terminating condition

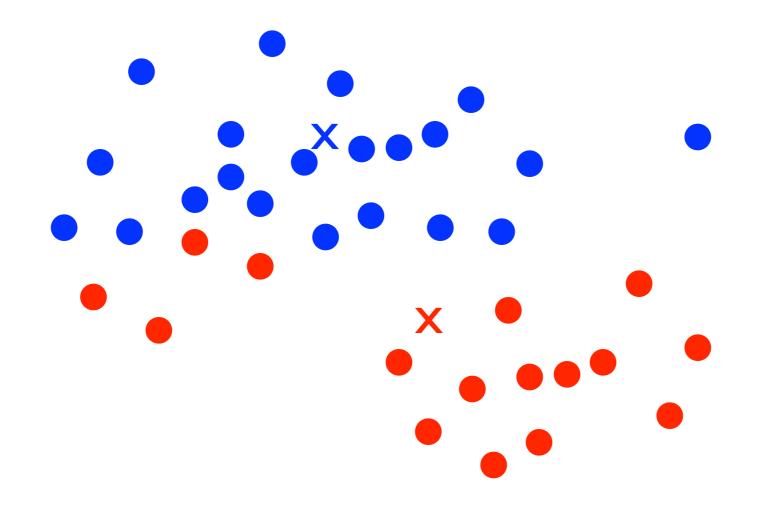
• Step 1: randomly select K documents (seeds)



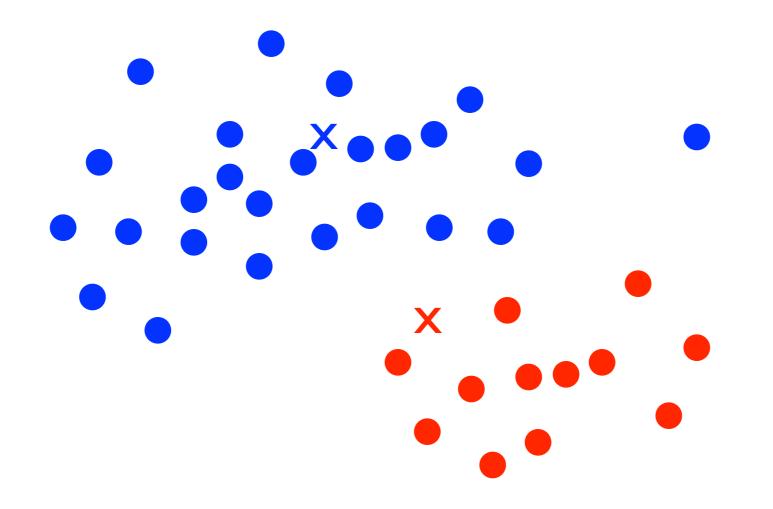
• Step 2: assign each document to its nearest seed



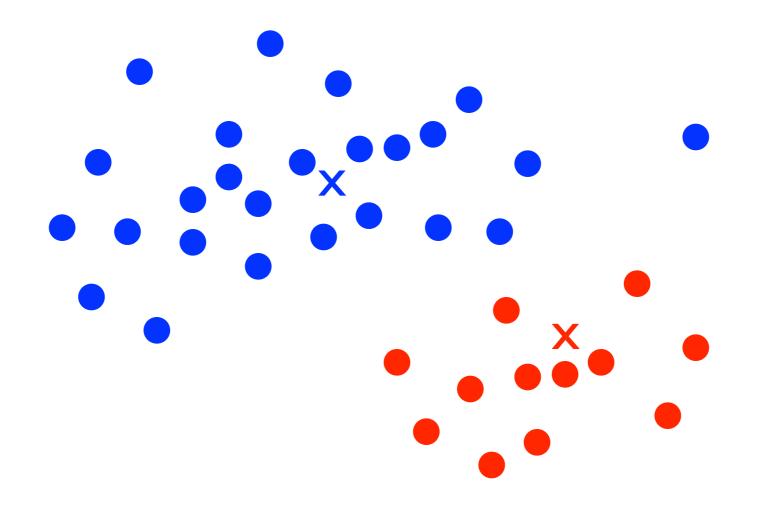
• Step 3: compute all K cluster centroids



