THE UNIVERSITY
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at CHAPEL HILL

Exploratory Analysis: Clustering

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

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

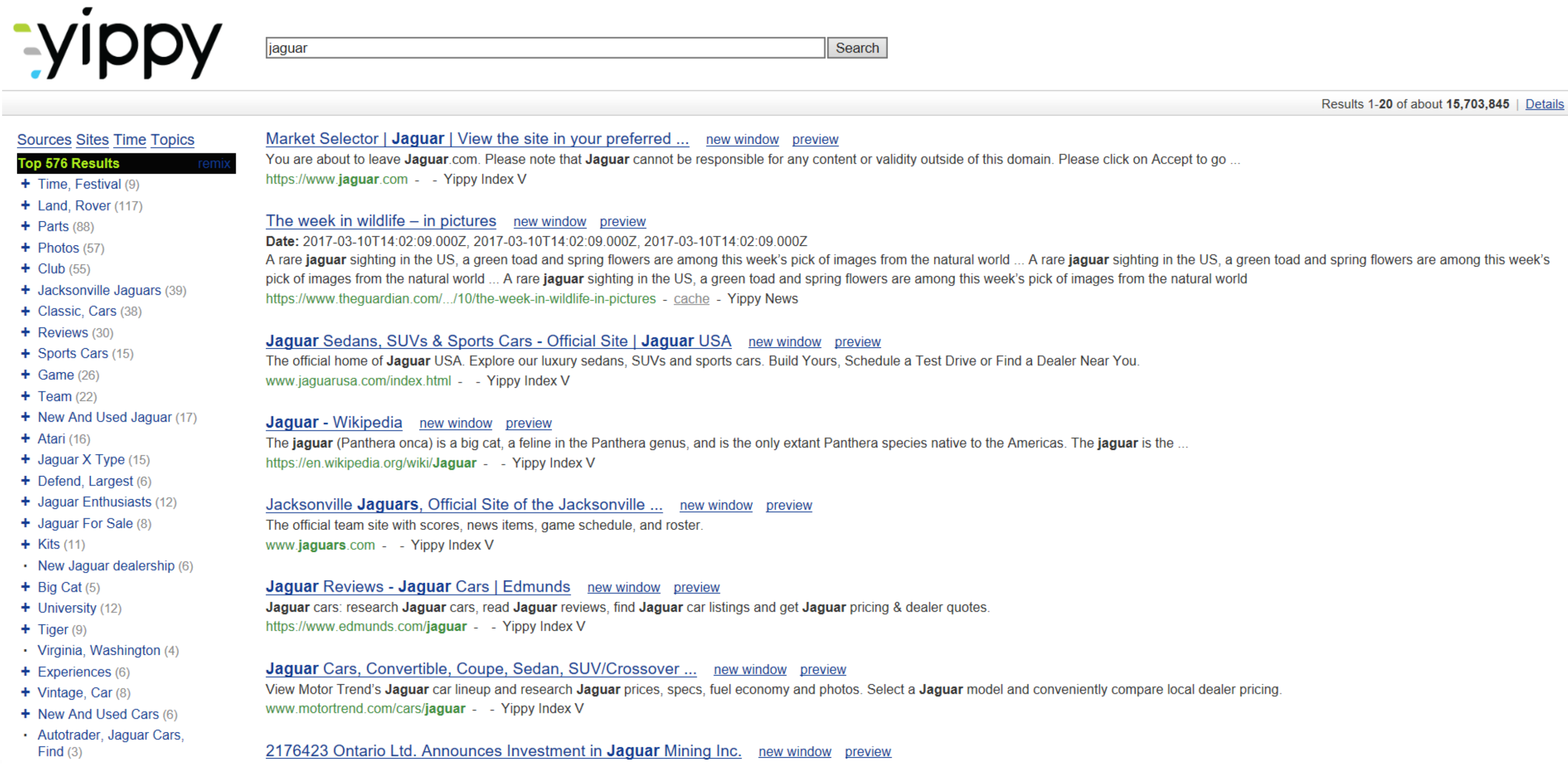
Clustering

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)

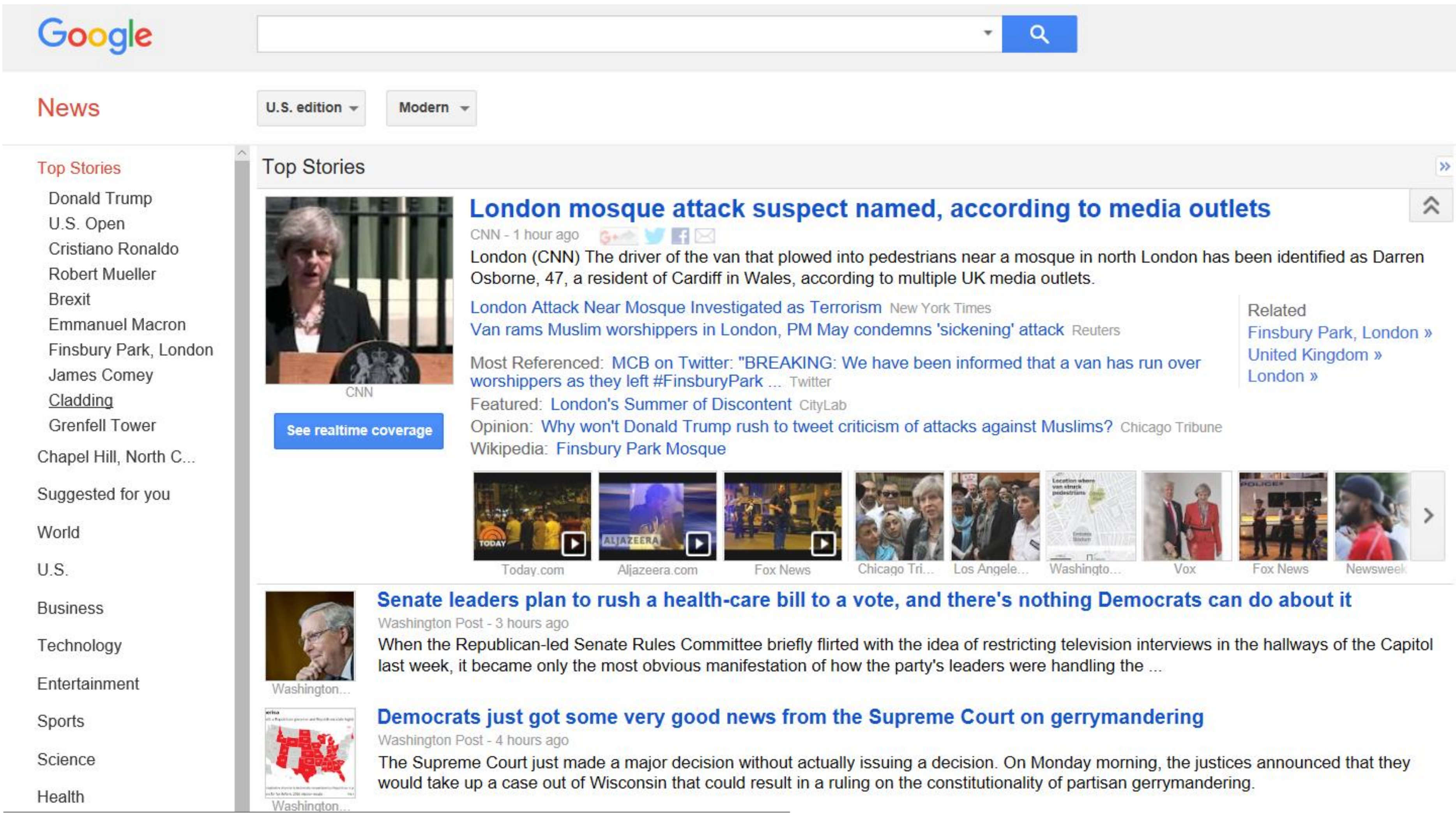
Clustering Applications

search engine results clustering



Clustering Applications

collection clustering



Clustering Applications

collection clustering

Clustering
objective

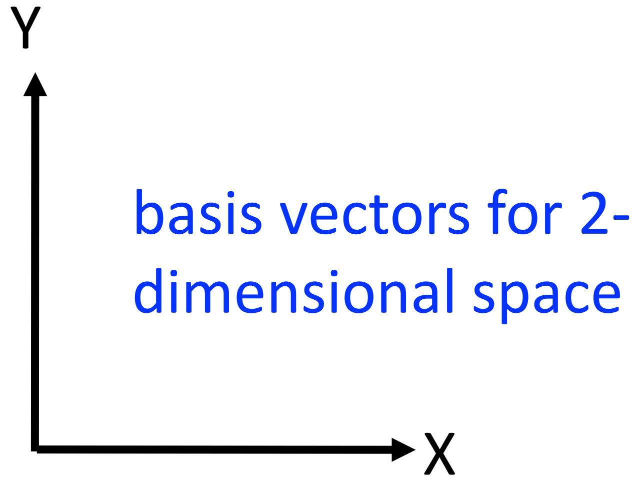
- Grouping documents or instances into subsets or clusters
- Documents within a the same cluster should be similar
- Documents from different clusters should be dissimilar

