# INTRODUCTION TO DATA SCIENCE

This lecture is
based on course by E. Fox and C. Guestrin, Univ of Washington

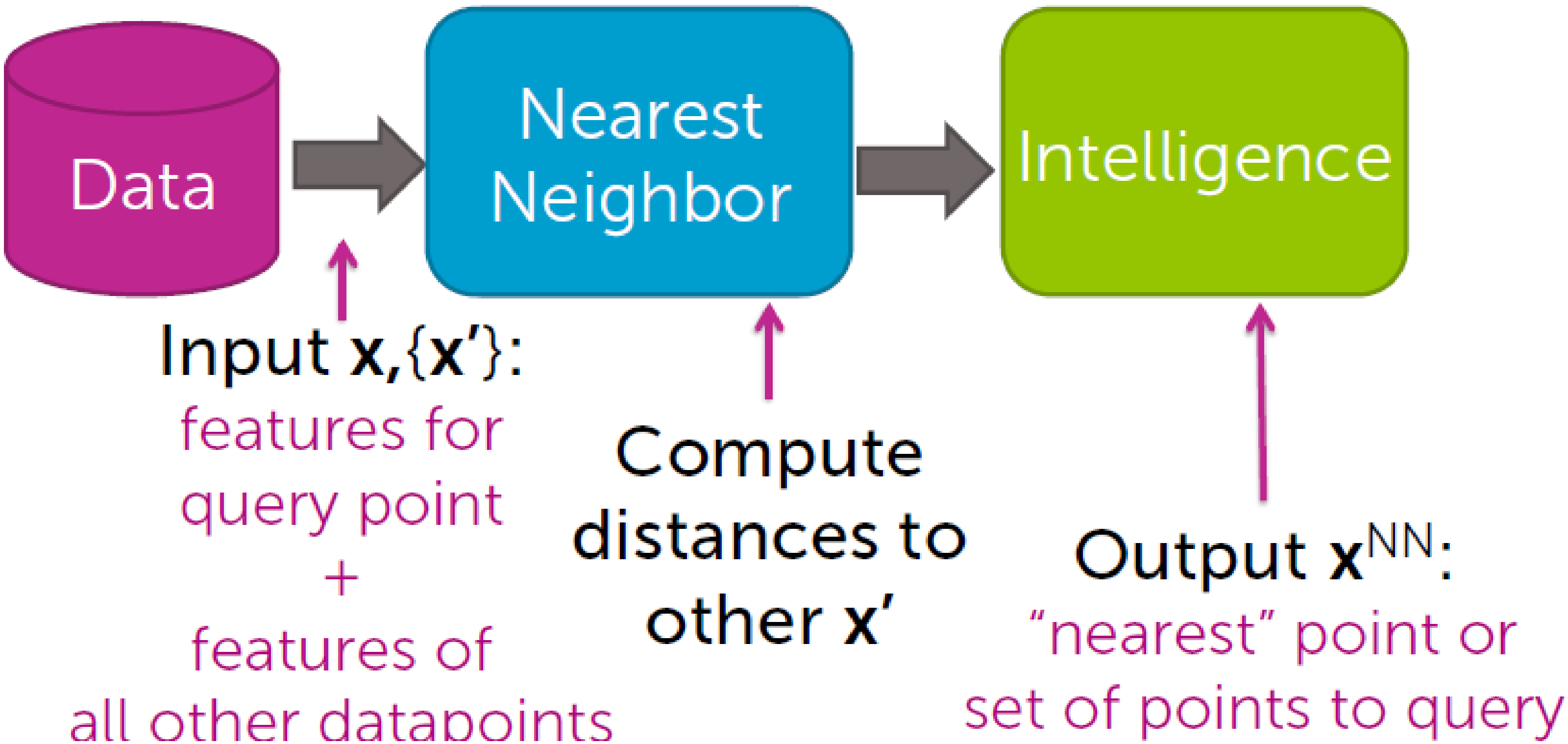
20/11, 27/11 2024

WFAiS UJ, Informatyka Stosowana
I stopień studiów

# What is retrieval?



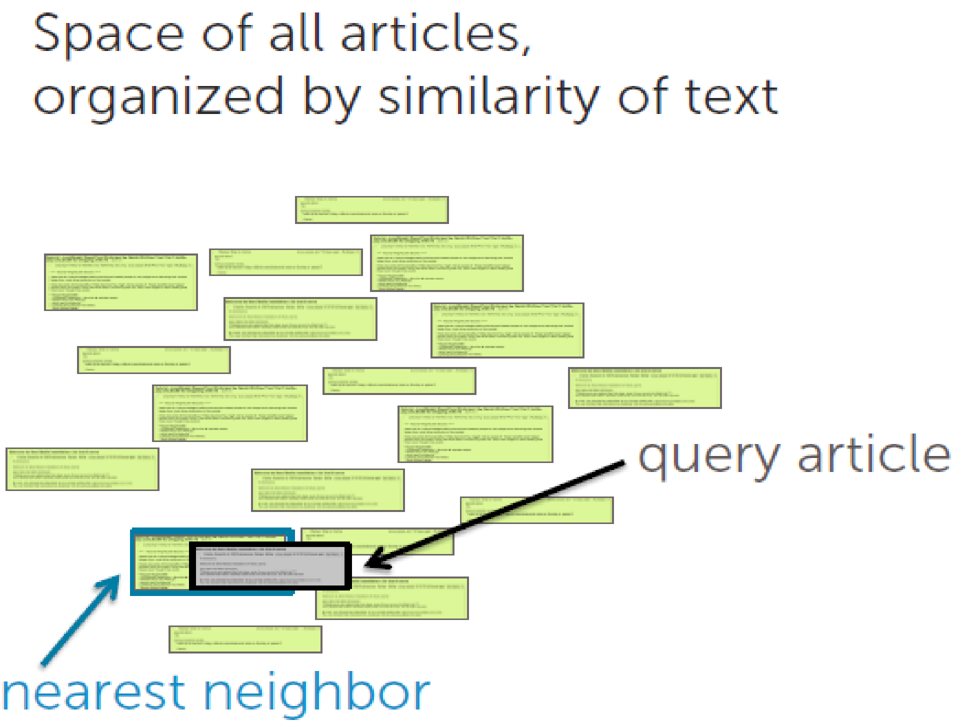
Search for related items



# What is retrieval?



## Retrieve "nearest neighbor" article

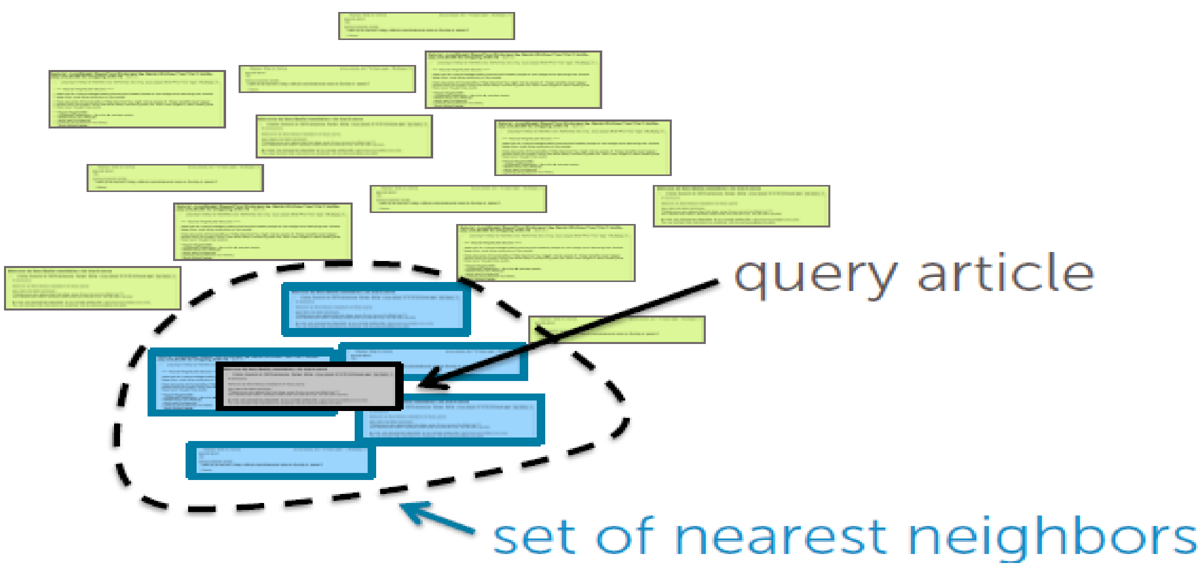


# What is retrieval?



## Or set of nearest neighbors

Space of all articles,
organized by similarity of text



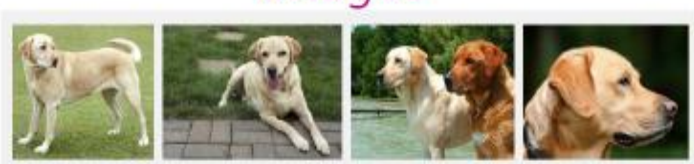
# Retrieval applications



Just about everything...

Products

Images



Streaming content:

- Songs
- Movies
- TV shows
- ...

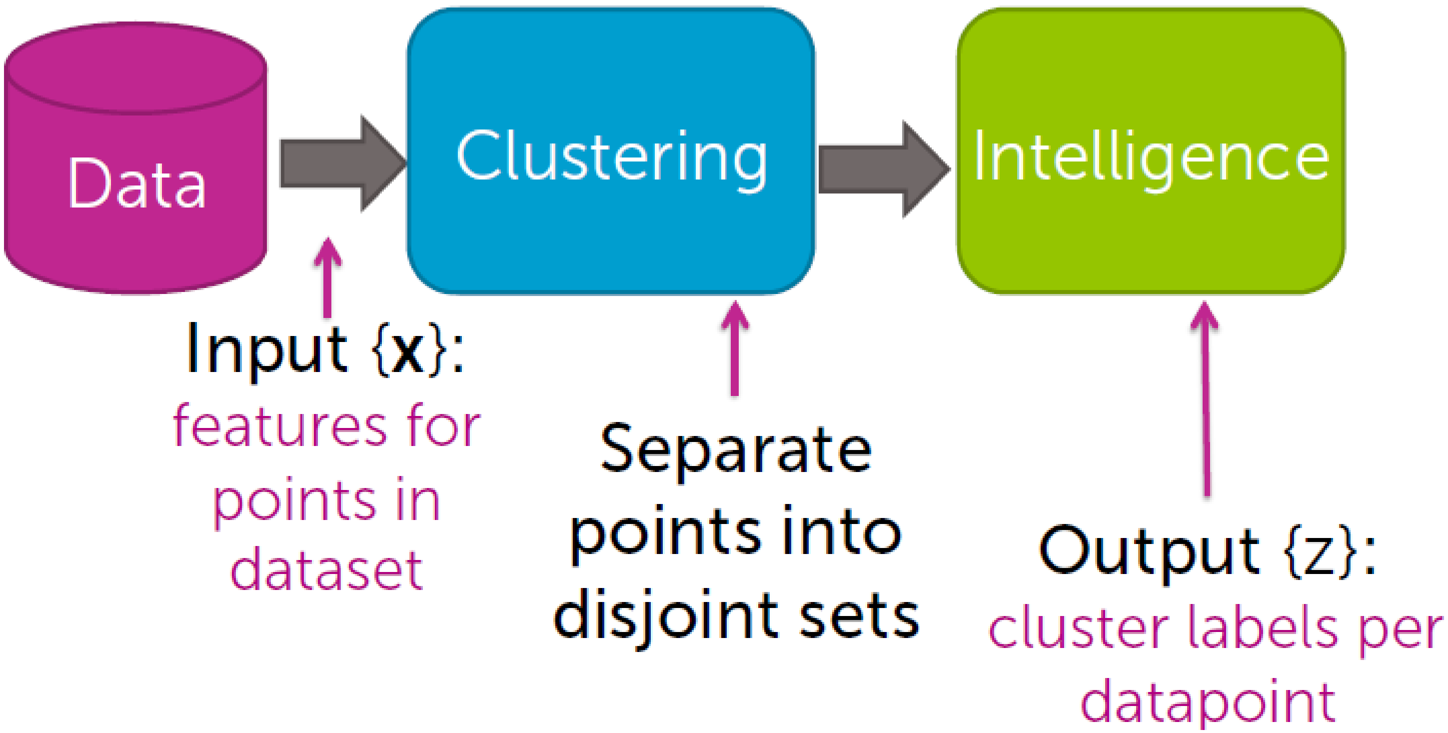
News articles


Social networks
(people you might want to connect with)

# What is clustering?



Discover groups of similar inputs



# Clustring applications



# Clustering applications

## Clustering images

For search, group as:

- Ocean
- Pink flower
- Dog
- Sunset
- Clouds
- …

# Impact of retrieval & clustering



- Foundational ideas
- Lots of information can be extracted using these tools (exploring user interests and interpretable structure relating groups of users based on observed behavior)