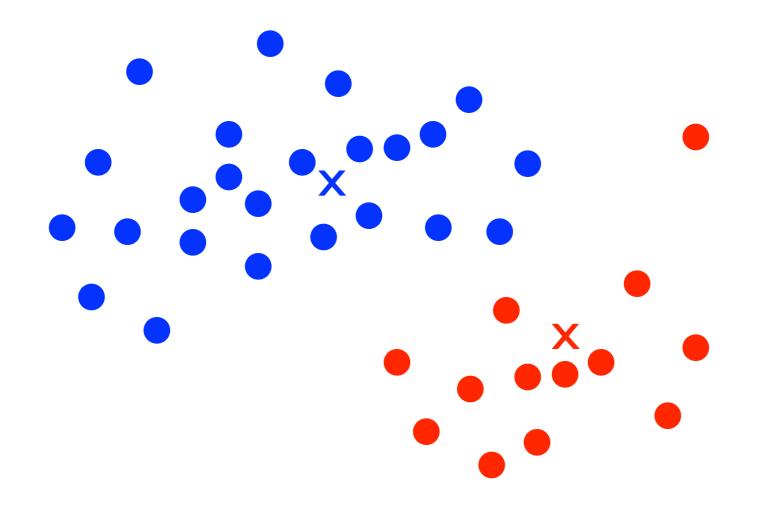
• Step 4: re-assign each document to its nearest centroid



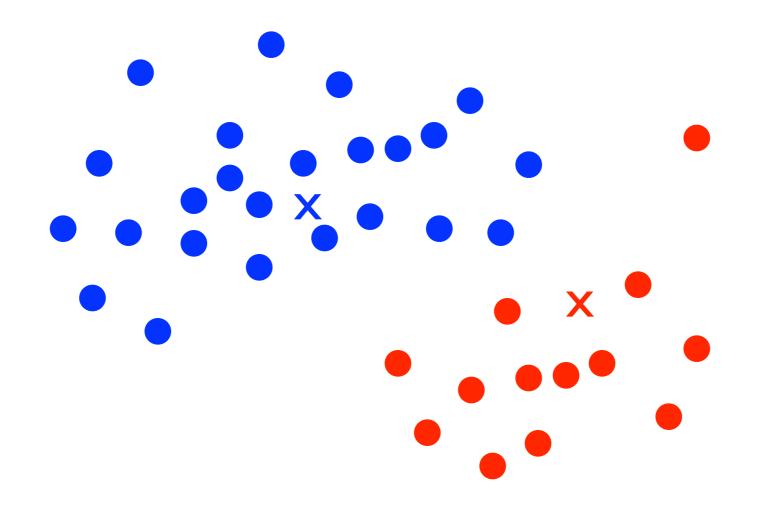
• Step 4: re-compute all K cluster centroids



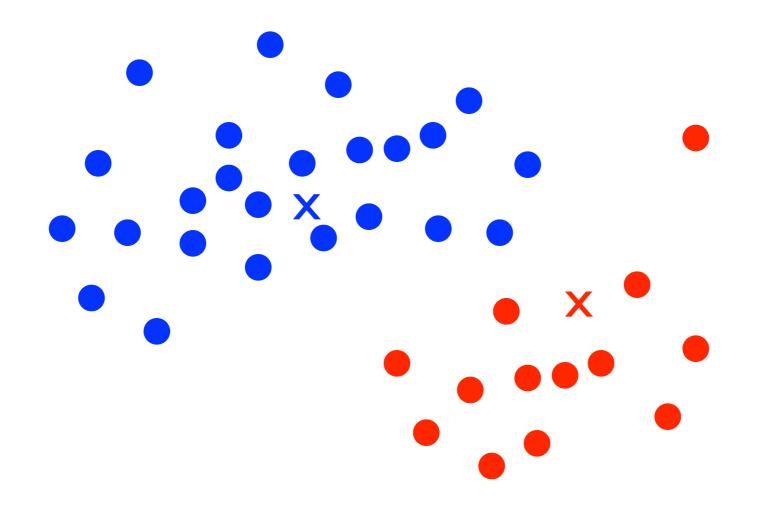
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• Step 4: re-compute all K cluster centroids