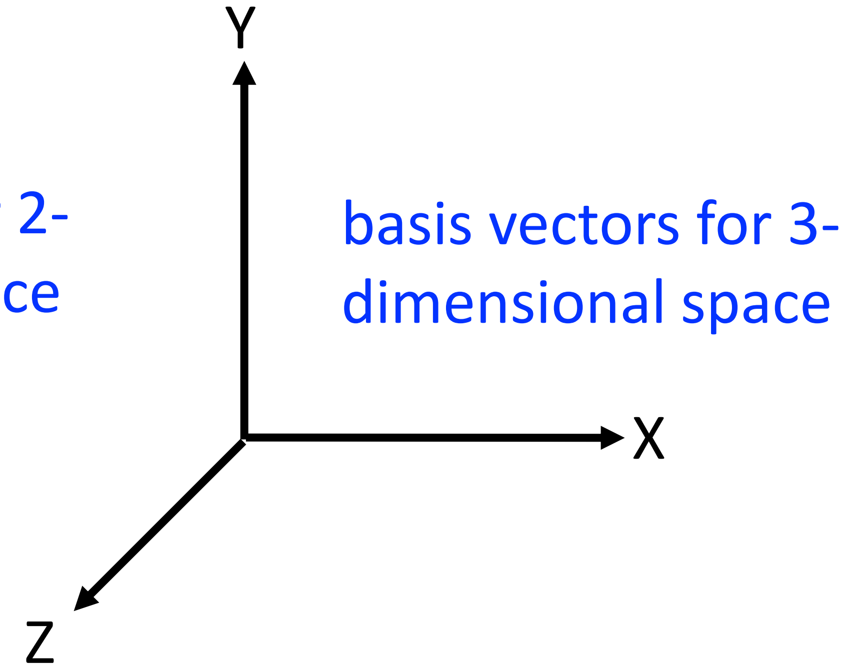
Clustering
basics

- 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

Vector Space Representation
review

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

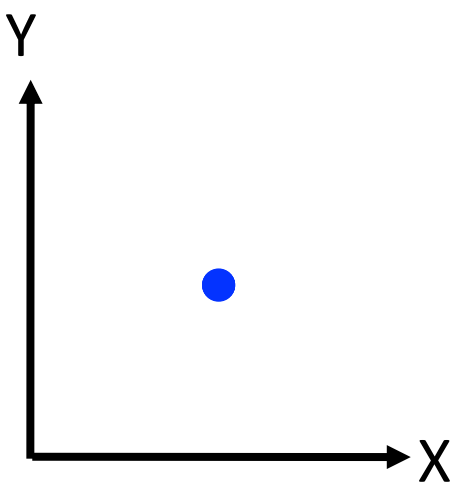


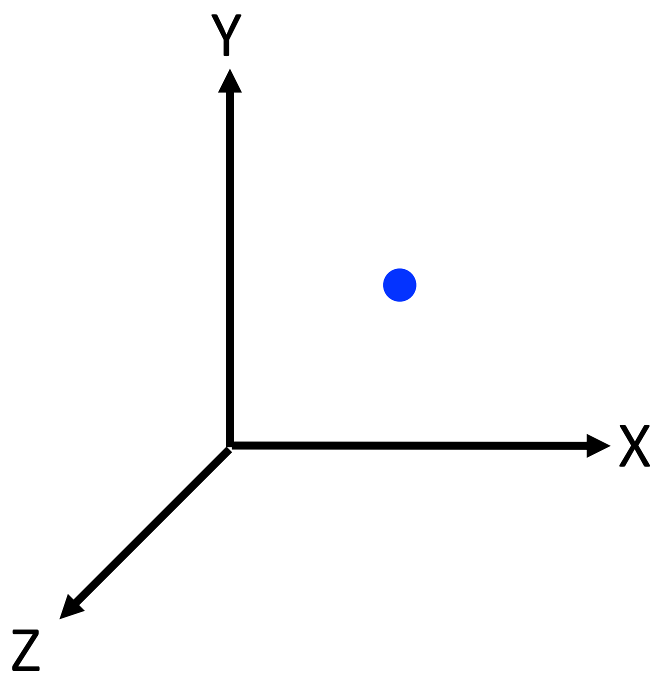


Vector Space Representation

review

- A vector is a point in a vector space

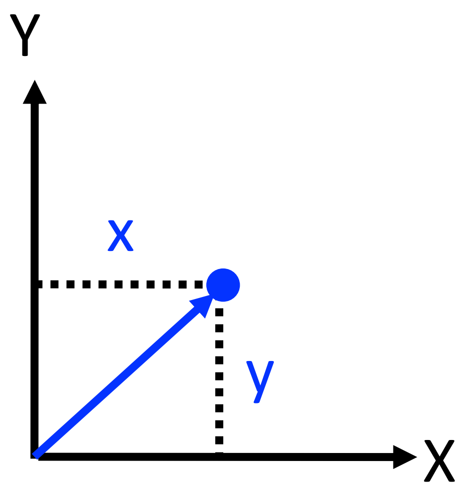


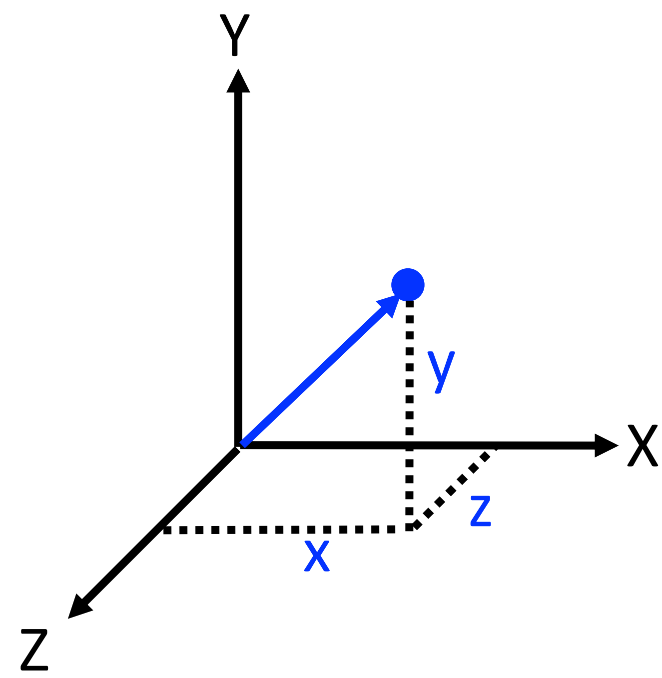


Vector Space Representation

review

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





Vector Space Representation

review

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

Vector Space Representation

review

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
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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 10-dimensional vector space

Vector Space Representation

review

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

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

Vector Space Representation

review

- Similarity = Euclidean Distance:

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

Vector Space Representation

review

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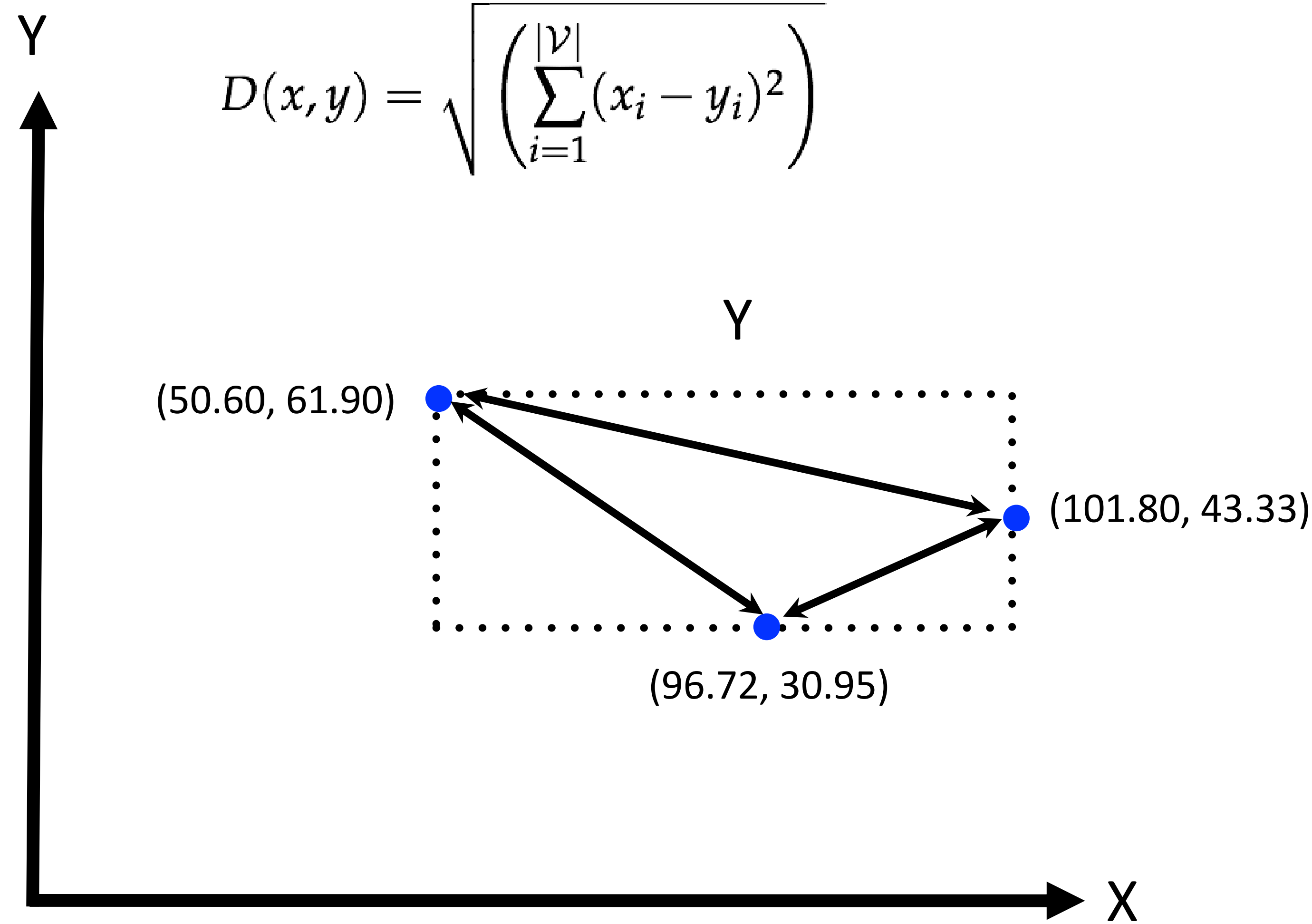
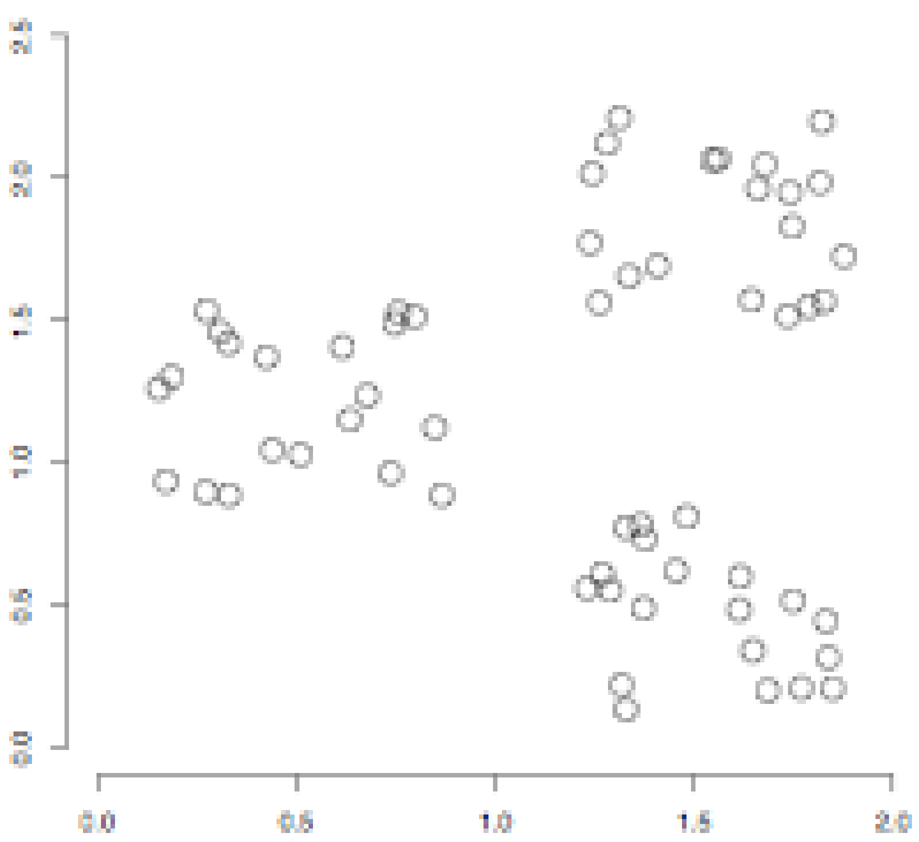