# Overwiew of content

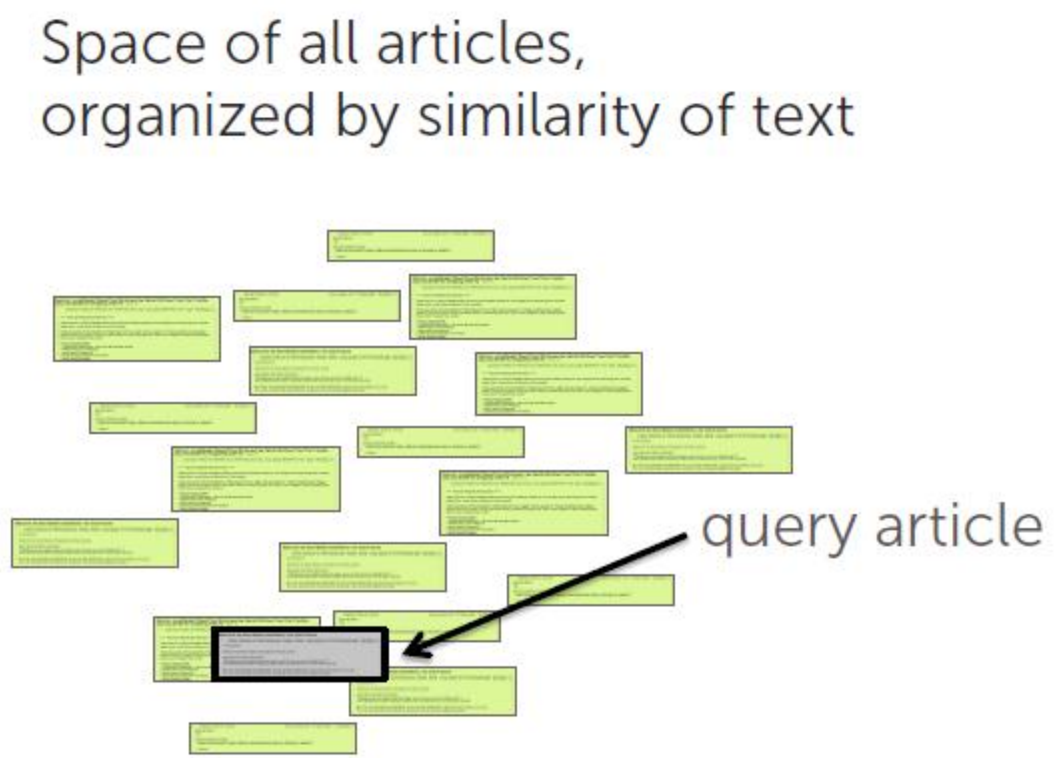


- **Models**
  - Nearest neighbors
  - Clustering
  - Mixture of Gaussians
  - Latent Dirichlet allocation
- **Algorithms**
  - KD-trees
  - Locality sensitive hashing
  - k-means
  - MapReduce
  - Expectation Maximization
  - Gibbs sampling
- **Core ML**
  - Distance metrics
  - Approximation algorithms
  - Unsupervised learning
  - Probabilistic modeling
  - Data parallel problems
  - Bayesian inference

# Retrieval
# as
# k-nearest neighbor search

# 1-NN search for retrieval

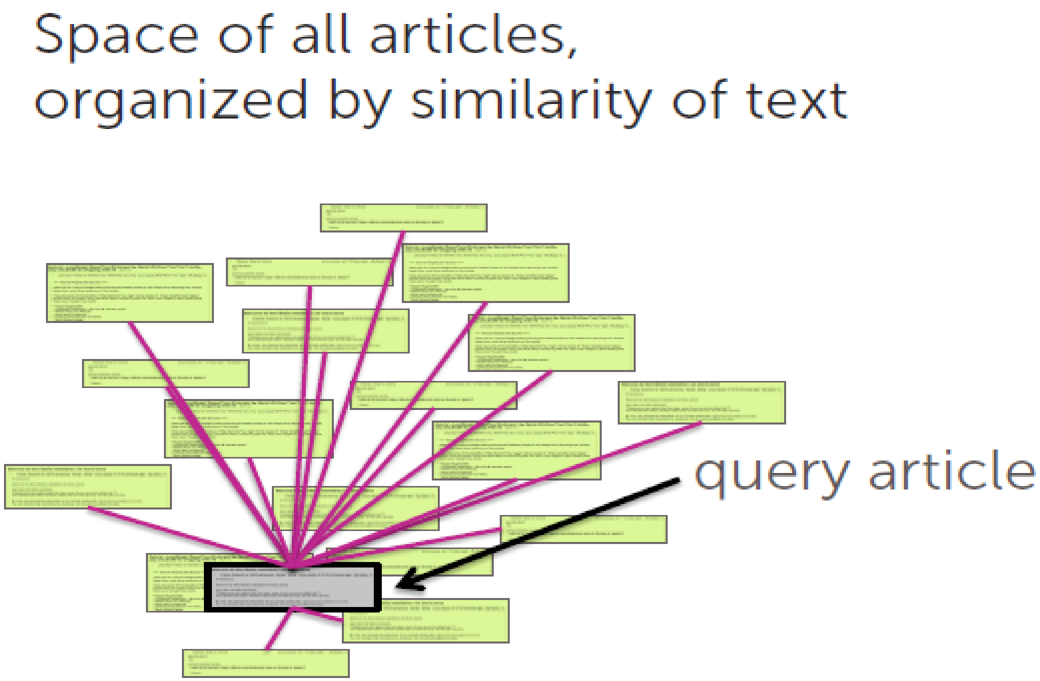




# 1-NN search for retrieval



## Compute distances to all docs

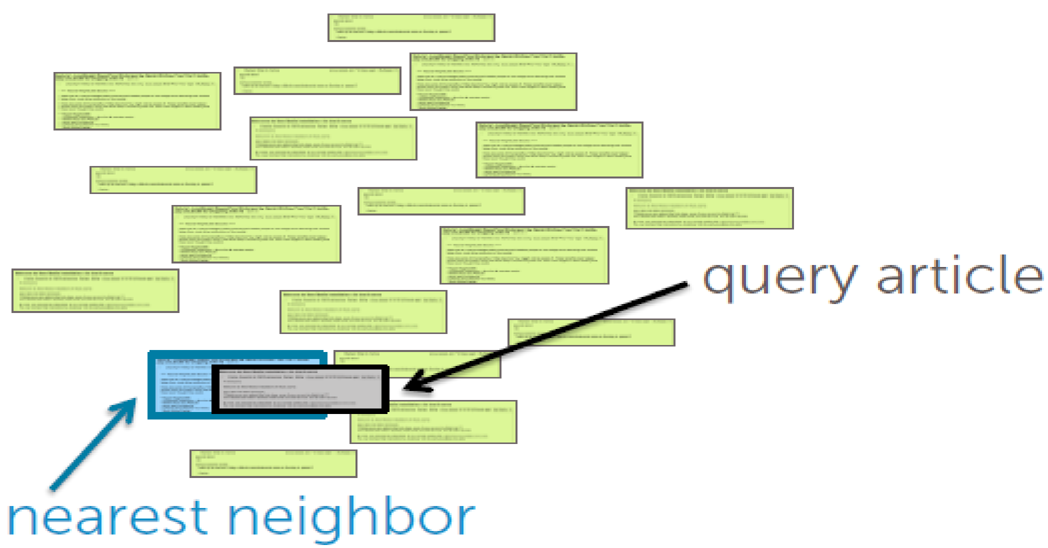


# 1-NN search for retrieval



## Retrieve "nearest neighbor"

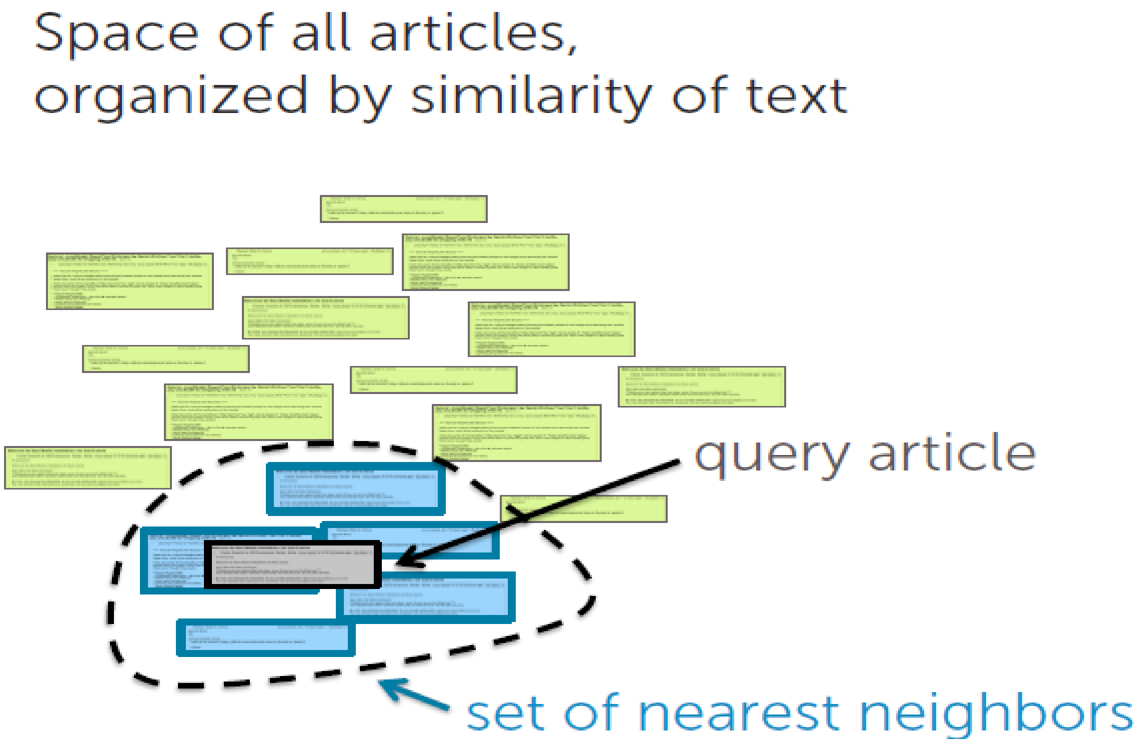
Space of all articles,
organized by similarity of text



# 1-NN search for retrieval



## Or set of nearest neighbors



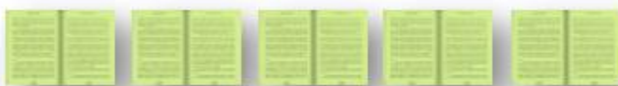
# 1-NN algorithm



## 1 – Nearest neighbor

- **Input:** Query article  : $\mathbf{x}_q$

  Corpus of documents (N docs)

   : $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$

- **Output:** *Most* similar article  $\leftarrow x^{NN}$

Formally: $x^{NN} = \min_{x_i} \text{distance}(x_q, x_i)$

# 1-NN algorithm



closest document

Initialize **Dist2NN** = ∞, = ∅

For i=1,2,…,N

query document $x_q$

$x_i$

Compute: δ = **distance(** , **)**

If δ < **Dist2NN**

document i from corpus

$x_i$

set =

set **Dist2NN** = δ

Return most similar document $\leftarrow x^{NN}$

closest document in corpus to query article

# k-NN algorithm



- **Input:** Query article  : $\mathbf{x}_q$

  Corpus of documents

   : $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$

- **Output:** *List of k* similar articles

Formally:

$$X^{NN} = \{x^{NN_1}, \ldots, x^{NN_k}\}$$

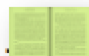
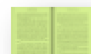
For all $x_i$ not in $X^{NN}$, $\text{distance}(x_i, x_q) \geq \max_{x^{NN_j},\, j=1,\ldots,k} \text{distance}(x^{NN_j}, x_q)$

# k-NN algorithm



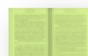
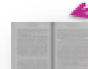
sort first **k documents**
by distance to query doc

Initialize **Dist2kNN** = sort($\delta_1,\ldots,\delta_k$) ← list of sorted distances

= rt( ,..  $_1$ )  $_k$ ← list of sorted docs

For i=k+1,…,N

query doc

Compute: $\delta$ = **distance(**  $_i$ **,**  $_q$ **)**

If $\delta$ < **Dist2kNN**[k] ← distance to $k^{th}$ NN (furthest NN in set)

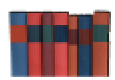
find j such that $\delta$ > **Dist2kNN**[j-1] but $\delta$ < **Dist2kNN**[j]

remove furthest house and shift queue:

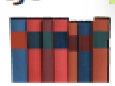
1:k] = -1]

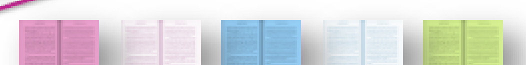
inserting new article

**Dist2kNN**[j+1:k] = **Dist2kNN**[j:k-1]

set **Dist2kNN**[j] = $\delta$ and [j] =  $_i$

closest k docs
to query doc

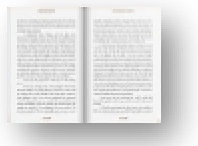
Return k most similar articles 



# Critical elements of NN search



Item (e.g., doc) representation

$\mathbf{x}_q \leftarrow$ 

Measure of distance between items:

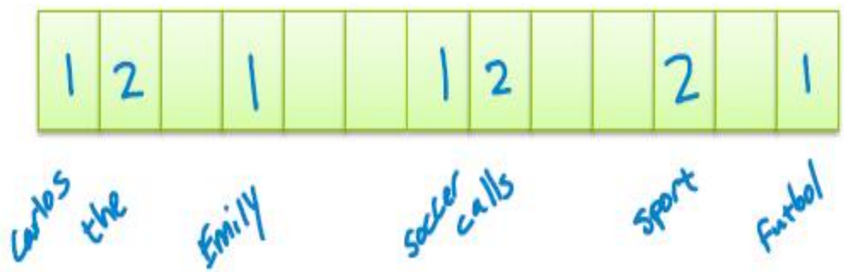
$\delta = \text{distance}(\mathbf{x}_i , \mathbf{x}_q)$