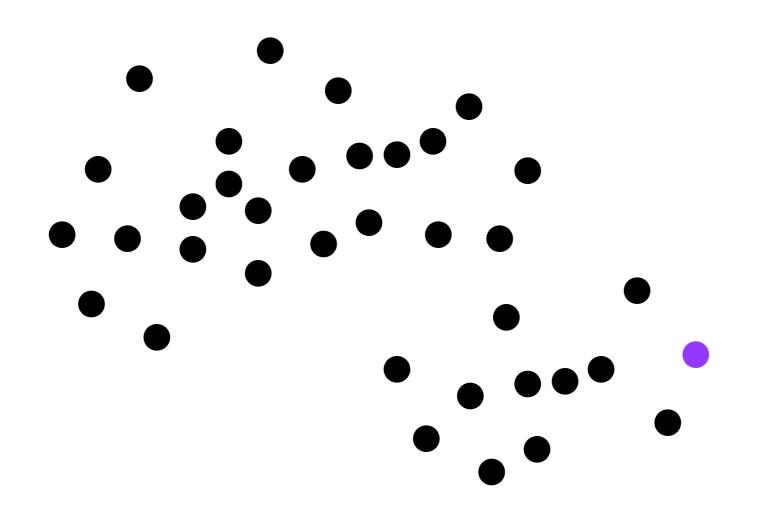
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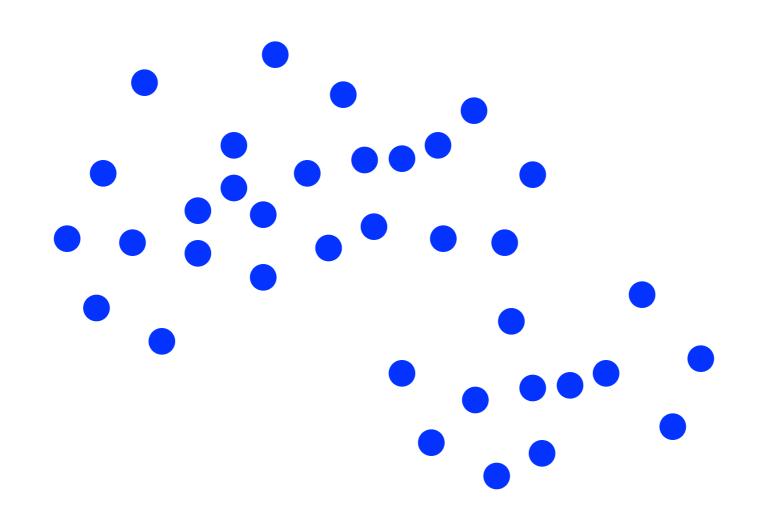


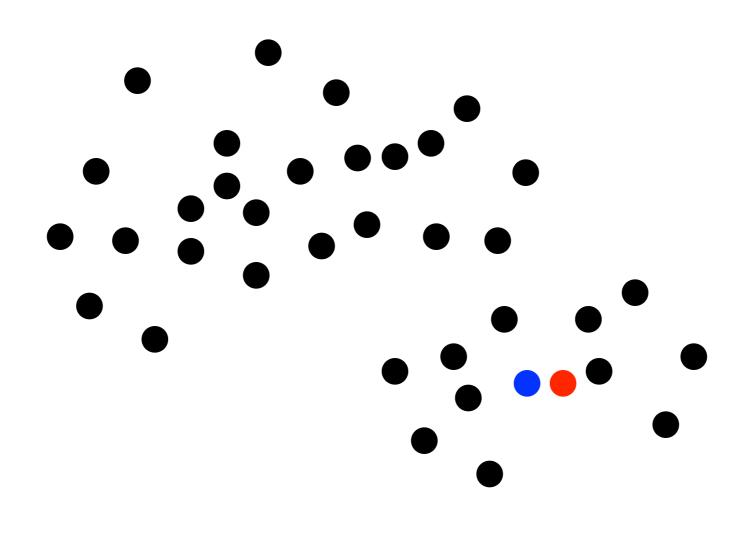
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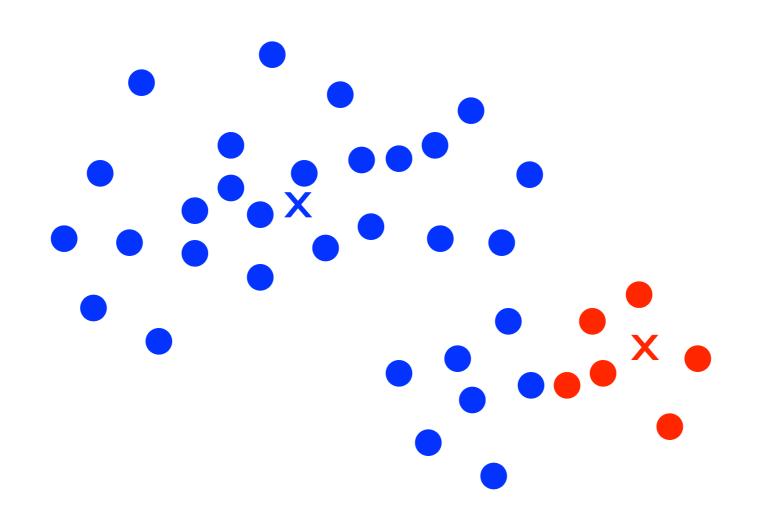
K-means Clustering potential drawback