Clustering

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



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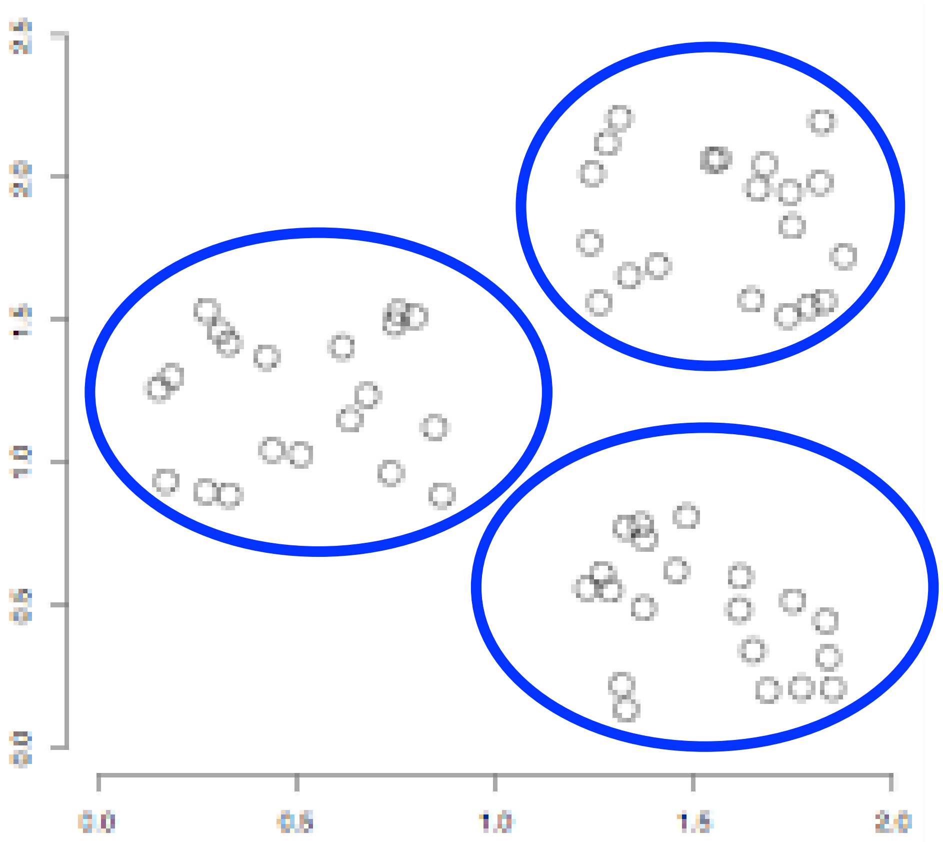
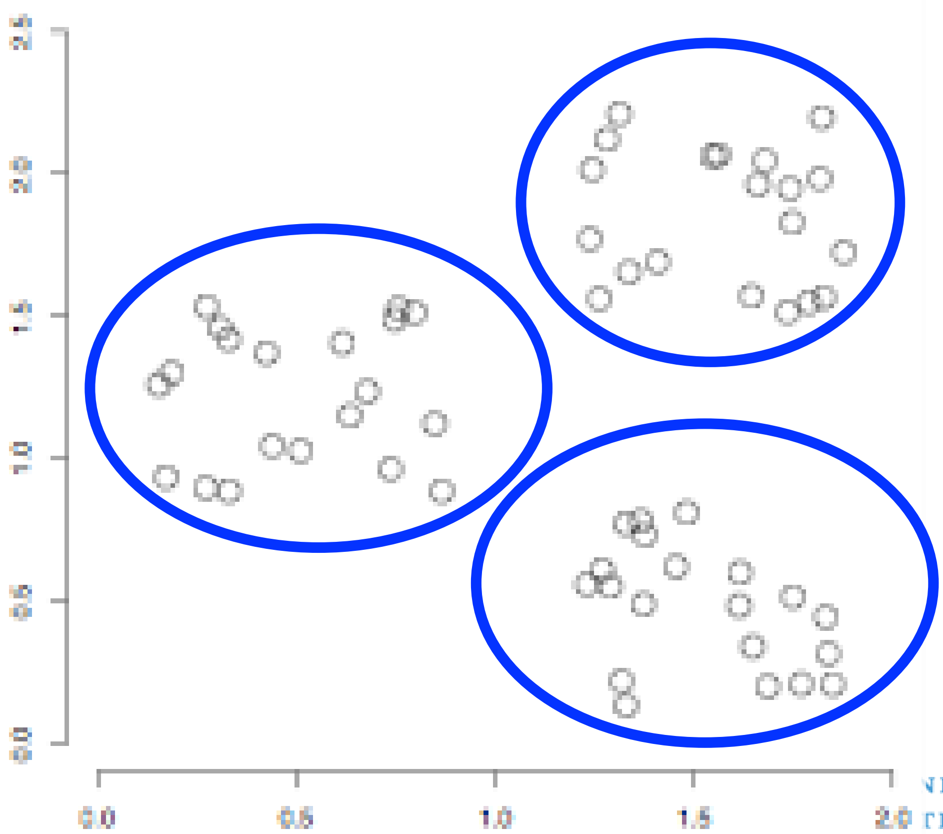


Clustering

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

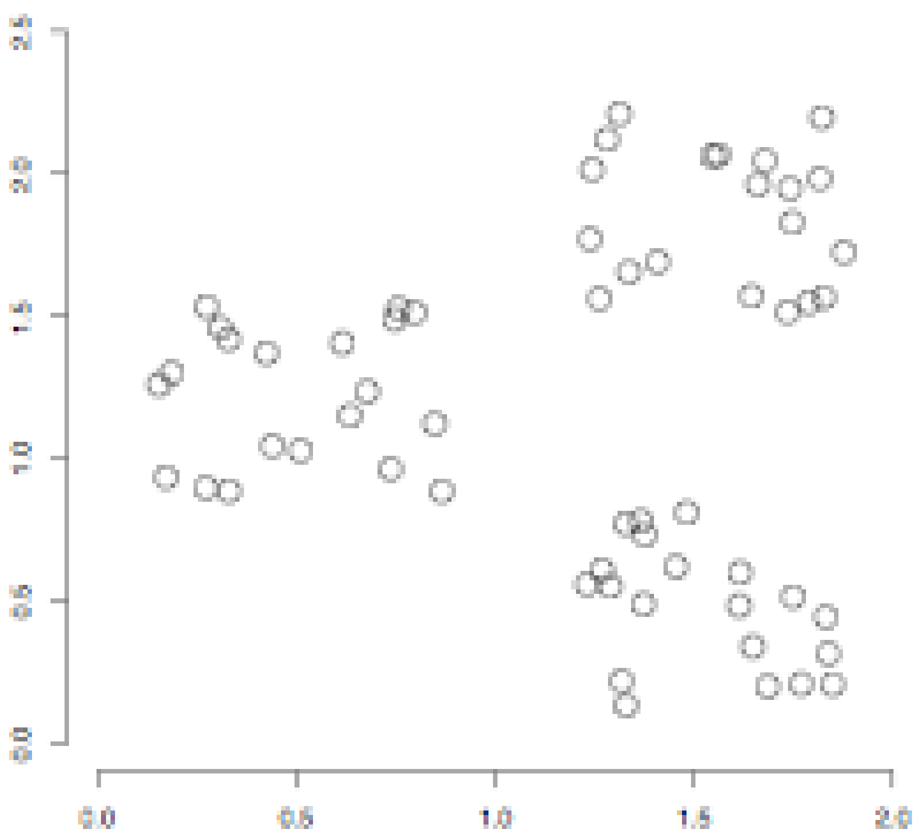


Clustering

- 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
  - and so on.

Clustering

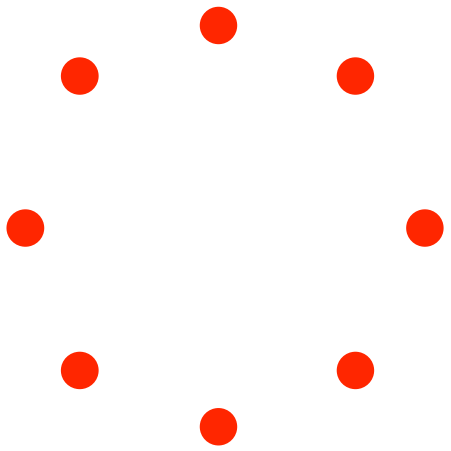
- Could this work?