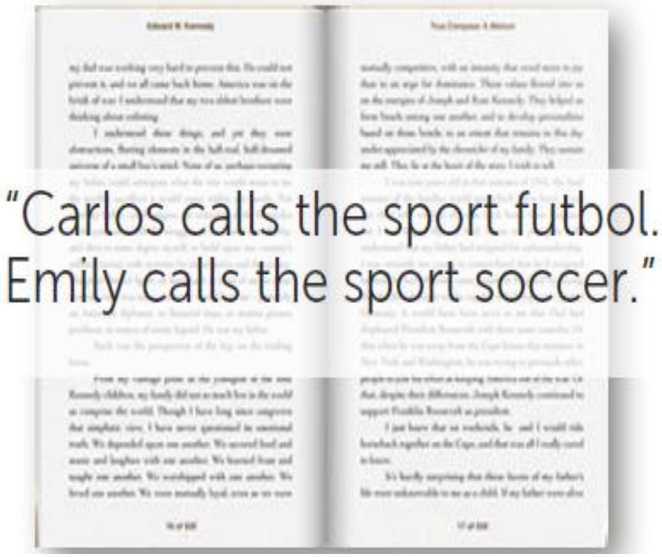
# Document representation



Bag of words model

- Ignore order of words
- Count # of instances of each word in vocabulary



# Document representation



## Issues with word counts – Rare words

Common words in doc: "the", "player", "field", "goal"

Dominate rare words like: "futbol", "Messi"

# Document representation



## TF-IDF document representation

Emphasizes important words

- Appears frequently in document (common locally)

Term frequency = word counts

- Appears rarely in corpus (rare globally)

Inverse doc freq. = $\log \frac{\#\text{ docs}}{1 + \#\text{ docs using word}}$

# TF-IDF document representation

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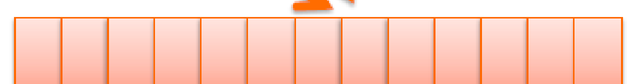

tf * idf

Trade off: local frequency vs. global rarity

# Distance metrics:



## Distance metrics:
## Defining notion of "closest"

In 1D, just Euclidean distance:

$$\boxed{\text{distance}(x_i, x_q) = |x_i - x_q|}$$

In multiple dimensions:

- can define many interesting distance functions
- most straightforwardly, might want to weight different dimensions differently

# Distance metrics:



## Weighting different features

Reasons:

– Some features are more relevant than others

**# bedrooms**
**# bathrooms**
**sq.ft. living**
sq.ft. lot
floors
**year built**
year renovated
waterfront

# Distance metrics:



## Weighting different features

Reasons:

– Some features are more relevant than others

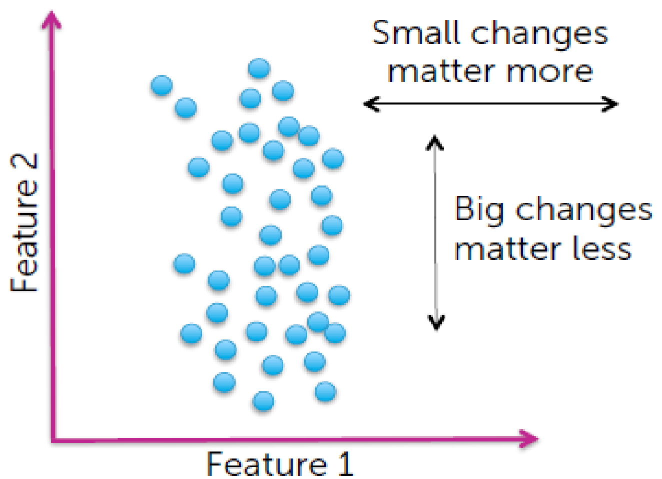
**title**
**abstract**
main body
**conclusion**

## Weighting different features

Reasons:

– Some features are more relevant than others

– Some features vary more than others




Specify weights as a function of feature spread

For feature j:

$$\frac{1}{\max_i(\mathbf{x}_i[j]) - \min_i(\mathbf{x}_i[j])}$$

# Distance metrics:



## Scaled Euclidean distance

Formally, this is achieved via

$$\boxed{\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{a_1(\mathbf{x}_i[1]-\mathbf{x}_q[1])^2 + \ldots + a_d(\mathbf{x}_i[d]-\mathbf{x}_q[d])^2}}$$

weight on each feature
(defining relative importance)

# Distance metrics:



## Effect of binary weights

$$\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{a_1(\mathbf{x}_i[1]-\mathbf{x}_q[1])^2 + \ldots + a_d(\mathbf{x}_i[d]-\mathbf{x}_q[d])^2}$$

Setting weights as 0 or 1
is equivalent to
**feature selection**

Feature engineering/
selection is
**important**, but **hard**

# Distance metrics:

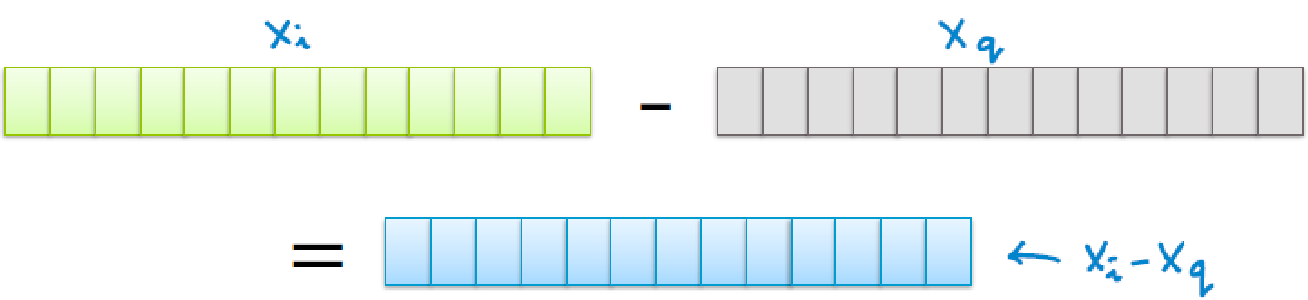


## (non-scaled) Euclidean distance

Defined in terms of inner product

$$\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{(\mathbf{x}_i - \mathbf{x}_q)^T (\mathbf{x}_i - \mathbf{x}_q)}$$

$$\sqrt{(\mathbf{x}_i[1] - \mathbf{x}_q[1])^2 + \dots + (\mathbf{x}_i[d] - \mathbf{x}_q[d])^2}$$



# Distance metrics:



## (non-scaled) Euclidean distance

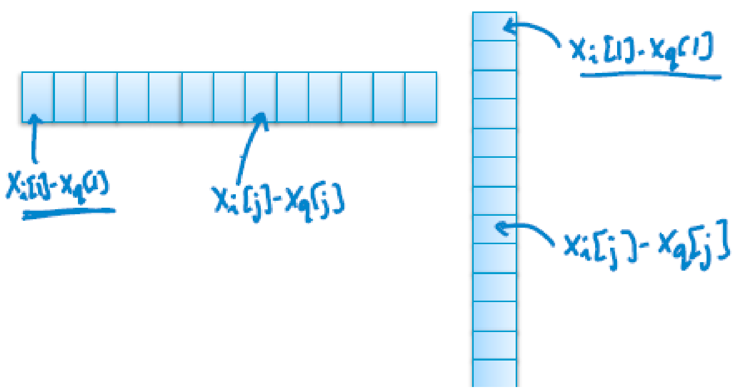
Defined in terms of inner product

$$\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{(\mathbf{x}_i - \mathbf{x}_q)^T(\mathbf{x}_i - \mathbf{x}_q)}$$

$$\sqrt{(\mathbf{x}_i[1] - \mathbf{x}_q[1])^2 + \ldots + (\mathbf{x}_i[d] - \mathbf{x}_q[d])^2}$$

take sq.rt.

distance$^2$ =



# Distance metrics:



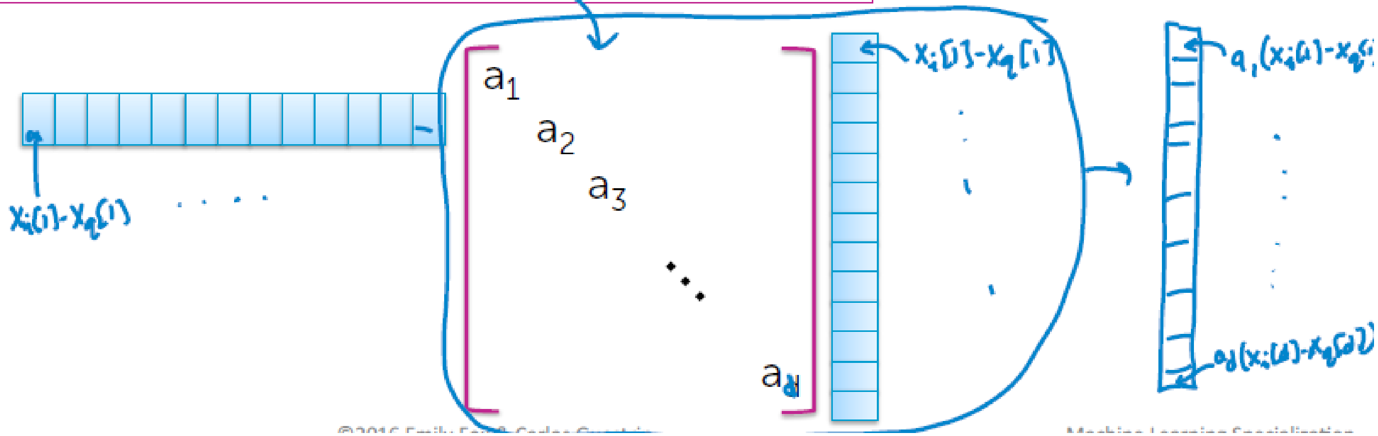
## Scaled Euclidean distance

Defined in terms of inner product

$$\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{(\mathbf{x}_i - \mathbf{x}_q)^T \mathbf{A} (\mathbf{x}_i - \mathbf{x}_q)}$$

$$\sqrt{a_1(\mathbf{x}_i[1]-\mathbf{x}_q[1])^2 + \ldots + a_d(\mathbf{x}_i[d]-\mathbf{x}_q[d])^2}$$

$\text{distance}^2 =$



# Distance metrics:



## Another natural inner product measure

$x_q$

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 5 | 3 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 0 | 0 | 0 | 2 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | 0 |

$x_i$

**Similarity**

$$= \mathbf{x}_i^T \mathbf{x}_q$$

$$= \sum_{j=1}^{d} \mathbf{x}_i[j]\, \mathbf{x}_q[j]$$

$$= 13$$

# Distance metrics:



## Another natural inner product measure

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 5 | 3 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |

**Similarity** = 0

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 1 | 0 | 0 | 0 | 9 | 0 | 0 | 6 | 0 | 4 | 0 |

# Distance metrics



## Cosine similarity – normalize

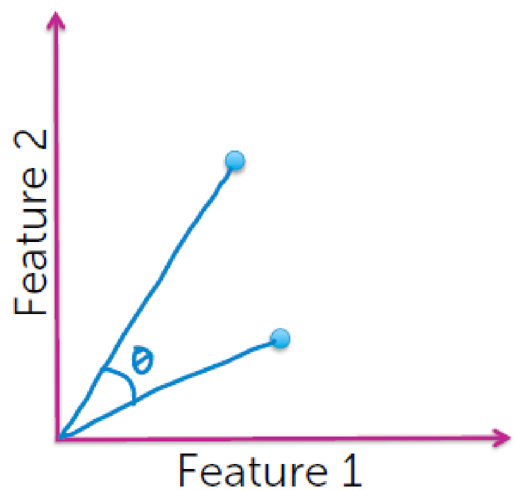
**Similarity** = $$\frac{\sum_{j=1}^{d} \mathbf{x}_i[j]\,\mathbf{x}_q[j]}{\sqrt{\sum_{j=1}^{d}(\mathbf{x}_i[j])^2}\sqrt{\sum_{j=1}^{d}(\mathbf{x}_q[j])^2}}$$

$$\frac{\mathbf{x}_i^{\mathsf{T}}\mathbf{x}_q}{||\mathbf{x}_i||\,||\mathbf{x}_q||} = \cos(\theta)$$

$$= \left(\frac{x_i}{||x_i||}\right)^{T}\left(\frac{x_q}{||x_q||}\right)$$ first normalize

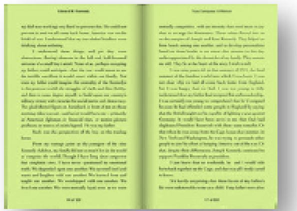
$a^T b = ||a||\,||b||\cos(\theta)$

- Not a proper distance metric
- Efficient to compute for sparse vecs



# Distance metrics

## Normalize



| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 5 | 3 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |

$\leftarrow x_i$

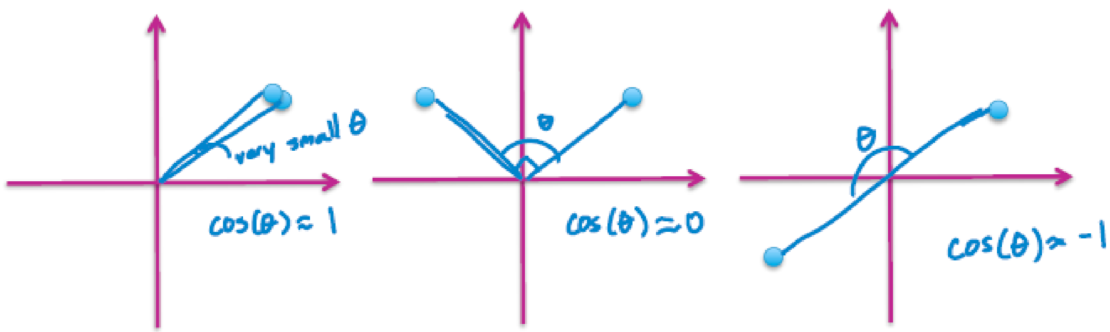
$$\sqrt{}(1^2 + 5^2 + 3^2 + 1^2) \leftarrow \|x_i\| = \sum_{j=1}^{d} x_i[j]^2$$

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1/6 | 0 | 0 | 0 | 5/6 | 3/6 | 0 | 0 | 1/6 | 0 | 0 | 0 | 0 |