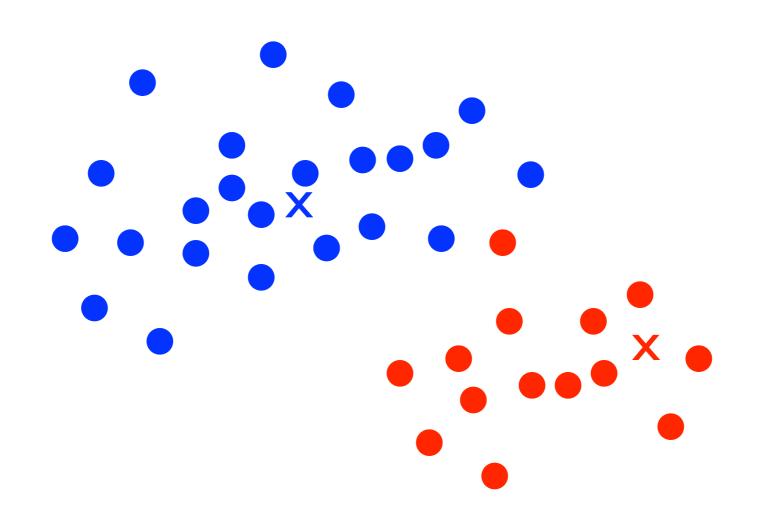
- The quality of the output clustering depends on the choice of K and on the initial seeds
- In many cases, the choice of K is pre-determined by the application
  - Search engine results clustering: grouping search engine results by topic
  - Collection clustering: grouping documents by topic to support navigation and exploration
- Later we'll see ways of setting K dynamically

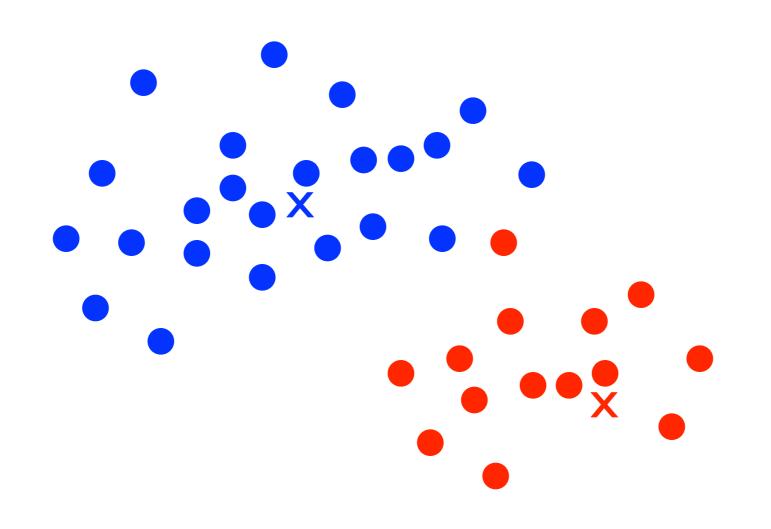


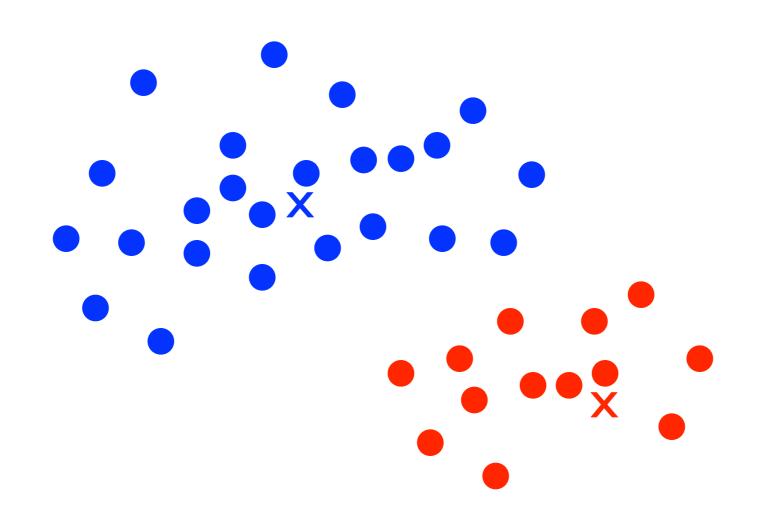












- It's difficult to know which seeds will yield a high-quality clustering
- However, it's usually a good idea to avoid seeds that are outliers
- How would you detect outliers?