K-Means Clustering

K-means Clustering
cluster centroid

- 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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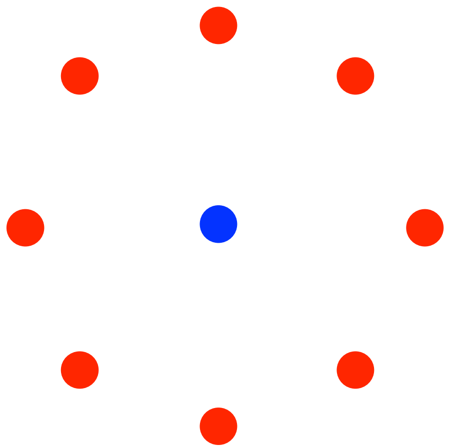

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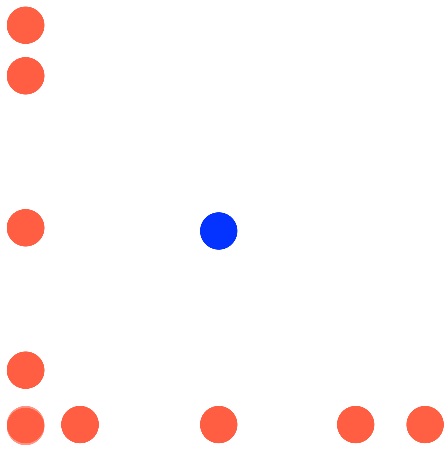

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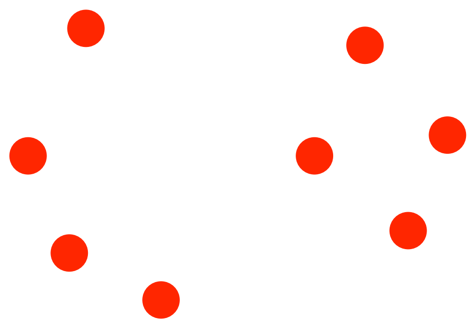

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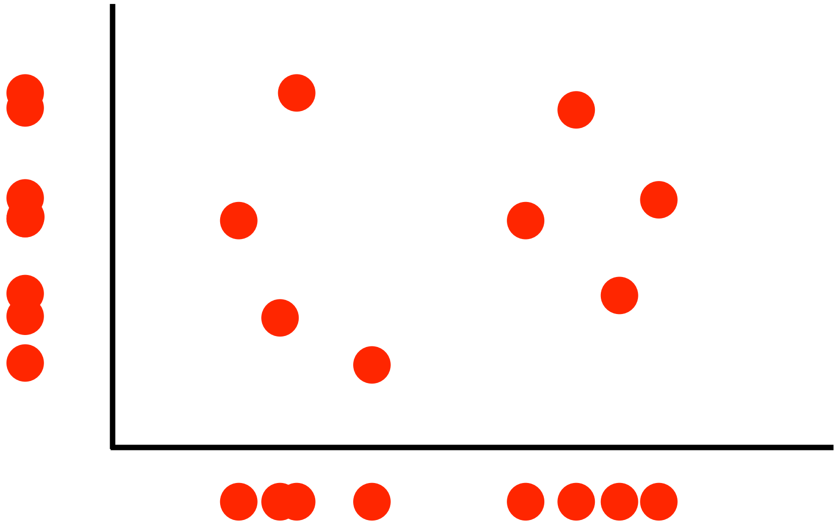

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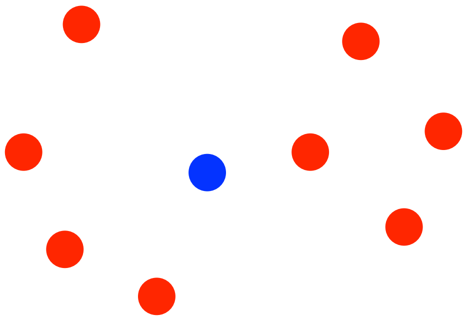


K-means Clustering

cluster centroid

docs assigned to cluster 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
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

docs assigned to cluster 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
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:

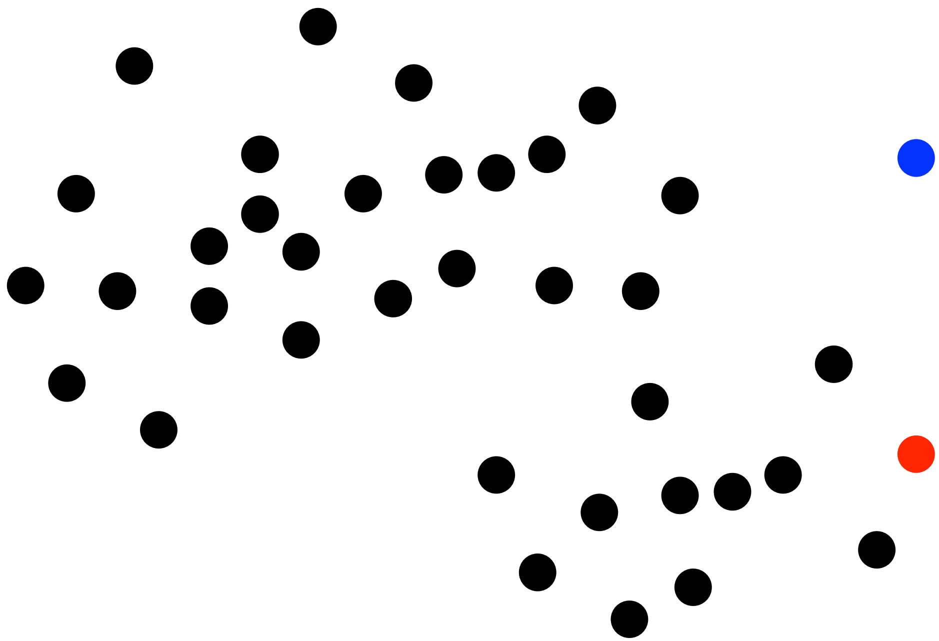
$$c_i = \frac{1}{|C|} \sum_{d \in C} d_i$$

K-means Clustering

- 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 <u>terminating condition</u>

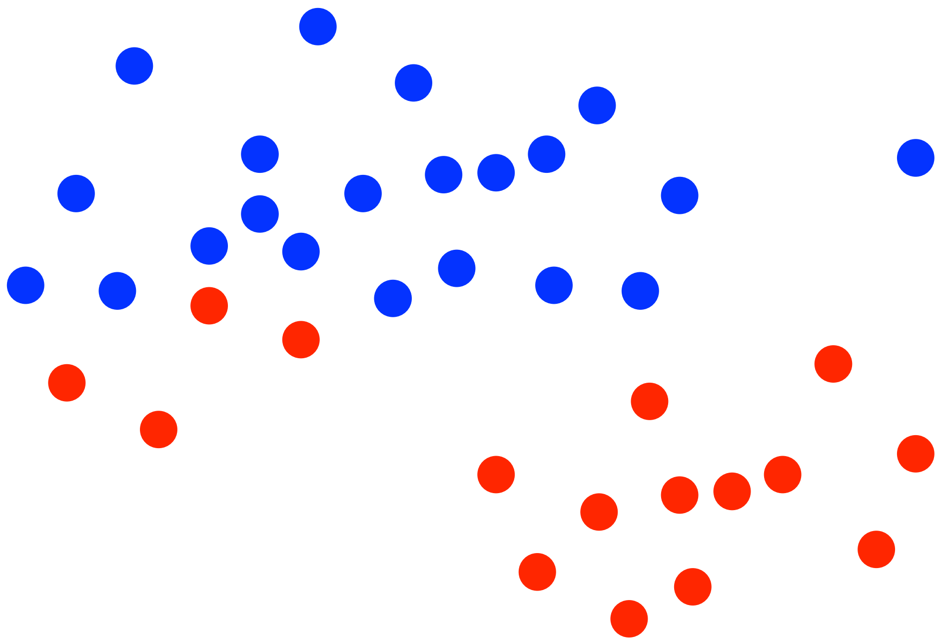
K-means Clustering

- Step 1: randomly select K documents (seeds)