# Distance metrics

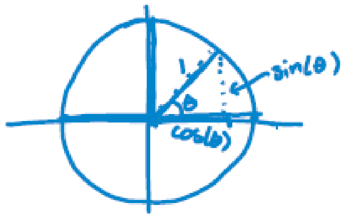


## Cosine similarity




In general, $-1 <$ similarity $< 1$

For positive features (like tf-idf)
$0 <$ similarity $< 1$ } our focus

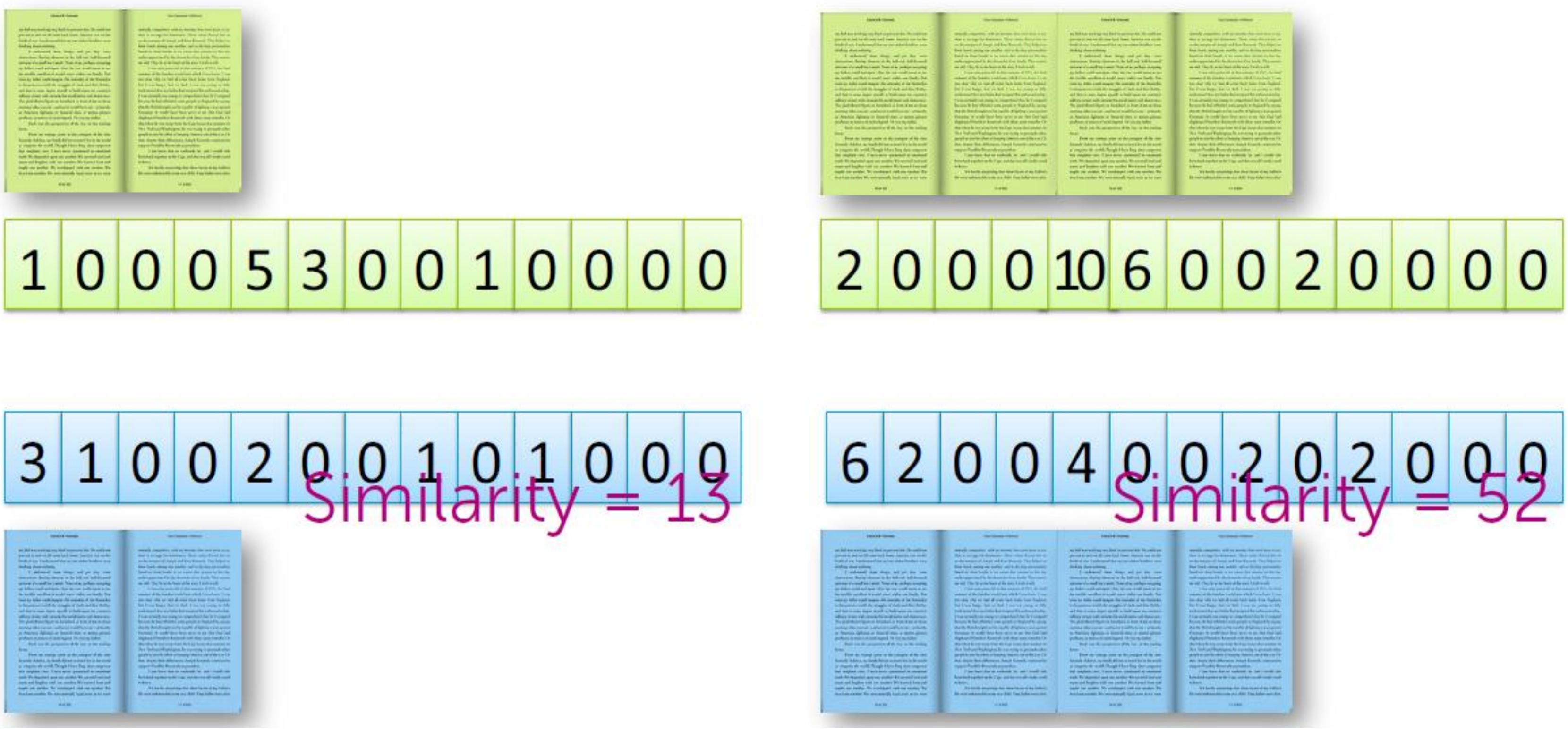



Define **distance = 1-similarity**

# Distance metrics



To normalize or not?



# Distance metrics



## In the normalized case

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1/6 | 0 | 0 | 0 | 5/6 | 3/6 | 0 | 0 | 1/6 | 0 | 0 | 0 | 0 |
| 3/4 | 1/4 | 0 | 0 | 1/2 | 0 | 0 | 1/4 | 0 | 1/4 | 0 | 0 | 0 |

Similarity = 13/24

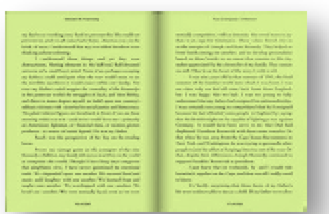
| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1/6 | 0 | 0 | 0 | 5/6 | 3/6 | 0 | 0 | 1/6 | 0 | 0 | 0 | 0 |
| 3/4 | 1/4 | 0 | 0 | 1/2 | 0 | 0 | 1/4 | 0 | 1/4 | 0 | 0 | 0 |

Similarity = 13/24

# Distance metrics



## But not always desired…

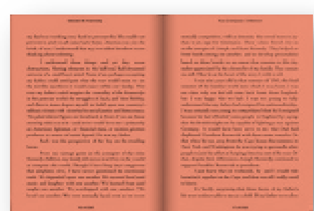


long document

short tweet

Normalizing can make dissimilar objects appear more similar

long document



long document

**Common compromise:**
Just cap maximum word counts

# Distance metrics



## Other distance metrics

– Mahalanobis
– rank-based
– correlation-based
– Manhattan
– Jaccard
– Hamming
– ...

# Combining distance metrics



**Example of document features:**

1. Text of document
   - Distance metric: Cosine similarity
2. # of reads of doc
   - Distance metric: Euclidean distance

Add together with user-specified weights

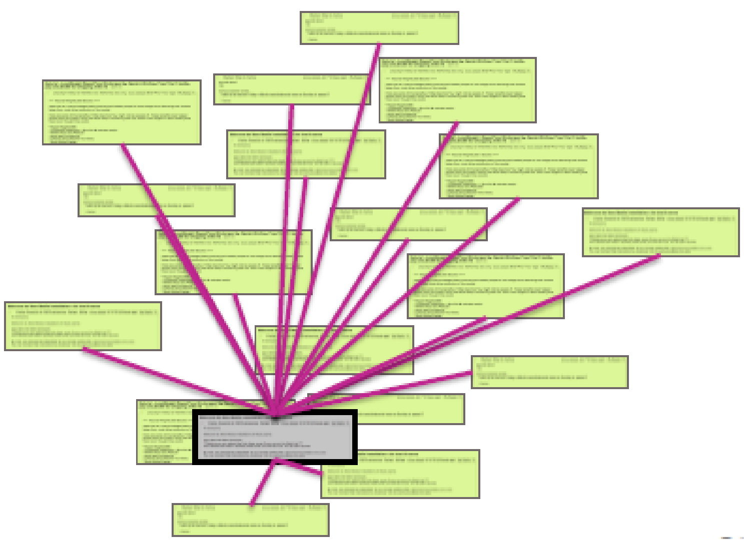
# Scaling up k-NN search by storing data in a KD-tree

# Complexity of brute-force search



Given a query point, scan through each point

- $O(N)$ distance computations per 1-NN query!
- $O(N\log k)$ per $k$-NN query!



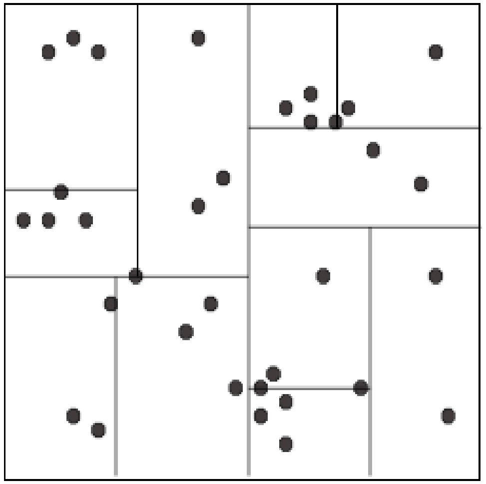
What if $N$ is huge???
(and many queries)

# KD-trees



Structured organization of documents

- Recursively partitions points into axis aligned boxes.



Enables more efficient pruning of search space

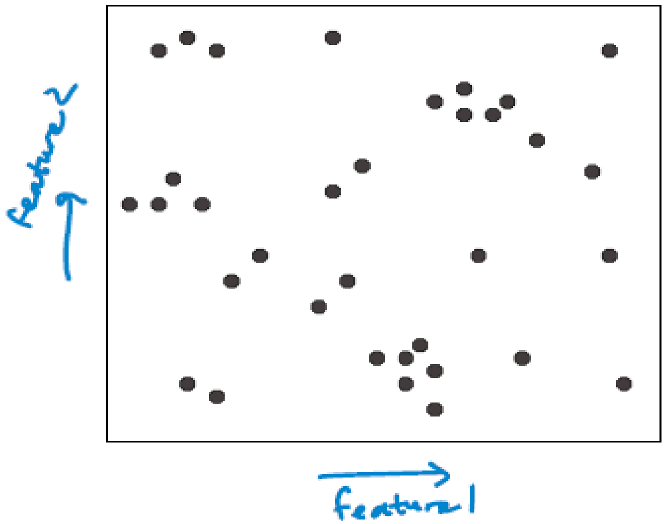
Works "well" in "low-medium" dimensions

- We'll get back to this...

# KD-trees



## KD-tree construction




Start with a list of d-dimensional points.

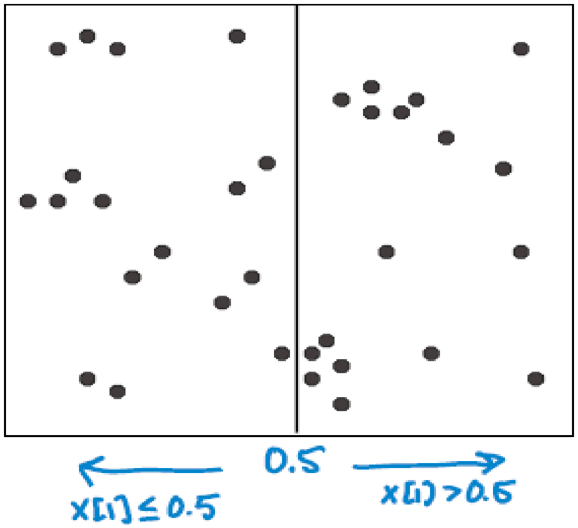
| Pt | **x**[1] | **x**[2] |
|---|---|---|
| 1 | 0.00 | 0.00 |
| 2 | 1.00 | 4.31 |
| 3 | 0.13 | 2.85 |
| ... | ... | ... |

obs. indices
feat. 1 (word 1)
feat. 2 (word 2)

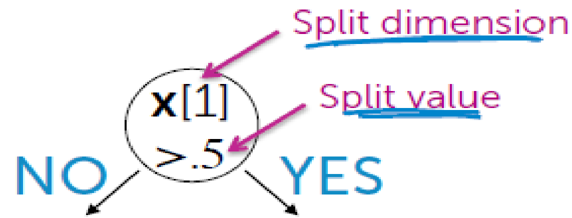
# KD-trees



## KD-tree construction




Split points into 2 groups




| Pt | **x**[1] | **x**[2] |
|---|---|---|
| 1 | 0.00 | 0.00 |
| 3 | 0.13 | 2.85 |
| ... | ... | ... |

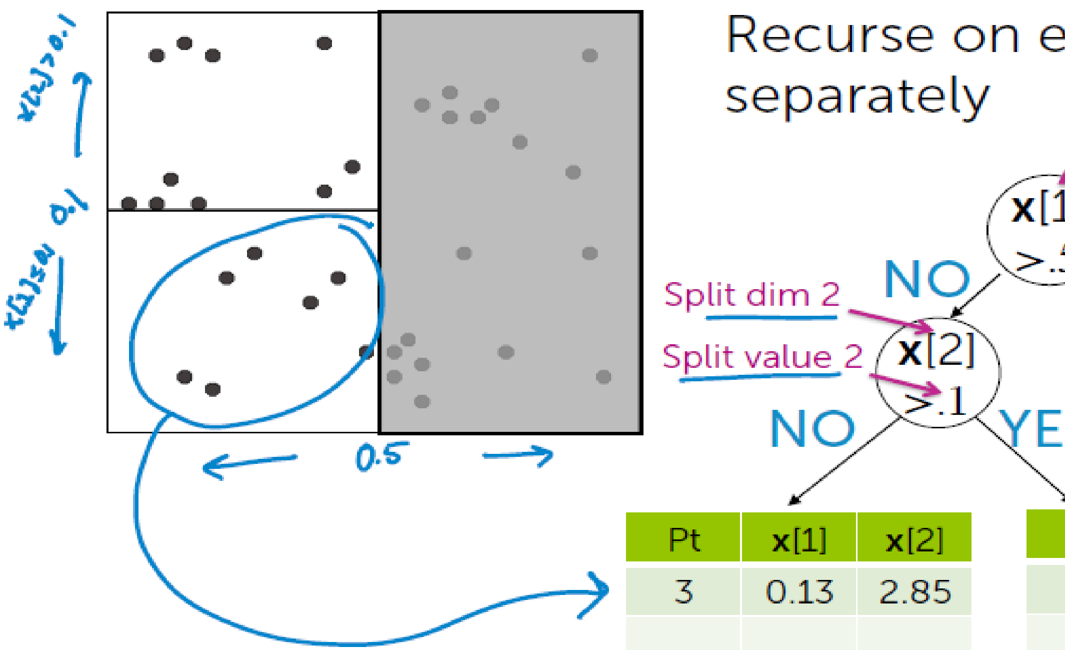
| Pt | **x**[1] | **x**[2] |
|---|---|---|
| 2 | 1.00 | 4.31 |
| ... | ... | ... |