## K-means Clustering clustering evaluation

- What does it mean for a clustering to be high quality anyway?
- What is the goal of clustering again?

### K-means Clustering internal evaluation

- In theory, a good clustering should have:
  - Similar documents in the same clusters
  - Different documents in different clusters

#### K-means Clustering internal evaluation

Clustering \_\_\_\_\_

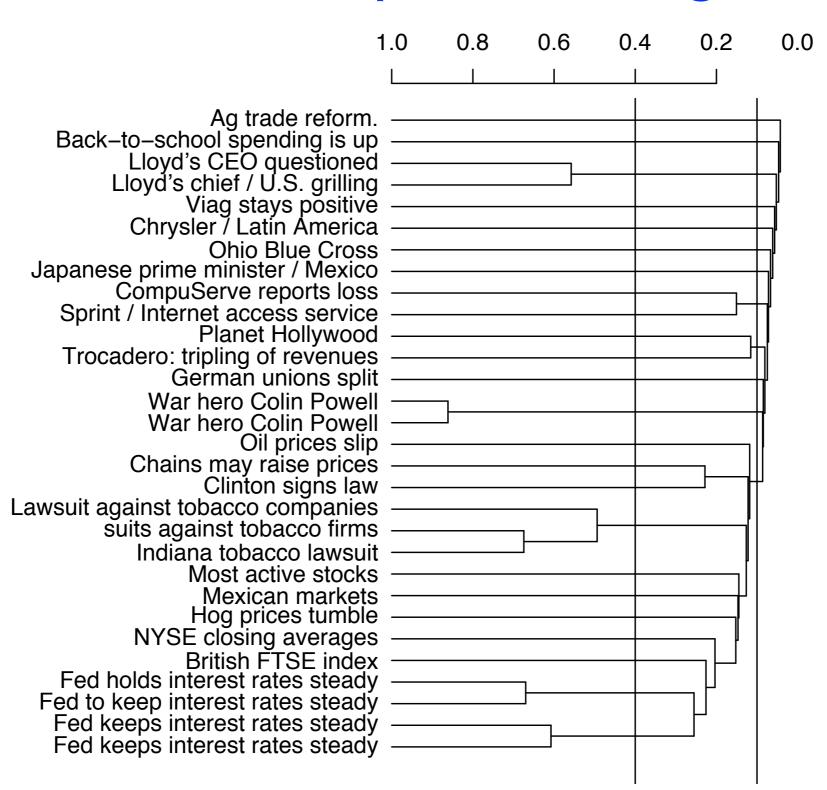
Average distance between all pairs of documents in <u>different clusters</u> Average distance between all pairs of documents in the <u>same cluster</u>

#### K-means Clustering improved k-means

• Given a set of documents and a value K, run Kmeans clustering N times and keep the clustering that produces the greatest difference between the intercluster distance and the intra-cluster distance

# Bottom-up Agglomerative Clustering

- While K-means requires setting K, bottom-up clustering groups the data in a hierarchical fashion
- We can then set K after the clustering is done or use a distance threshold to set K dynamically (more on this later)

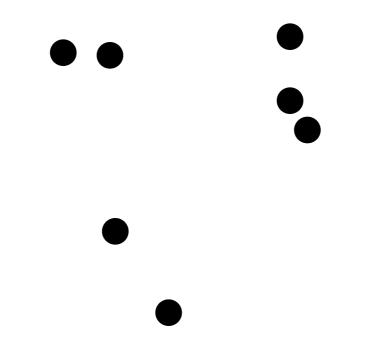


- Input: data
- Output: cluster hierarchy
- Algorithm:
  - Step 1: consider every document its own cluster
  - Step 2: compute the distance between all cluster pairs
  - Step 3: merge/combine the nearest two clusters into one
  - Step 4: repeat steps 2 and 3 until every document is in one cluster

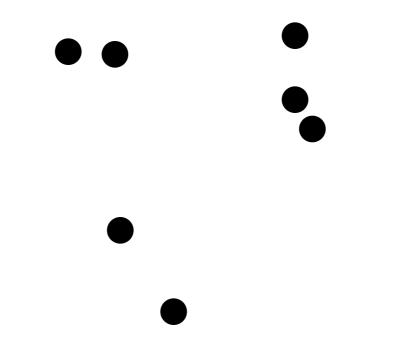
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- Computing the distance between two clusters
- Single-Link: the distance between the two nearest documents
- Complete-Link: the distance between the two documents that are farthest apart
- Average-Link: the average distance between all document pairs in the two different clusters
  - this is equivalent to using the distance between the two cluster centroids