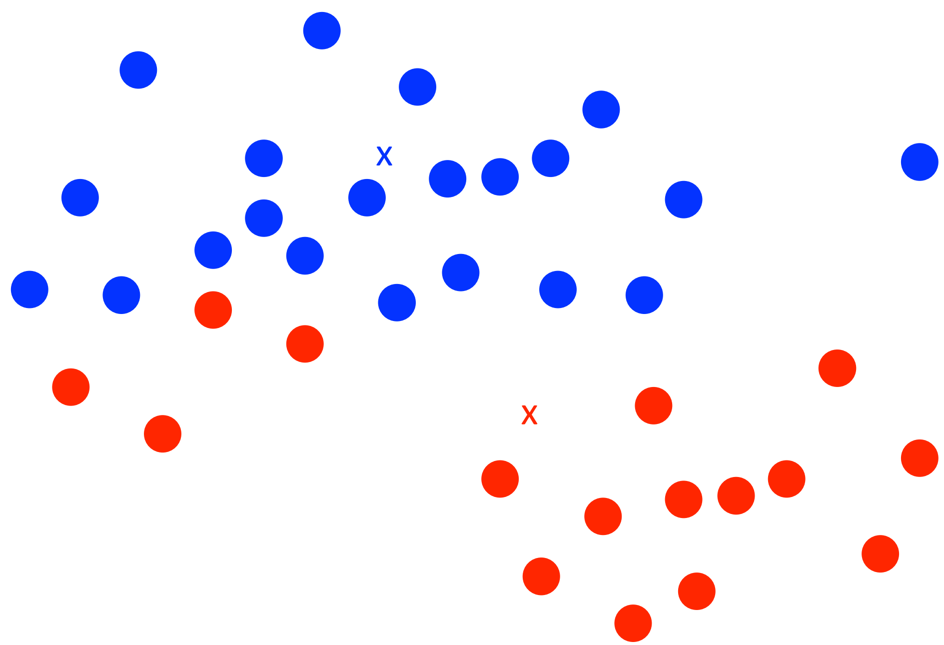
K-means Clustering

- Step 2: assign each document to its nearest seed



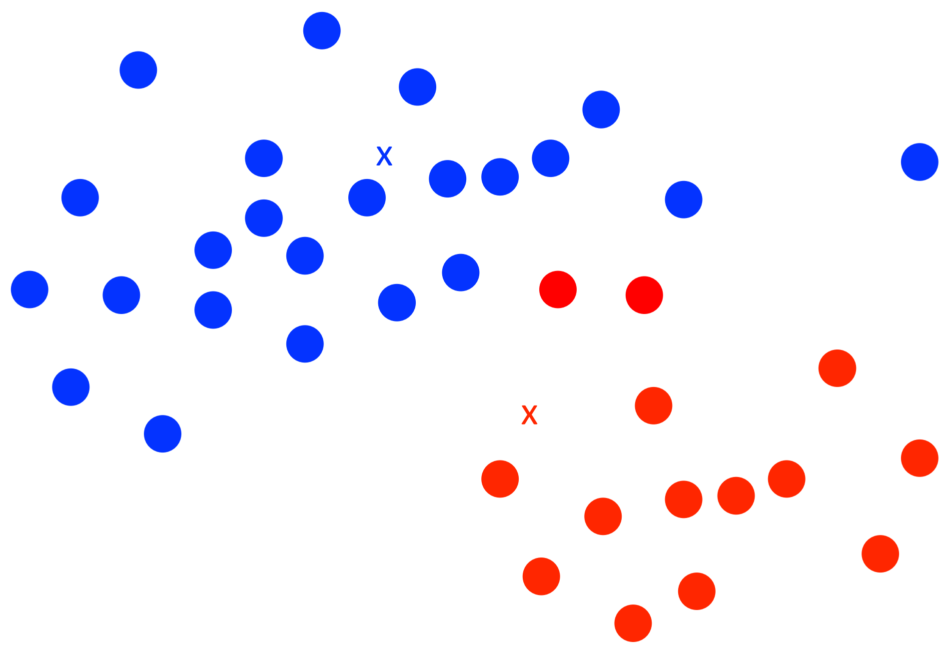
K-means Clustering

- Step 3: compute all K cluster centroids



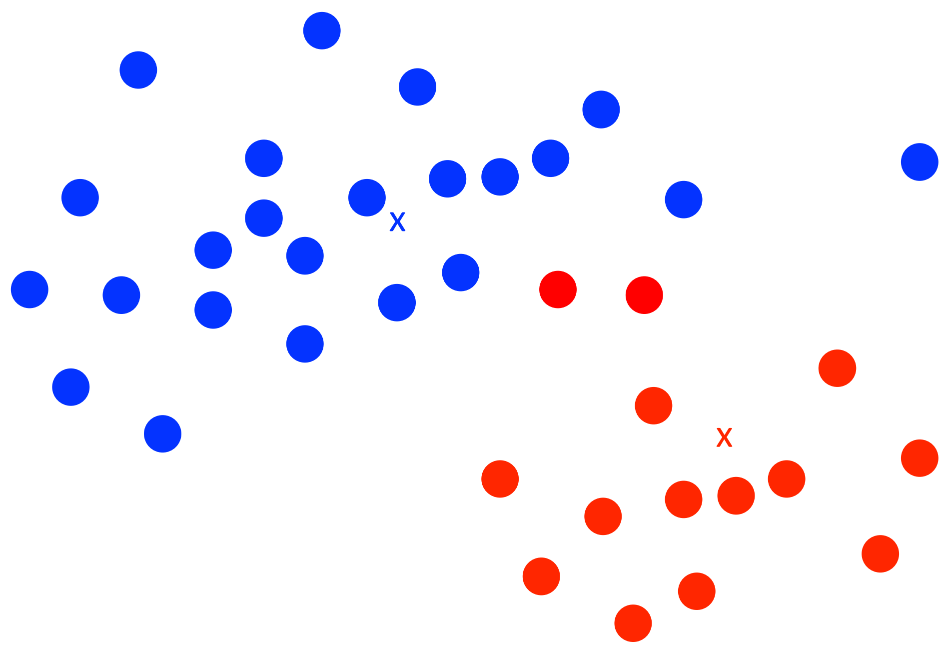
K-means Clustering

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



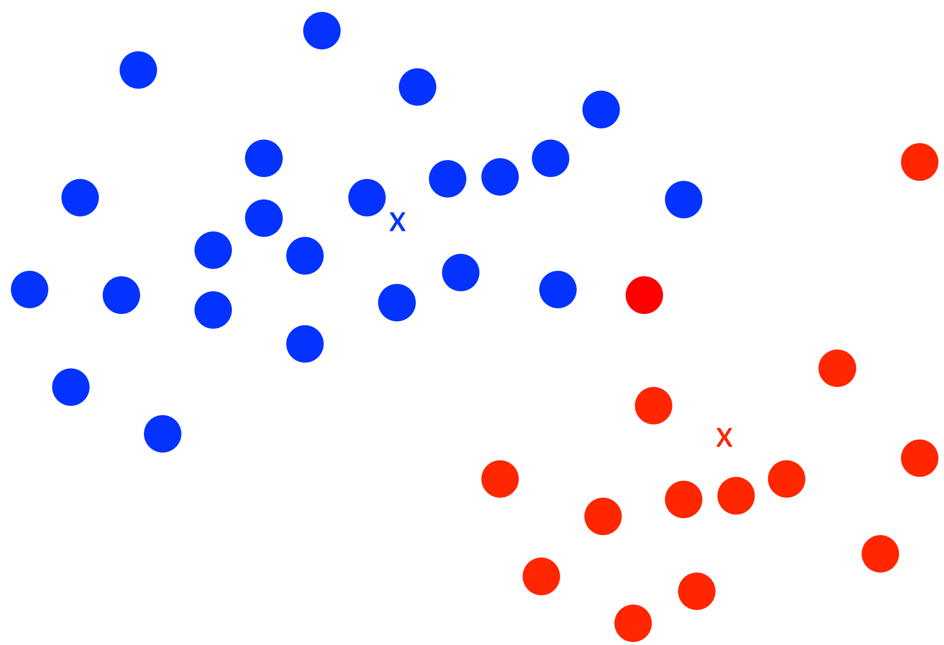
K-means Clustering

- Step 4: re-compute all K cluster centroids



K-means Clustering

- Step 5: re-assign each document to its nearest centroid



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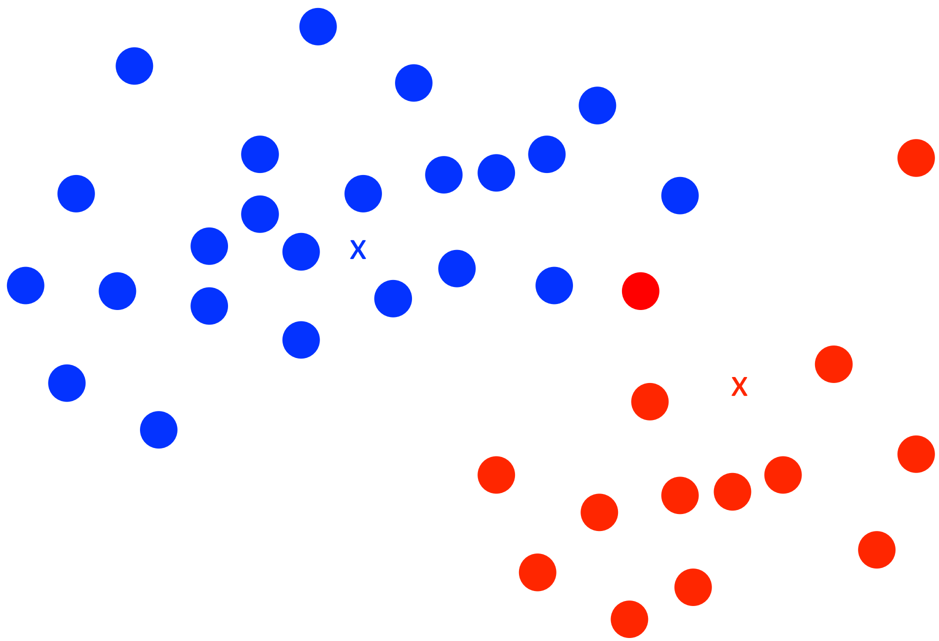
K-means Clustering

- Step 4: re-compute all K cluster centroids



K-means Clustering

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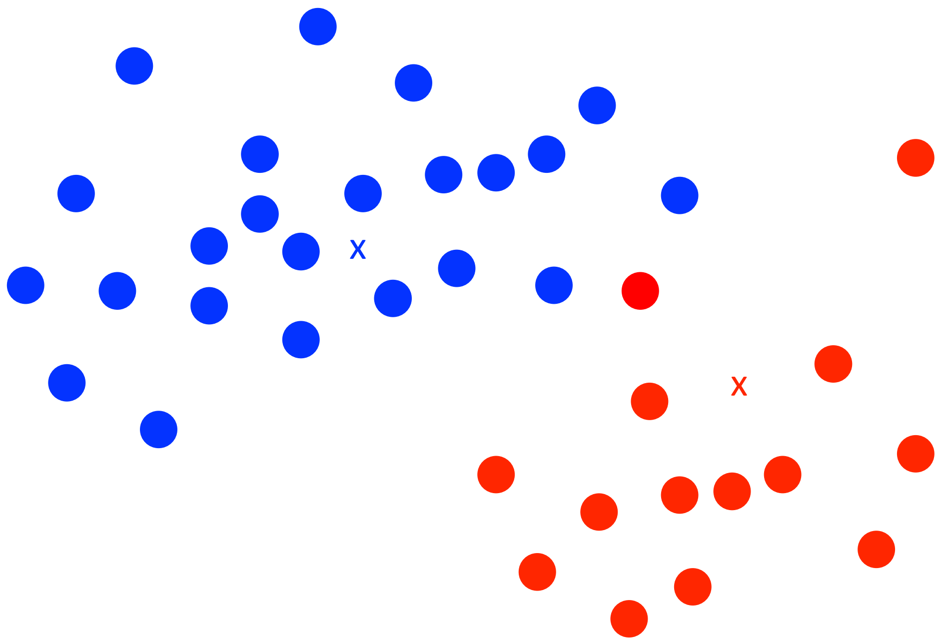