# KD-trees



## KD-tree construction

Recurse on each group separately

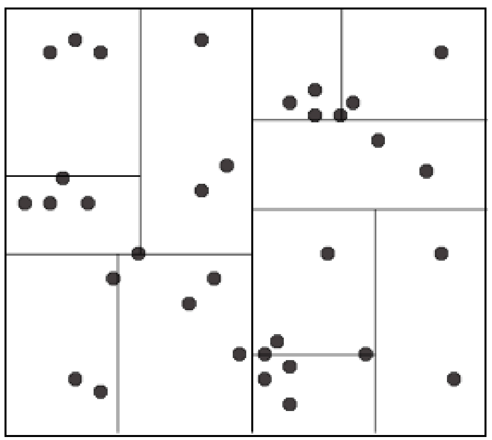


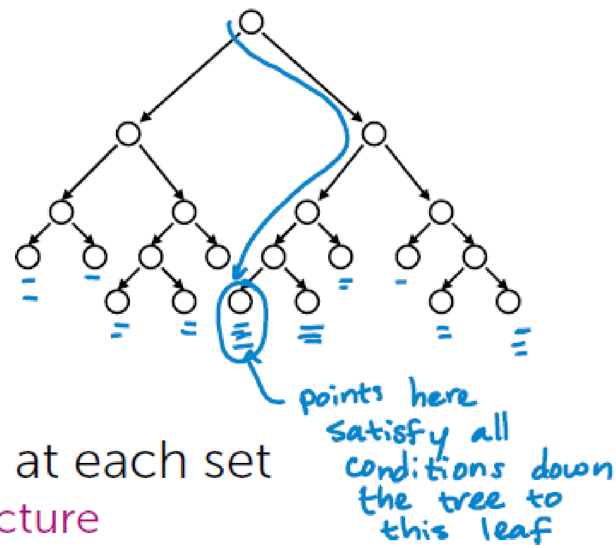

| Pt | x[1] | x[2] |
|---|---|---|
| 2 | 1.00 | 4.31 |
| ... | ... | ... |

| Pt | x[1] | x[2] |
|---|---|---|
| 3 | 0.13 | 2.85 |
| ... | ... | ... |

| Pt | x[1] | x[2] |
|---|---|---|
| 1 | 0.00 | 0.00 |
| ... | ... | ... |

# KD-tree construction






Continue splitting points at each set

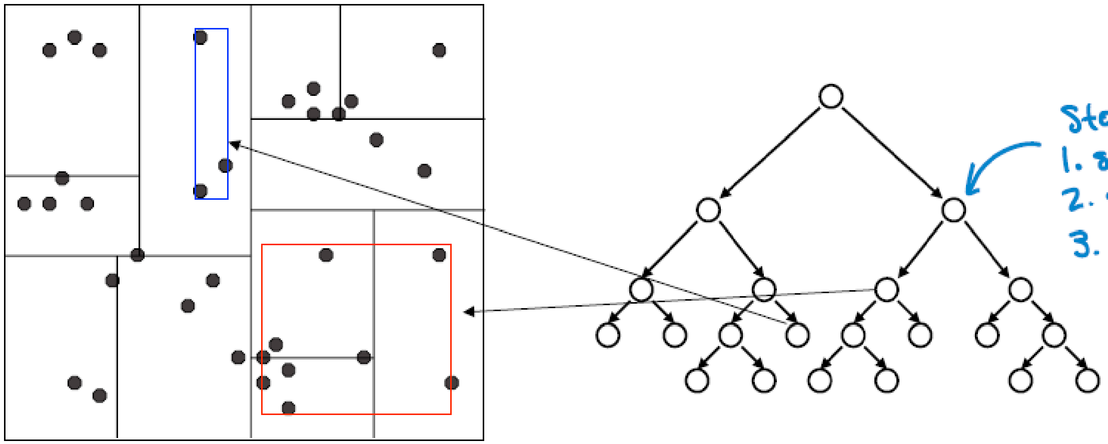
- Creates a binary tree structure

Each leaf node contains a list of points

# KD-trees



## KD-tree construction



Store:
1. split dim?
2. split value
3. bounding box that is as small as possible while containing pts

Keep one additional piece of info at each node:

#3 – The (tight) bounds of points at or below node

# KD-tree construction choices

Use heuristics to make splitting decisions:

- Which dimension do we split along?

  widest (or alternate)

- Which value do we split at?

  median (or center point of box, ignoring data in box)

- When do we stop?