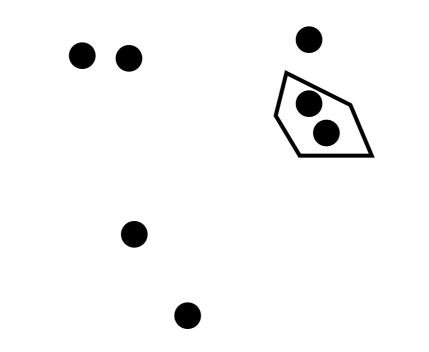
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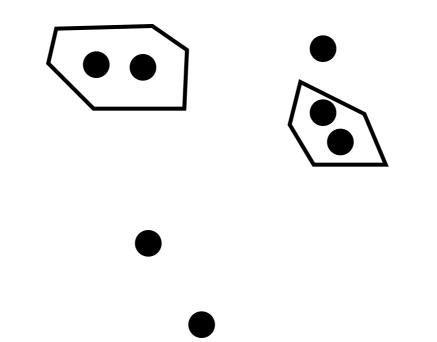
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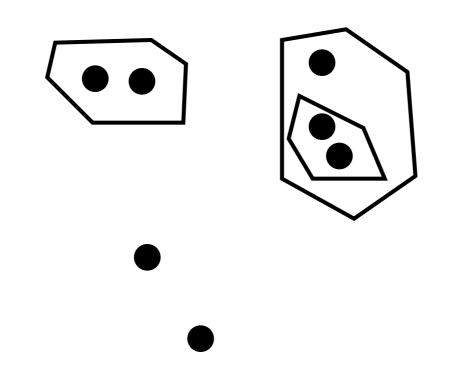
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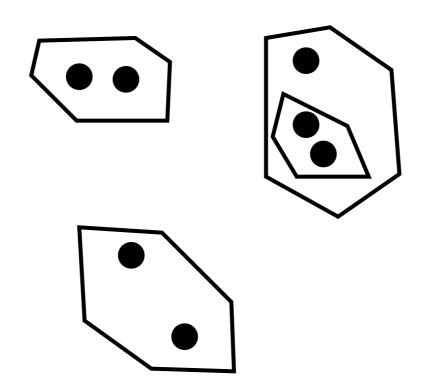


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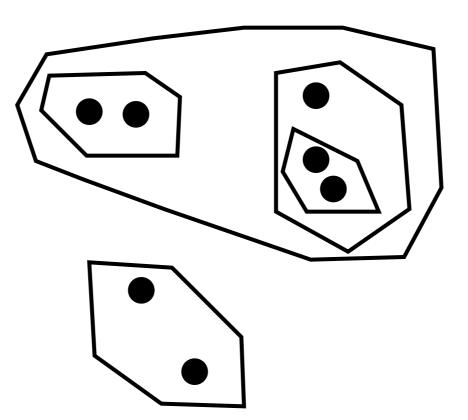
### Bottom-up Clustering single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