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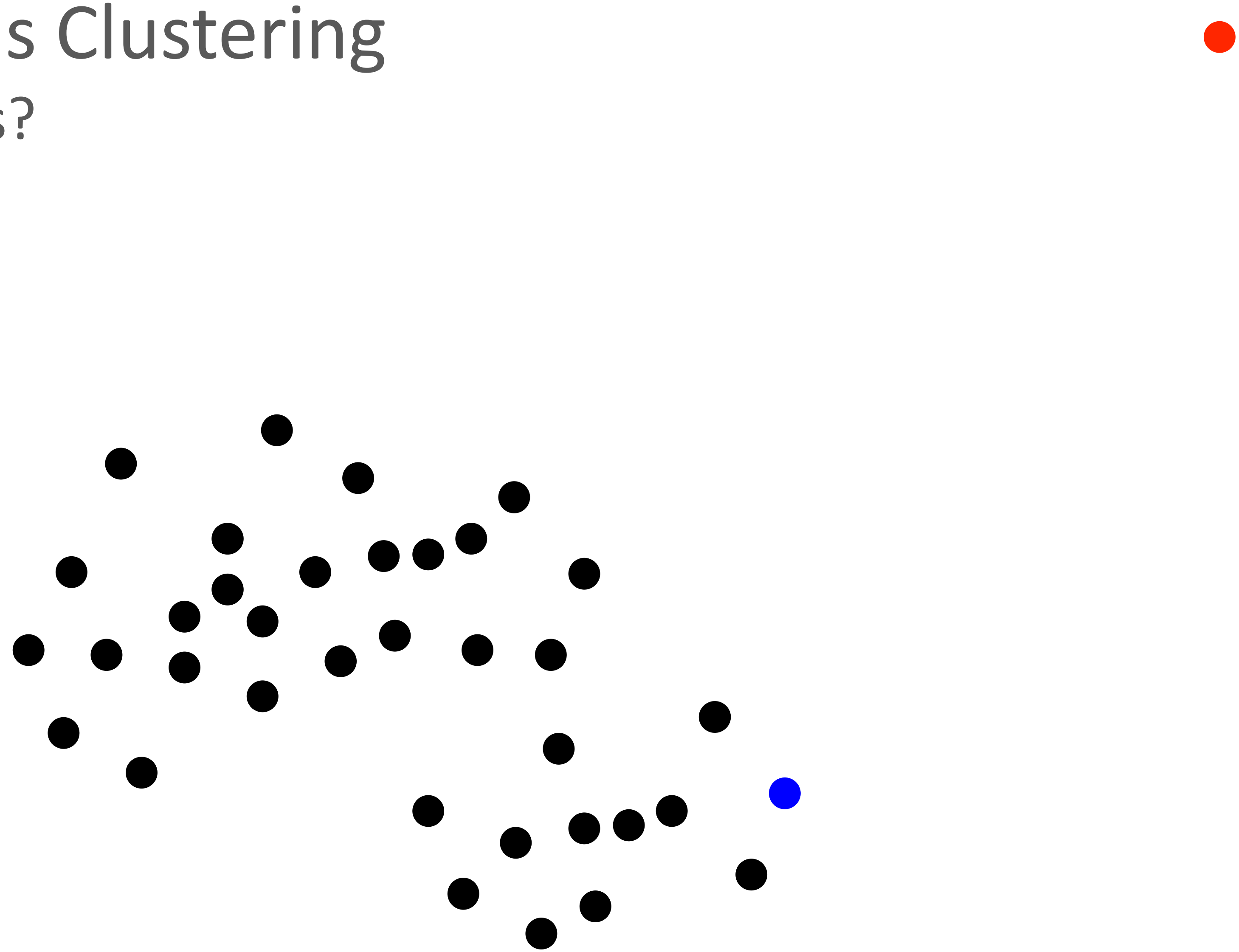
K-means Clustering
potential drawback

- 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

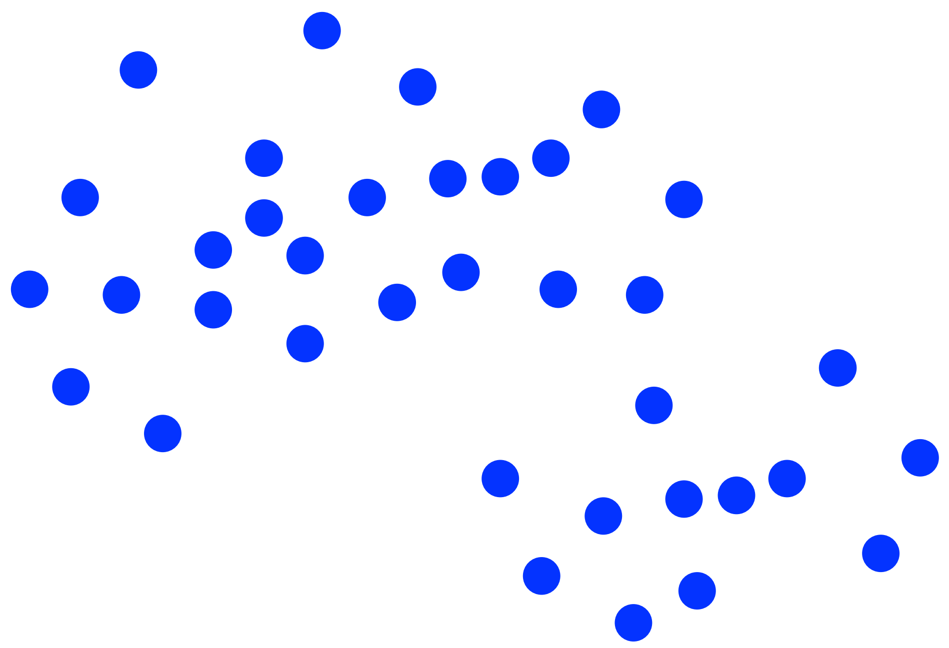
K-means Clustering

bad seeds?



K-means Clustering

bad seeds?



K-means Clustering

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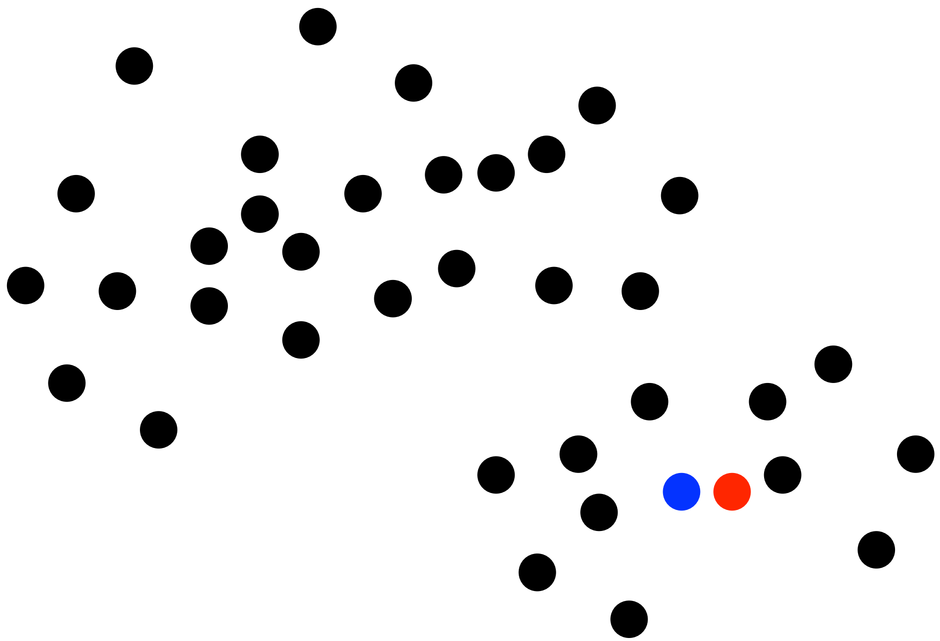

K-means Clustering

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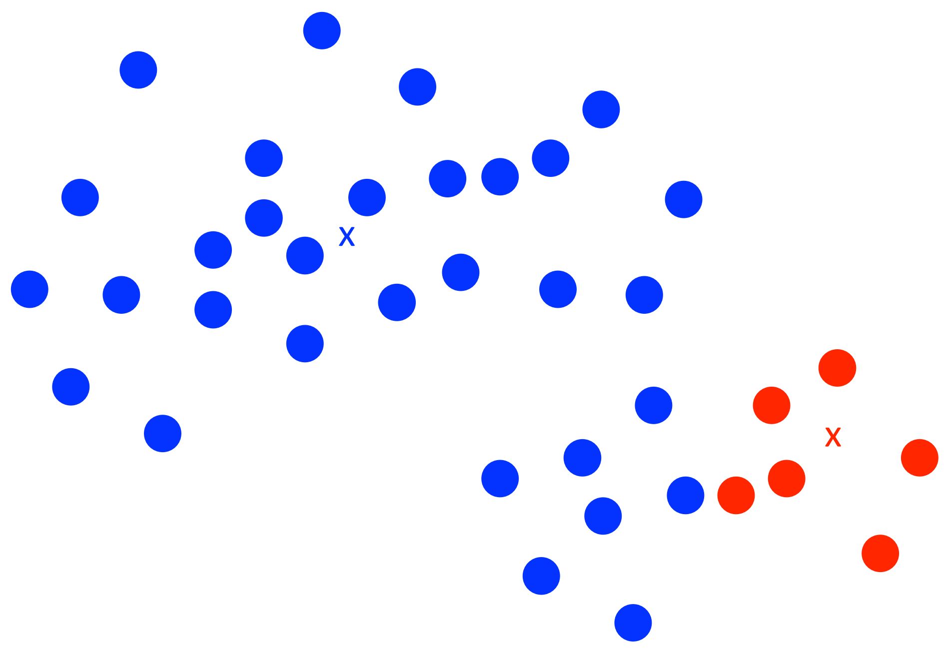
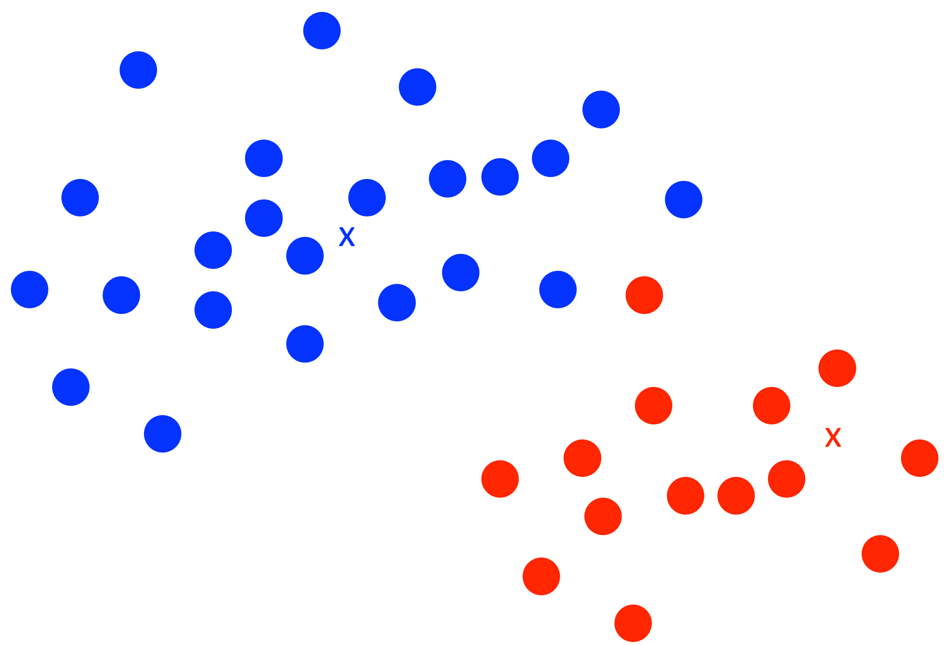


K-means Clustering

bad seeds?