  fewer than m pts left

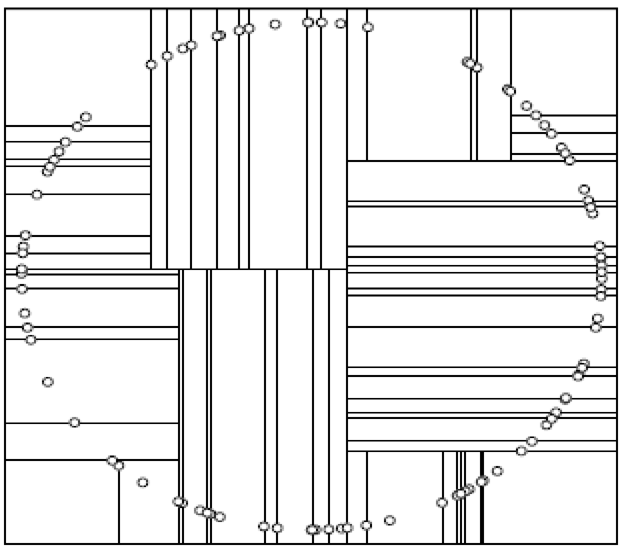
  or

  box hits minimum width

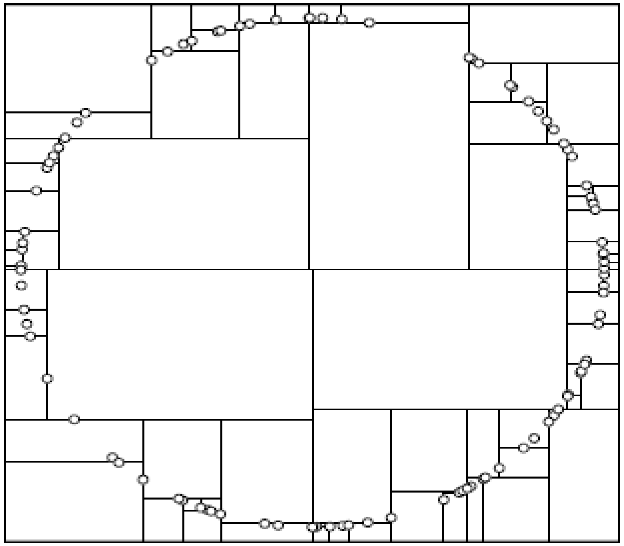
# KD-trees



## Many heuristics…



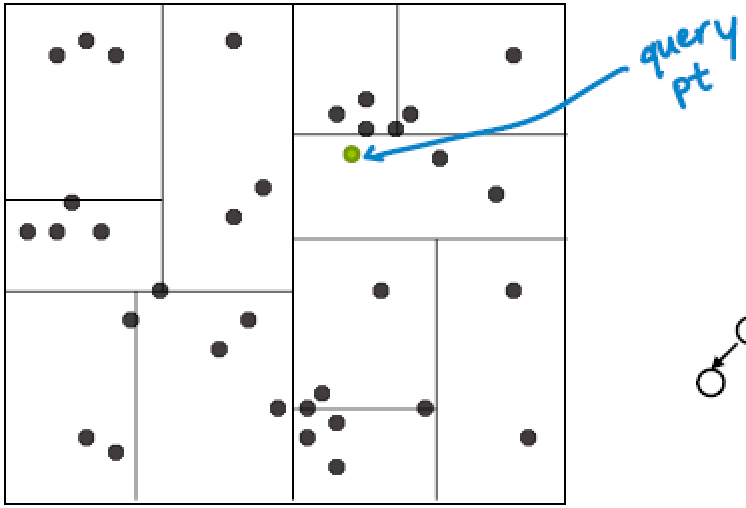
median heuristic

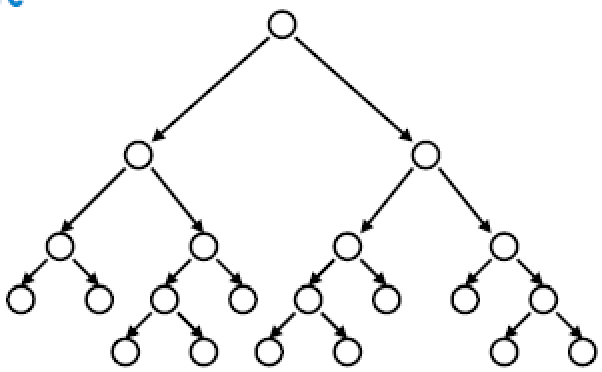


center-of-range heuristic

# Nearest neighbor with KD-trees



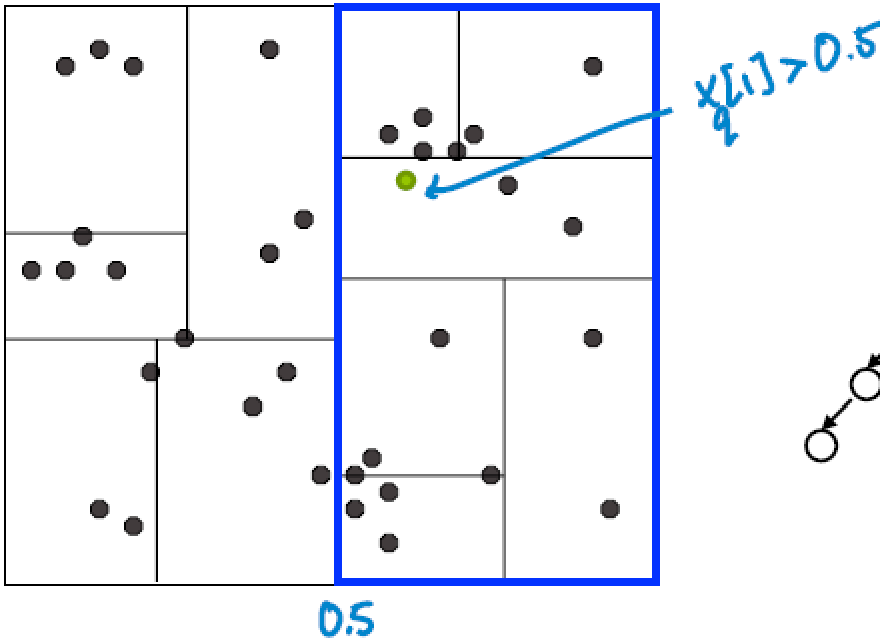


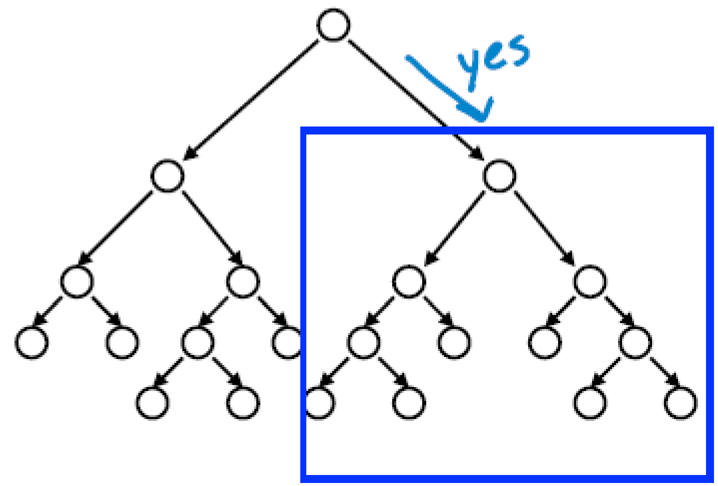



Traverse tree looking for nearest neighbor to query point

# Nearest neighbor with KD-trees



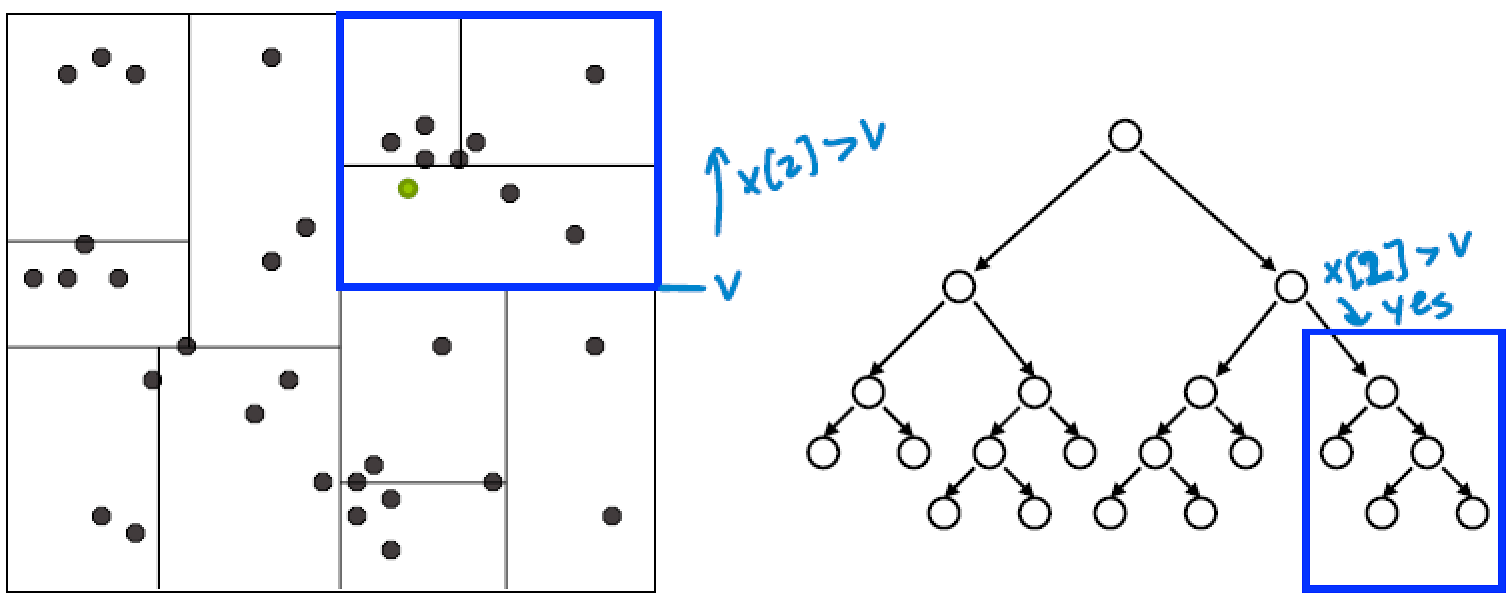



1. Start by exploring leaf node containing query point

# Nearest neighbor with KD-trees

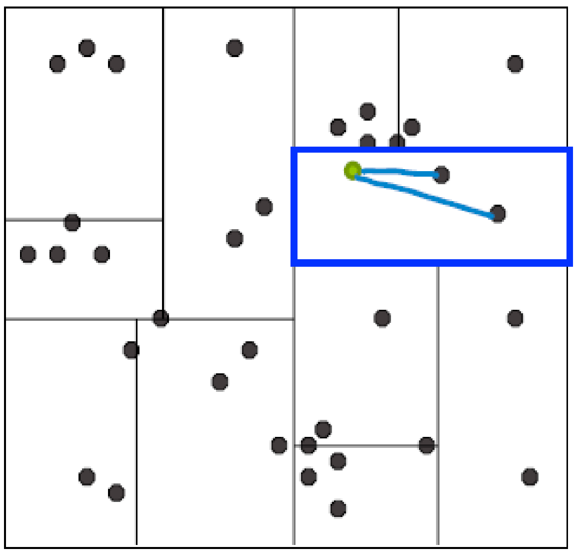


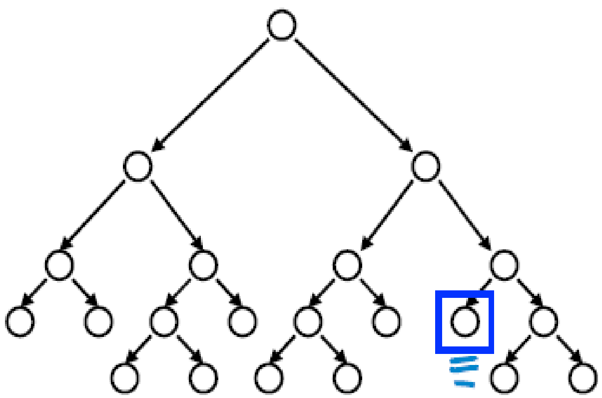



1. Start by exploring leaf node containing query point

# Nearest neighbor with KD-trees



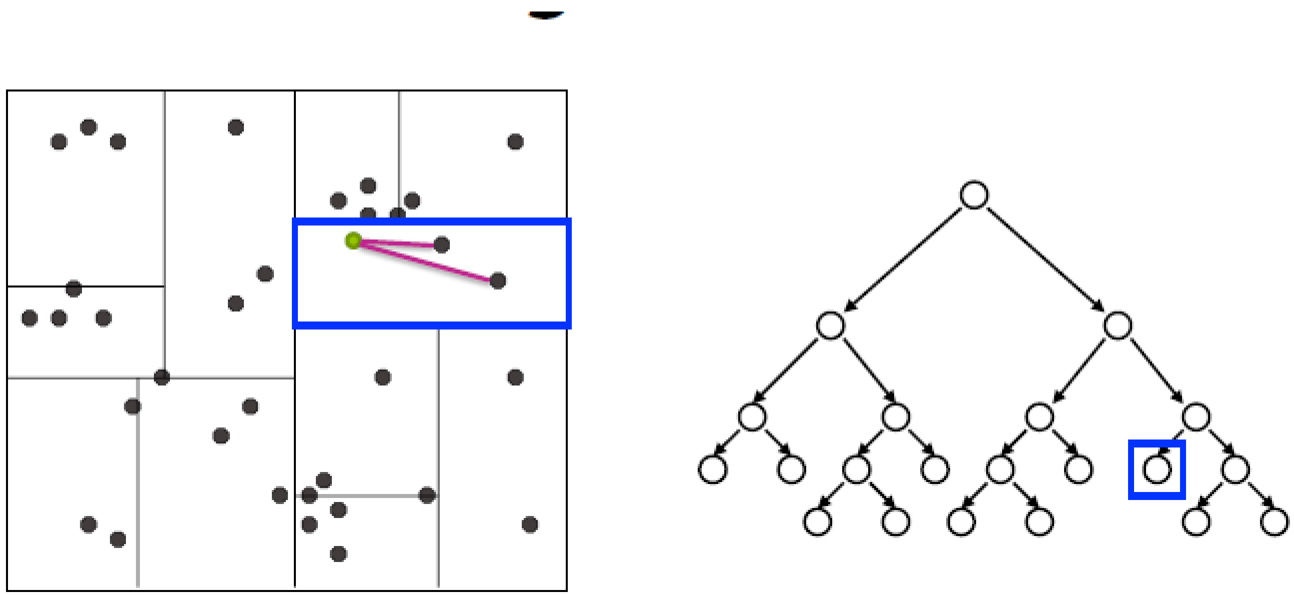




1. Start by exploring leaf node containing query point

# Nearest neighbor with KD-trees

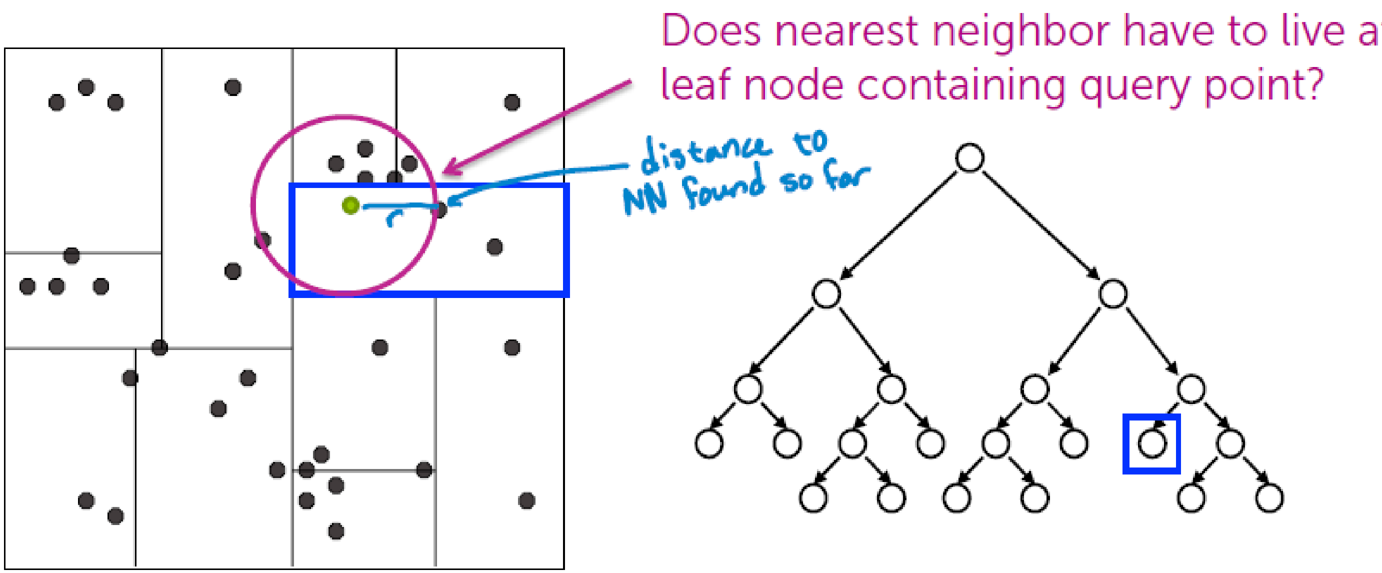




1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node

# Nearest neighbor with KD-trees

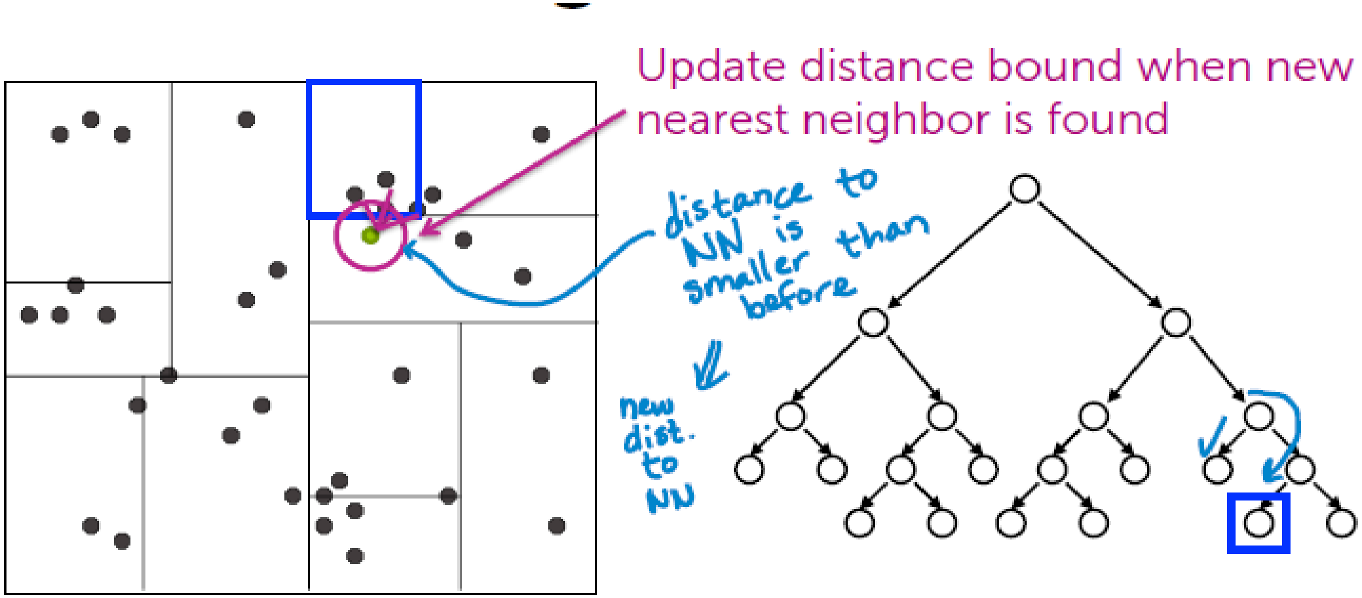





1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node

# Nearest neighbor with KD-trees

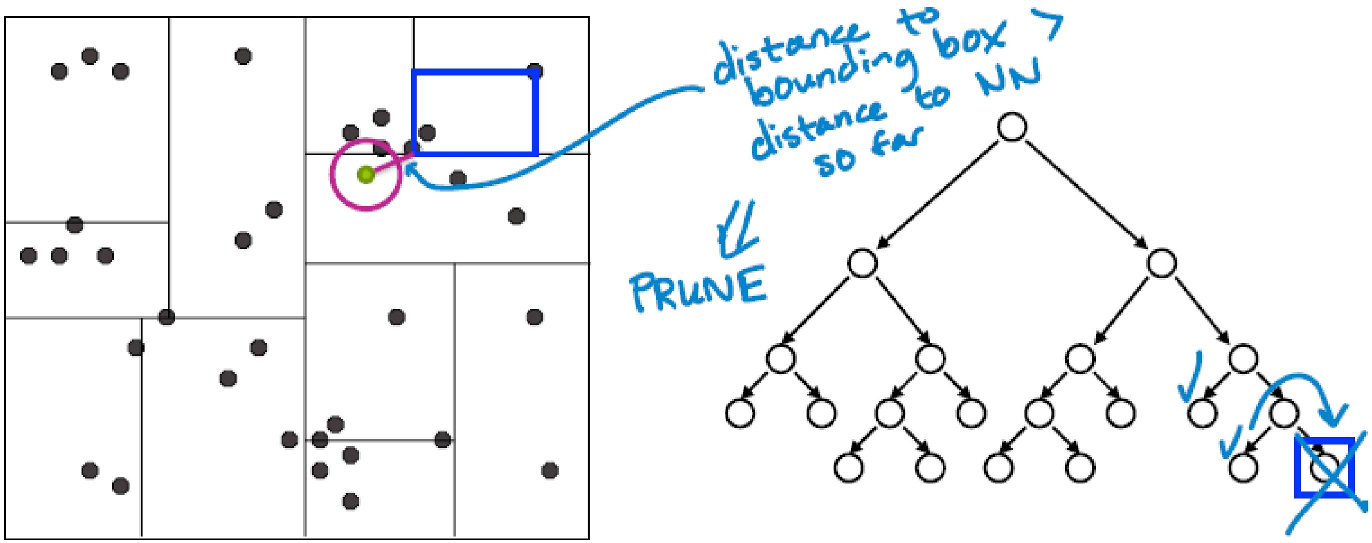





1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node
3. Backtrack and try other branch at each node visited