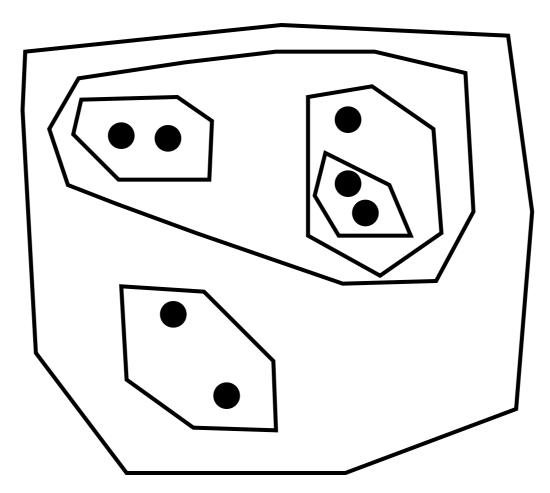
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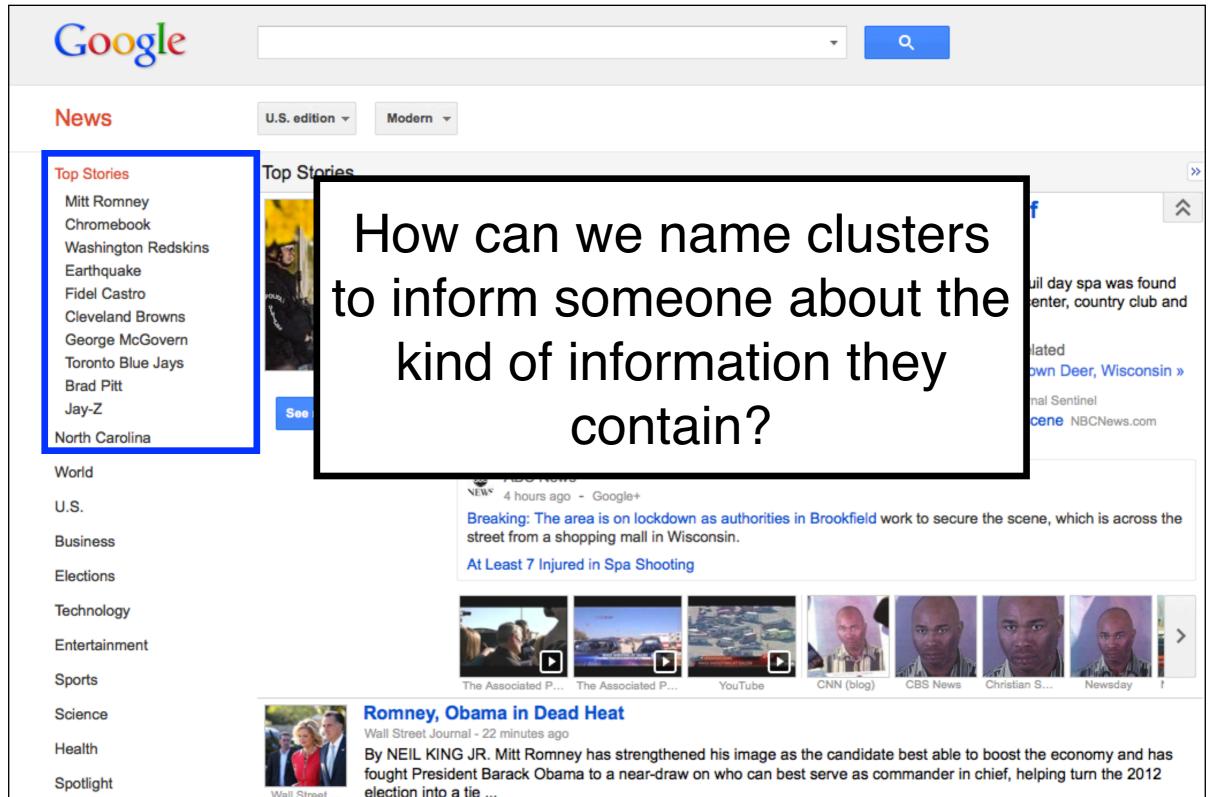


## Bottom-up Clustering

- Setting K dynamically
- Instead of setting K, we could set a distance threshold T
- Stop merging/combining clusters when the distance between the two nearest clusters > T
- Using a distance threshold can help prevent "concept drift" (especially with single-link clustering)
  - text mining --> inls 613 --> unc --> basketball

Labeling Clusters

### Clustering Applications collection clustering



### Labeling Clusters A simple solution

- Construct a vocabulary of terms and/or phrases (n-grams) that are frequent in the data
- Assign each cluster the term(s) or phrase(s) with the highest mutual information

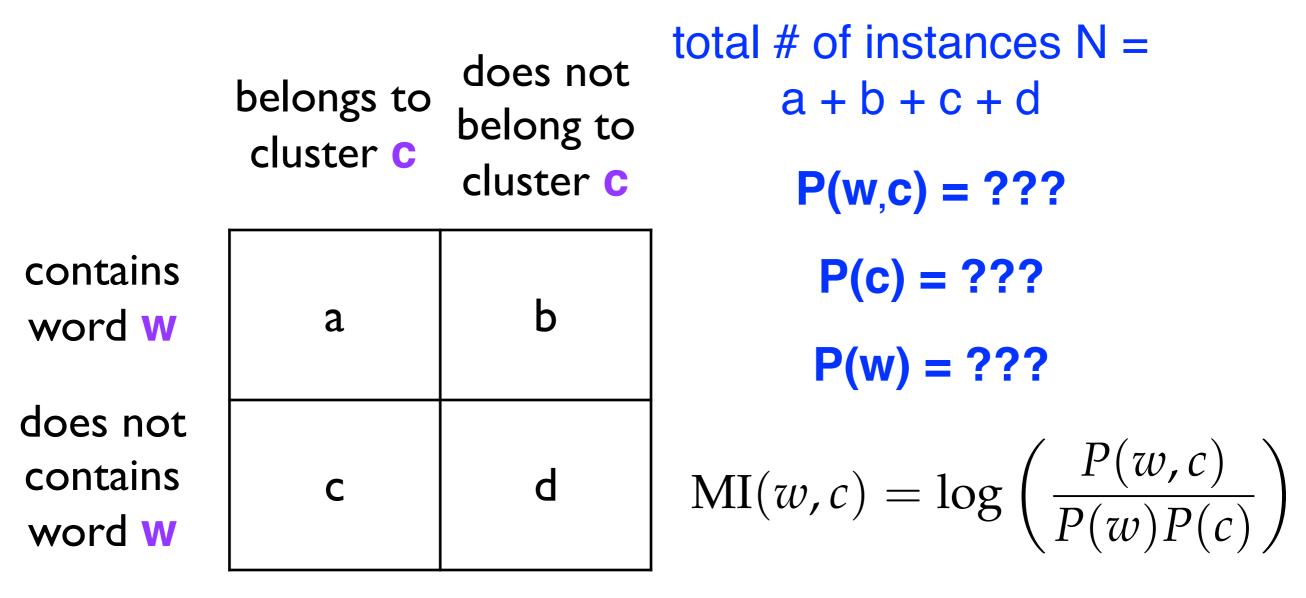
$$MI(w,c) = \log\left(\frac{P(w,c)}{P(w)P(c)}\right)$$