K-means Clustering

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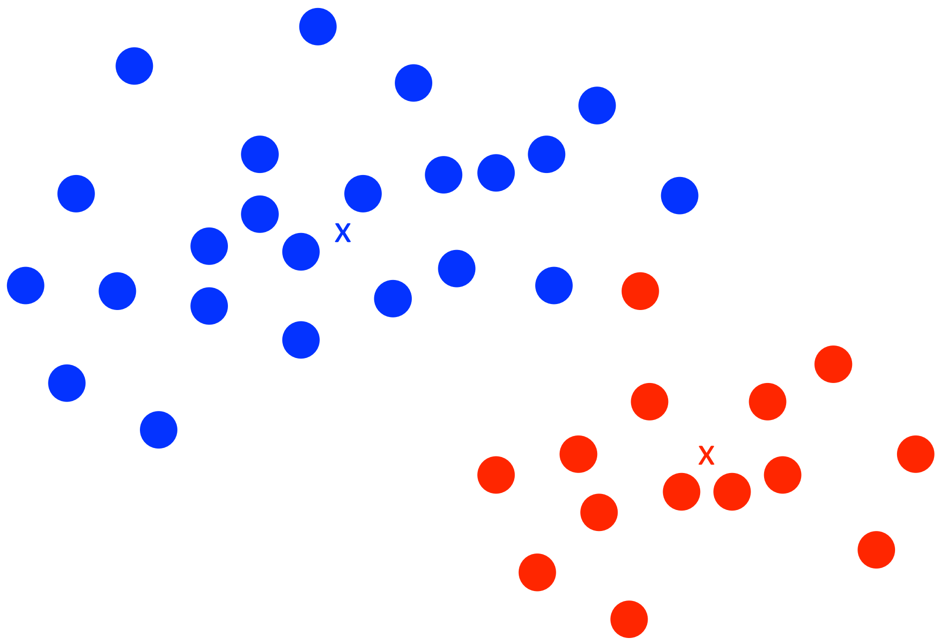
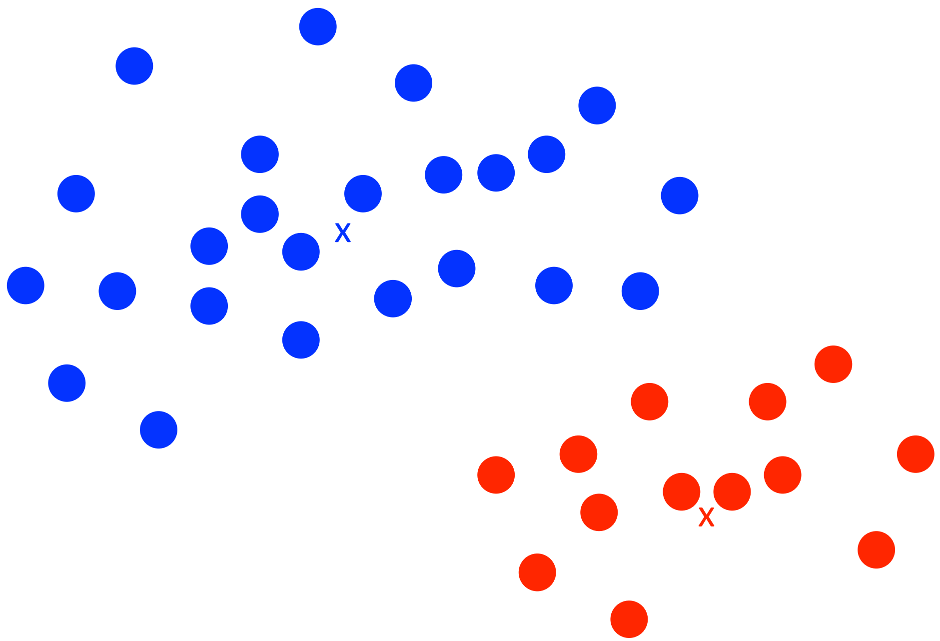


K-means Clustering

bad seeds?



K-means Clustering

bad seeds

- 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 Quality = (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>)

Inter-cluster distance   Intra-cluster distance

K-means Clustering
improved k-means

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

Bottom-up Agglomerative Clustering

Bottom-up 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)

Bottom-up Clustering

- 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

Bottom-up Clustering

- Input: data
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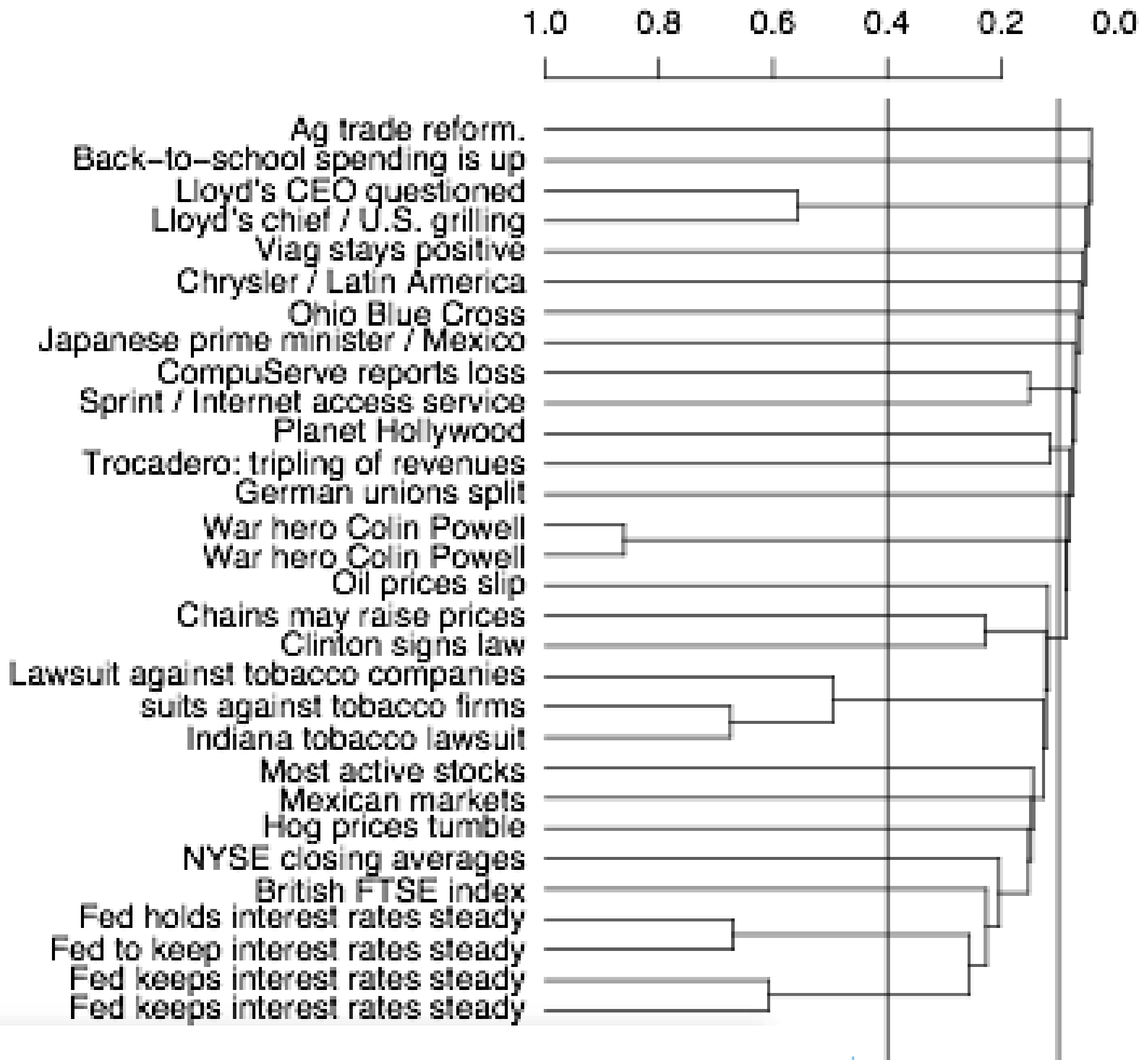
Bottom-up Clustering

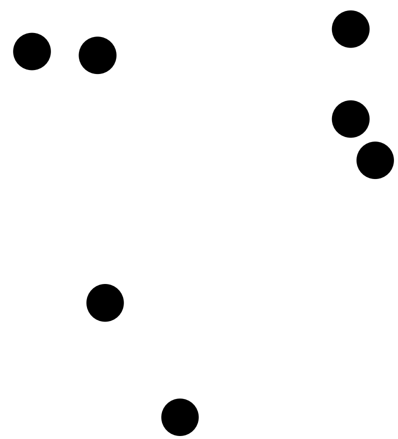


Bottom-up Clustering

- 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

Bottom-up Clustering
single-link

- Step 1: consider each document its own cluster



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Bottom-up Clustering

single-link

- Step 2: compute the distance between all cluster pairs
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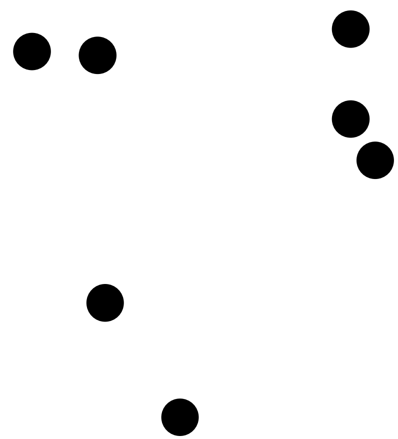

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Bottom-up Clustering

single-link

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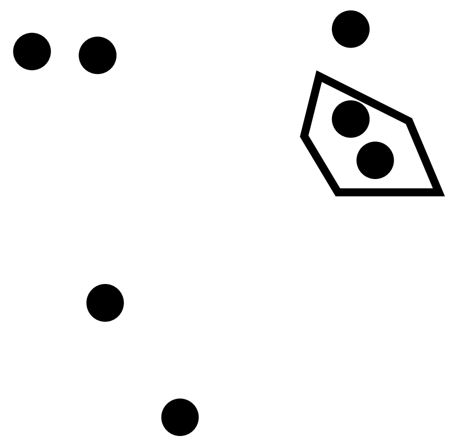