# Nearest neighbor with KD-trees

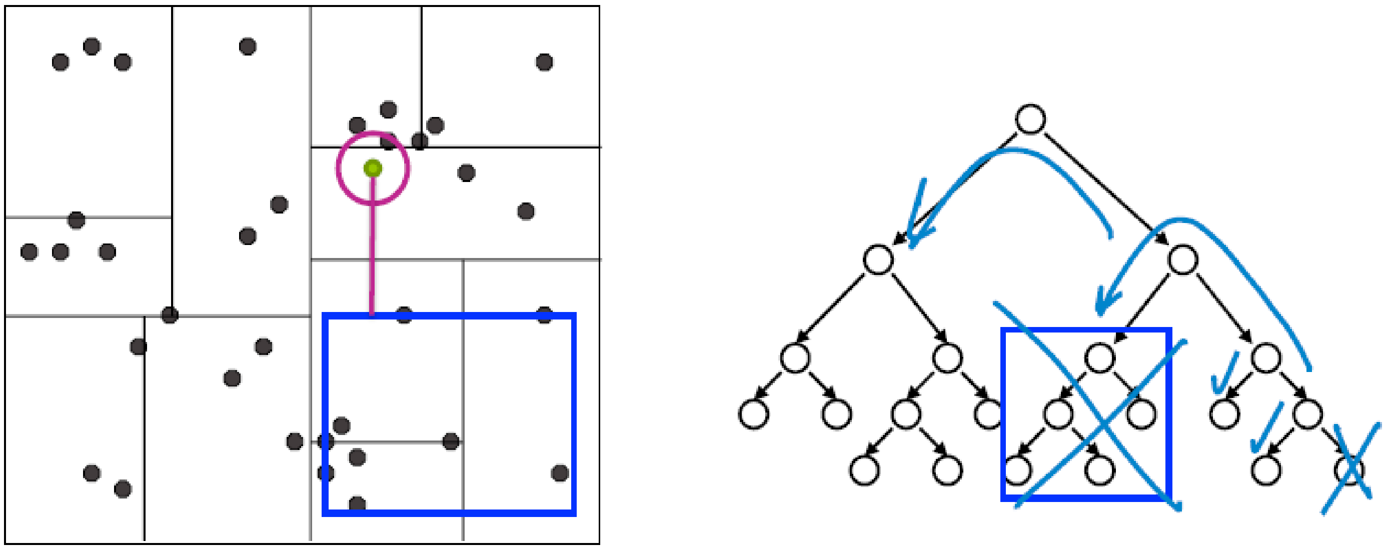





Use distance bound and bounding box of each node to prune parts of tree that cannot include nearest neighbor

# Nearest neighbor with KD-trees

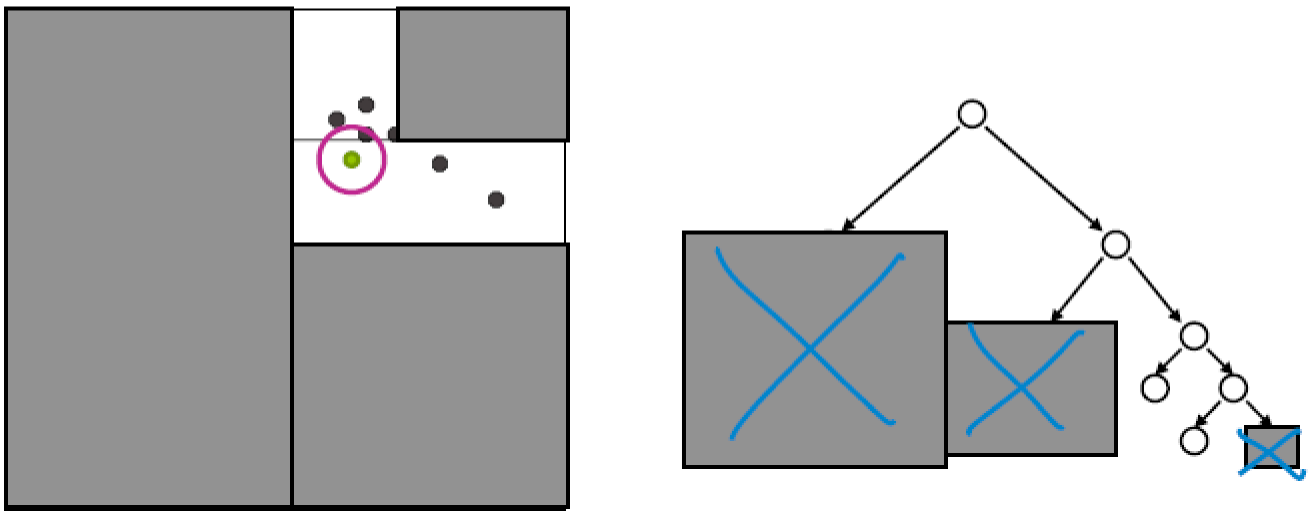




Use distance bound and bounding box of each node to prune parts of tree that cannot include nearest neighbor

# Nearest neighbor with KD-trees





Use distance bound and bounding box of each node to prune parts of tree that cannot include nearest neighbor

# Nearest neighbor with KD-trees



## Complexity

For (nearly) balanced, binary trees...

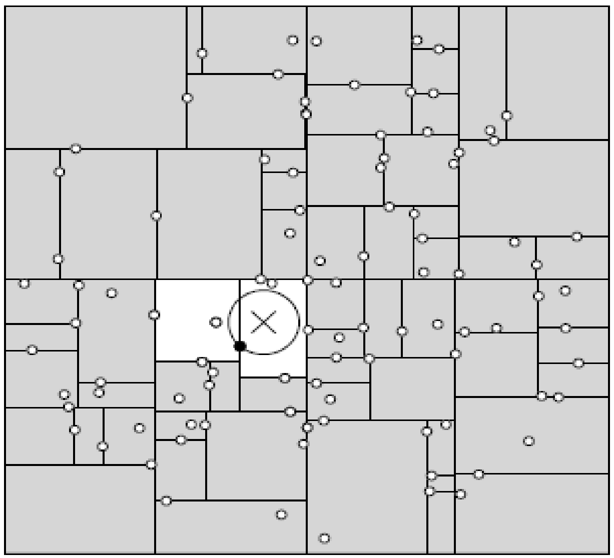
- Construction
  - Size: 2N−1 nodes if 1 datapt at each leaf → $O(N)$
  - Depth: $O(\log N)$
  - Median + send points left right: $O(N)$ at every level of the tree
  - Construction time: $O(N \log N)$
- 1-NN query
  - Traverse down tree to starting point: $O(\log N)$
  - Maximum backtrack and traverse: $O(N)$ in worst case
  - Complexity range: $O(\log N) \rightarrow O(N)$

Under some assumptions on distribution of points, we get O(logN) but exponential in d

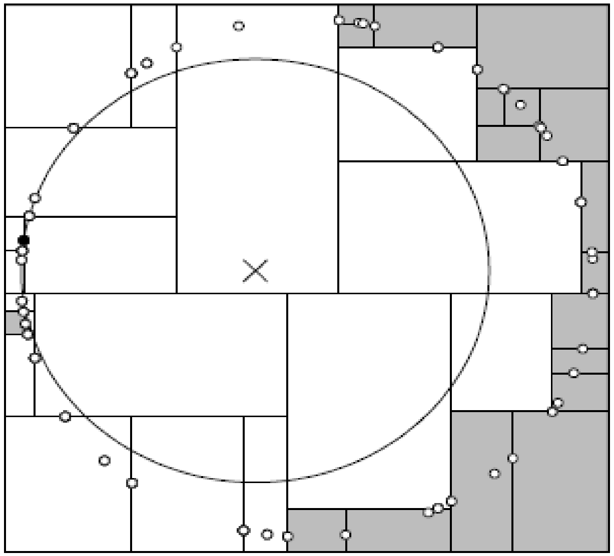
# Nearest neighbor with KD-trees



## Complexity



pruned many
(closer to O(log N) )



pruned few
(closer to O(N) )

# Complexity for N queries



- Ask for nearest neighbor to each doc

  N queries

- Brute force 1-NN:

  $O(N^2)$

- kd-trees:

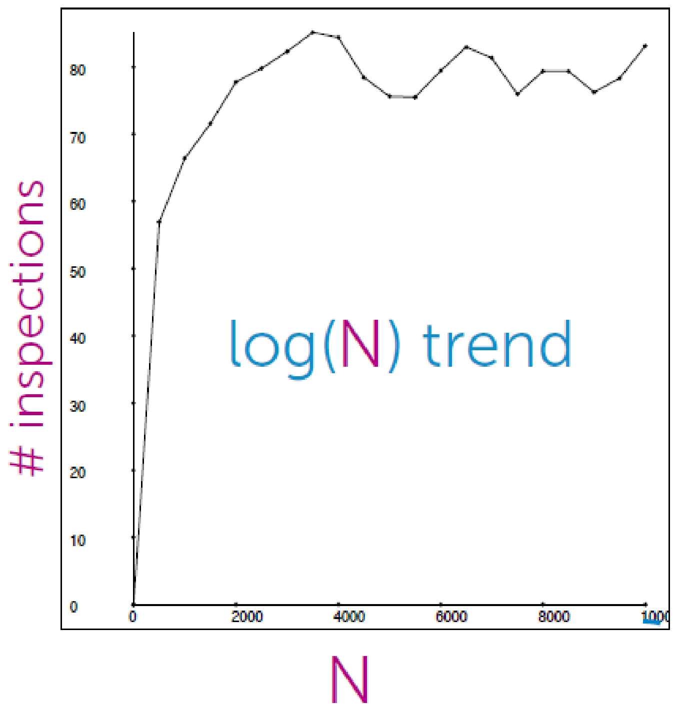
  $O(N \log N) \longrightarrow O(N^2)$

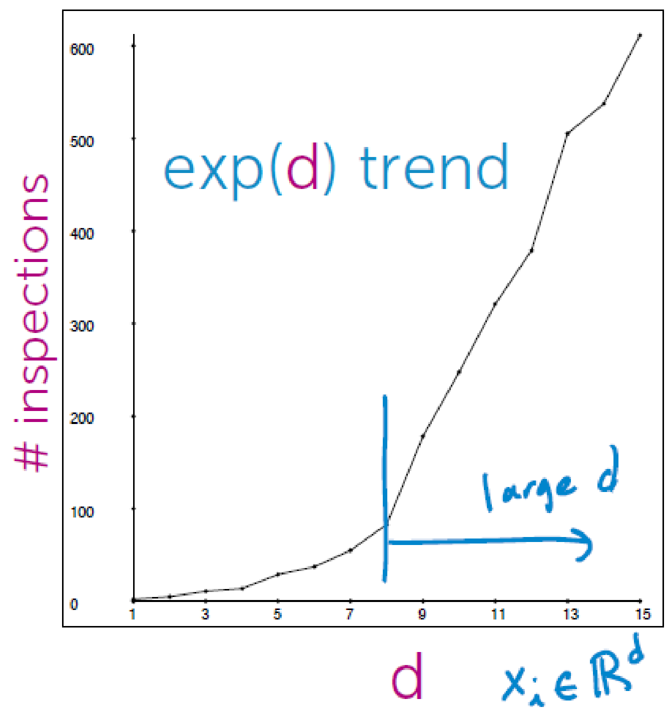
  potentially very large savings for large N!

# Complexity for N queries



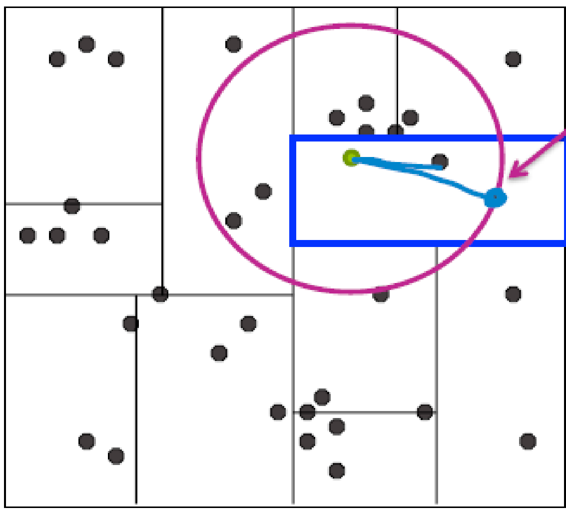
## Inspections vs. N and d



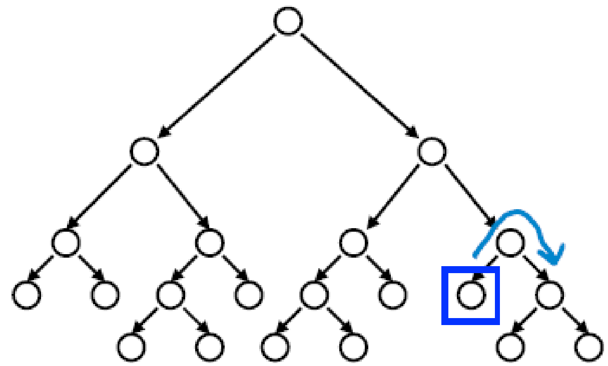



# k-NN with KD-trees





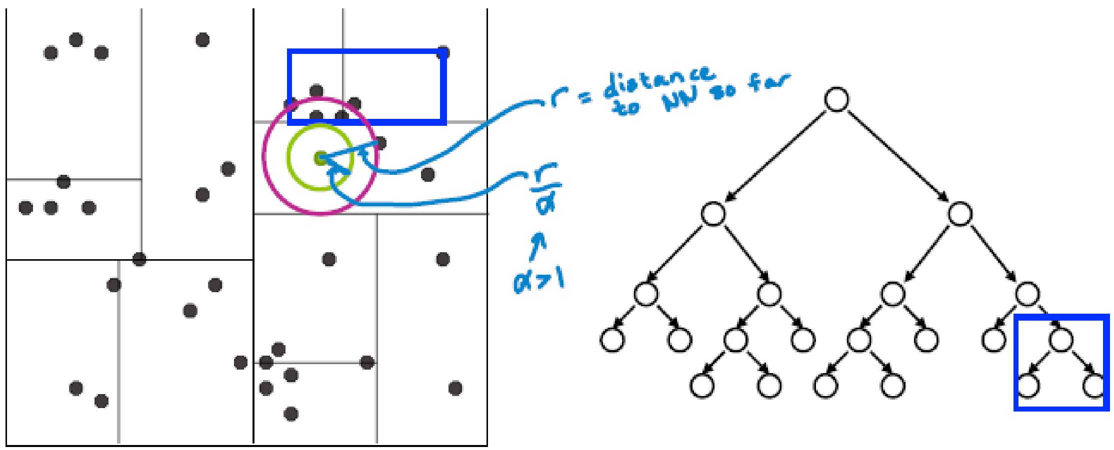
distance to 2nd nearest neighbor in 2-NN example

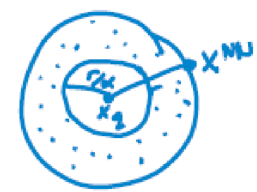


Exactly same algorithm, but maintain distance to furthest of current *k* nearest neighbors

# Approximate k-NN with KD-trees





**Before:** Prune when distance to bounding box > r

**Now:** Prune when distance to bounding box > $r/\alpha$

Prunes more than allowed, but can guarantee that if we return a neighbor at distance r, then there is no neighbor closer than $r/\alpha$

Bound loose...In practice, often closer to optimal.