- **P(w,c)**: the probability that a document contains word **w** and belongs to cluster **c**
- **P(w)**: the probability that word **w** occurs in a document from any cluster
- P(c): the probability that a document belongs to cluster c

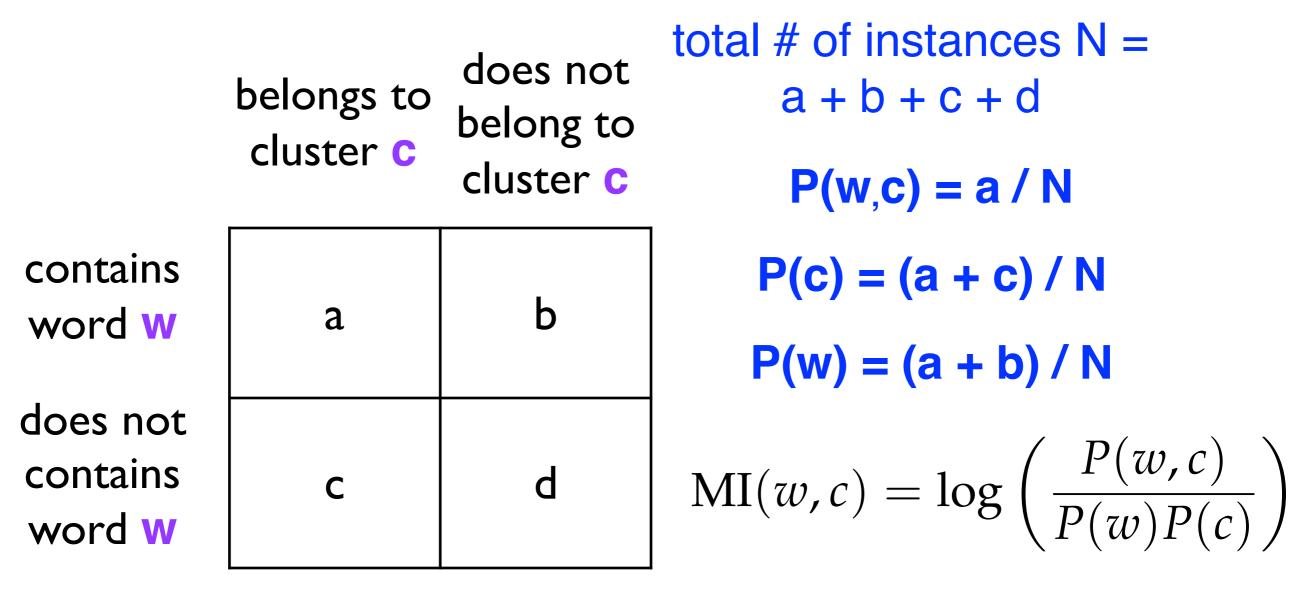
$$MI(w,c) = \log\left(\frac{P(w,c)}{P(w)P(c)}\right)$$

- If P(w,c) = P(w) P(c), it means that the word w is independent of cluster c
- If P(w,c) > P(w) P(c), it means that the word w is not independent of of cluster c

• Every document falls under one of these quadrants



• Every document falls under one of these quadrants



# Summary

- Clustering: grouping similar documents (or instances) into subsets
- Exploratory analysis: the goal is to discover common and uncommon properties of the data
- K-means and Agglomerative Bottom-up Clustering (there are many, many others)
- Labeling clusters