Bottom-up Clustering

single-link

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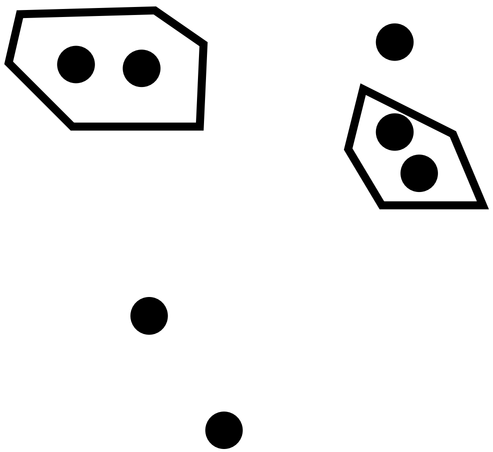

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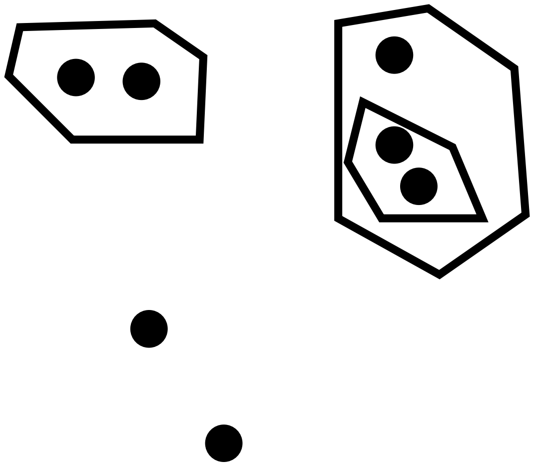

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single-link

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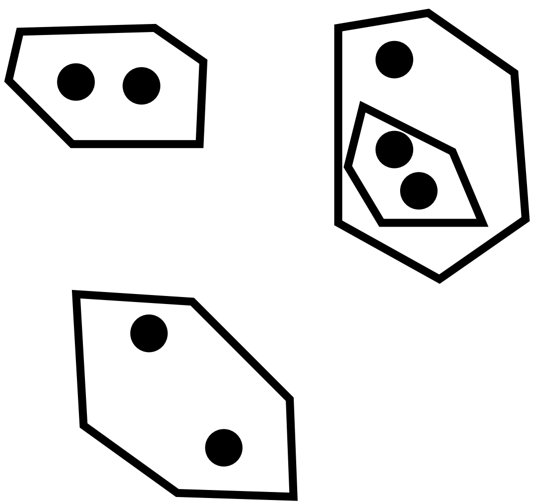
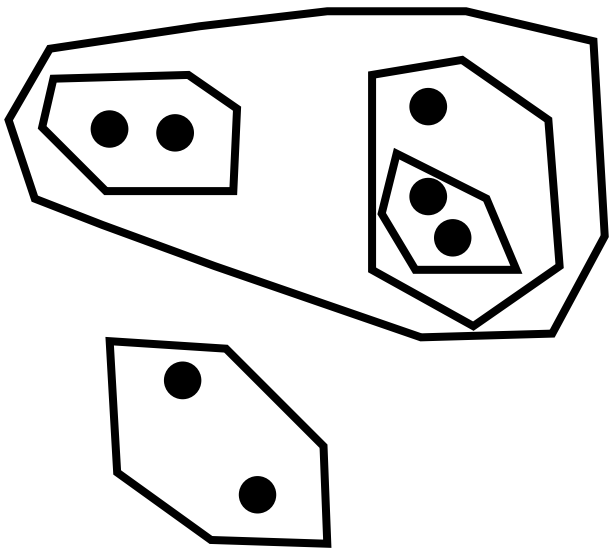


Bottom-up Clustering

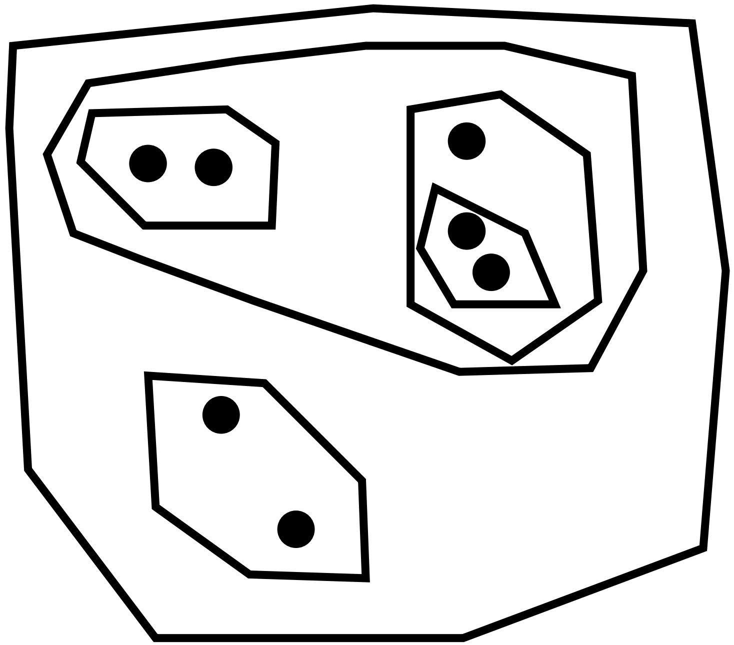
single-link

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



Bottom-up Clustering
single-link

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



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 --> HiDAV --> unc --> basketball

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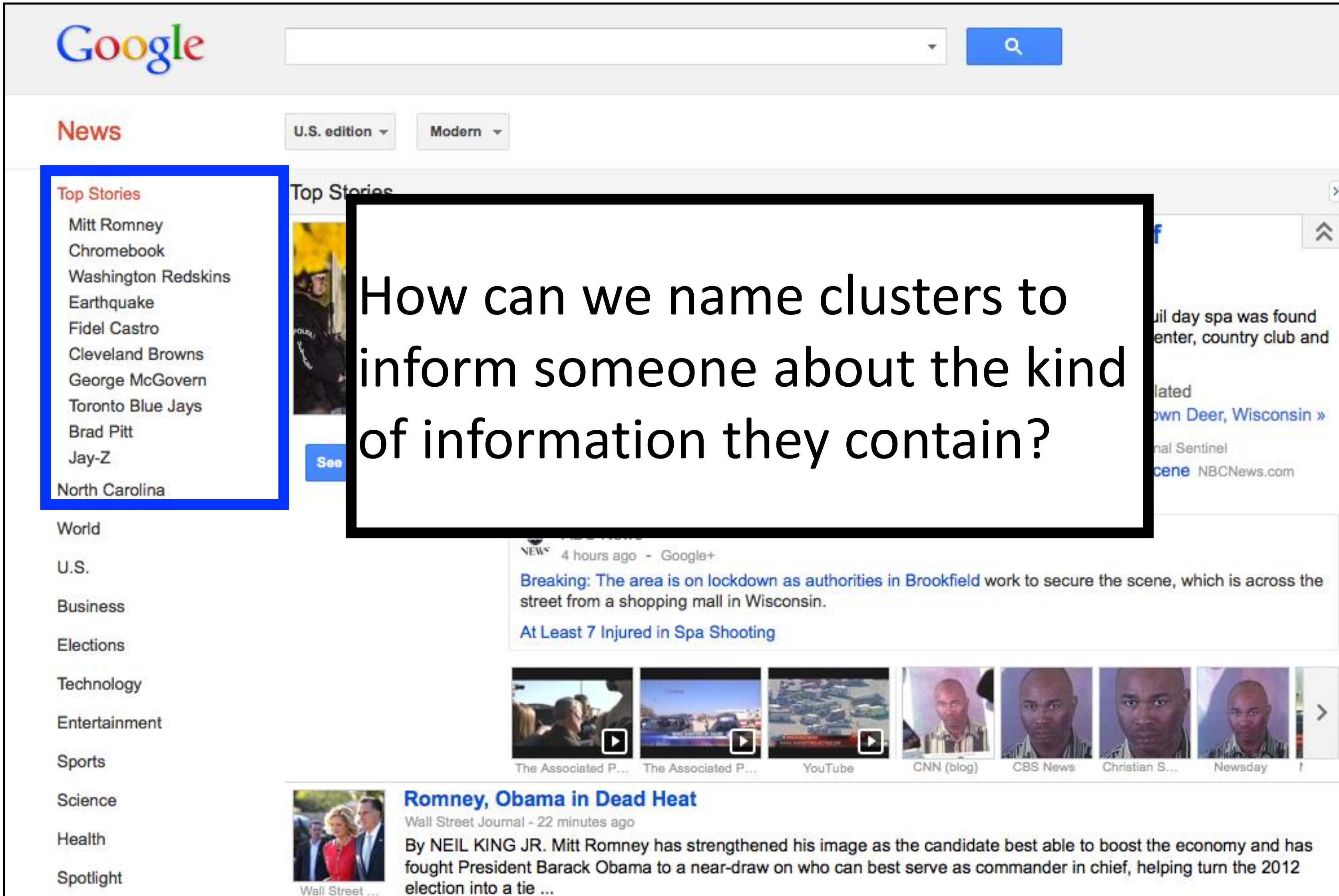
Labeling Clusters

Clustering Applications

collection clustering



How can we name clusters to inform someone about the kind of information they contain?

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

Mutual Information

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

- **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**

Mutual Information

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

- If **$P(w,c) = P(w)\ P(c)$**, it means that the word **w** is <u>independent</u> of cluster **c**
- If **$P(w,c) > P(w)\ P(c)$**, it means that the word **w** is not <u>independent</u> of of cluster **c**

Mutual Information

- Every document falls under one of these quadrants

	belongs to cluster **c**	does not belong to cluster **c**
contains word **w**	a	b
does not contains word **w**	c	d

total # of instances N = a + b + c + d

P(w, c) = a / N

P(c) = (a + c) / N

P(w) = (a + b) / N

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

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

The Future of Text Mining

Link

Too Many Barriers? It really Matter Where to Apply and How to Start.

Link

Challenge with Something You Really Like

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Any Questions?

No More Next Class