Saves lots of search time at little cost in quality of NN!

# Closing remarks on KD-trees



Tons of variants of kd-trees

- On construction of trees
  (heuristics for splitting, stopping, representing branches...)
- Other representational data structures for fast NN search
  (e.g., ball trees,...)

Nearest Neighbor Search

- Distance metric and data representation crucial to answer returned

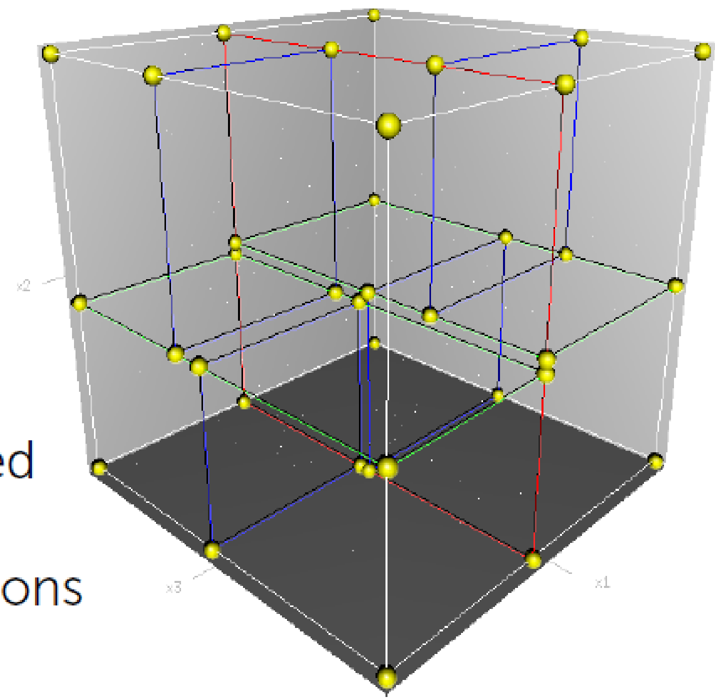
**For both,** high-dim spaces are hard!

- Number of kd-tree searches can be exponential in dimension
  - Rule of thumb... $N >> 2^d$... Typically useless for large d.
- Distances sensitive to irrelevant features
  - Most dimensions are just noise → everything is far away
  - Need technique to learn which features are important to given task

# KD-tree in high dimmensions



- Unlikely to have any data points close to query point
- Once “nearby” point is found, the search radius is likely to intersect many hypercubes in at least one dim
- Not many nodes can be pruned
- Can show under some conditions that you visit at least $2^d$ nodes



# Moving away from exact NN search



- Approximate neighbor finding…
  - Don't find exact neighbor, but that's okay for many applications

Out of millions of articles, do we need the closest article or just one that's pretty similar?

Do we even fully trust our measure of similarity???

- Focus on methods that provide good probabilistic guarantees on approximation

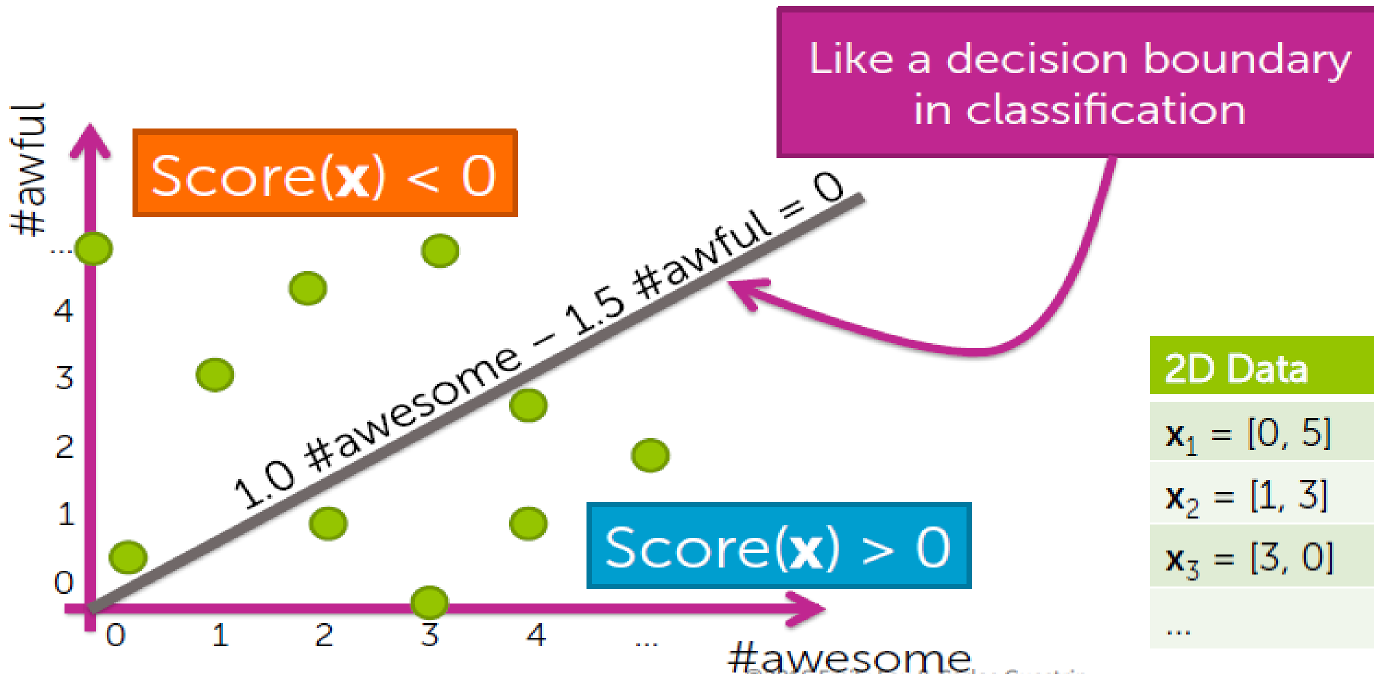
# Locality Sensitive Hashing (LHS) as alternative to KD-trees

# Locality sensitive hashing



## Simple "binning" of data into 2 bins

Score(**x**) = 1.0 #awesome – 1.5 #awful

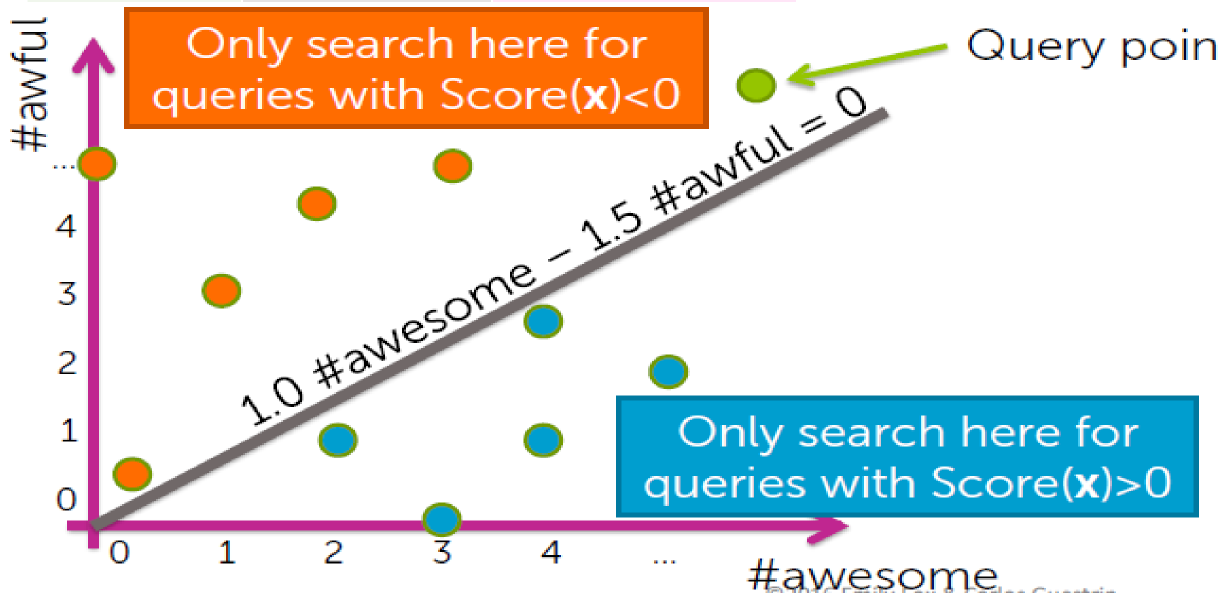



| 2D Data | Sign(Score) |
|---|---|
| $\mathbf{x}_1 = [0, 5]$ | -1 |
| $\mathbf{x}_2 = [1, 3]$ | -1 |
| $\mathbf{x}_3 = [3, 0]$ | 1 |
| ... | ... |

# Using bins for NN search

| 2D Data | Sign(Score) | Bin index |
|---|---|---|
| $\mathbf{x}_1$ = [0, 5] | -1 | 0 |
| $\mathbf{x}_2$ = [1, 3] | -1 | 0 |
| $\mathbf{x}_3$ = [3, 0] | 1 | 1 |
| ... | ... | ... |

candidate neighbors if Score($\mathbf{x}$)<0



# Using score for NN search

| 2D Data | Sign(Score) | Bin index |
|---|---|---|
| $\mathbf{x}_1$ = [0, 5] | -1 | 0 |
| $\mathbf{x}_2$ = [1, 3] | -1 | 0 |
| $\mathbf{x}_3$ = [3, 0] | 1 | 1 |
| … | … | … |

candidate neighbors if Score(x)<0

| Bin | 0 | 1 |
|---|---|---|
| List containing indices of datapoints: | {1,2,4,7,...} | {3,5,6,8,...} |

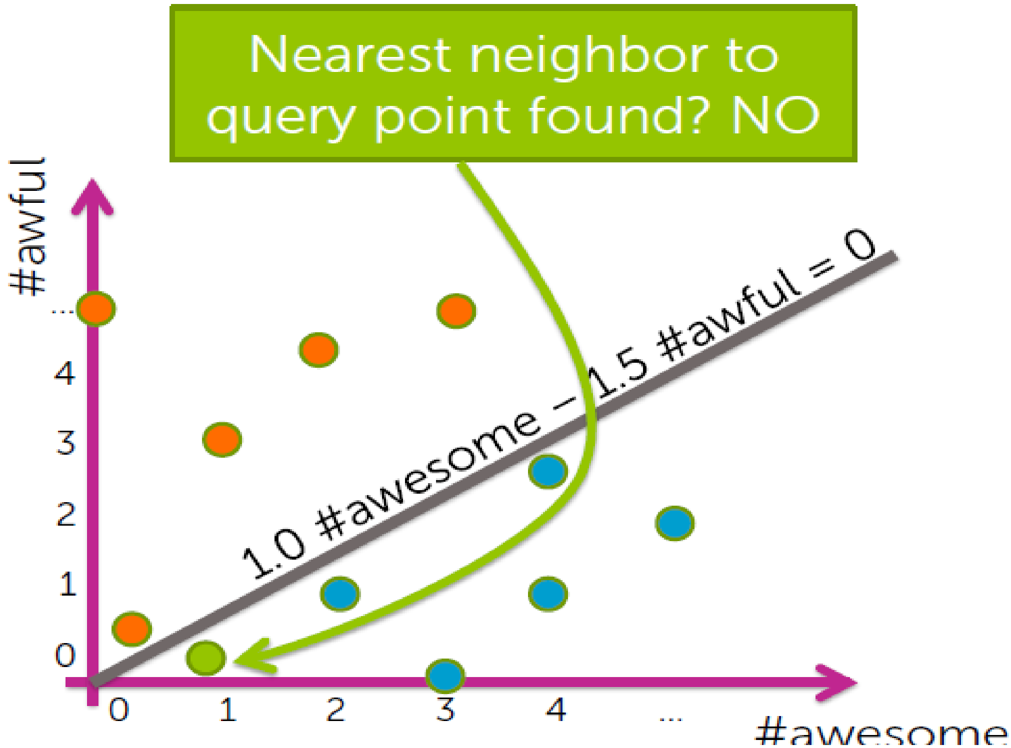
HASH TABLE

search for NN amongst this set

# Locality sensitive hashing



## Provides approximate NN



# Locality sensitive hashing



## Three potential issues with simple approach

1. Challenging to find good line
2. Poor quality solution:
   - Points close together get split into separate bins
3. Large computational cost:
   - Bins might contain many points, so still searching over large set for each NN query

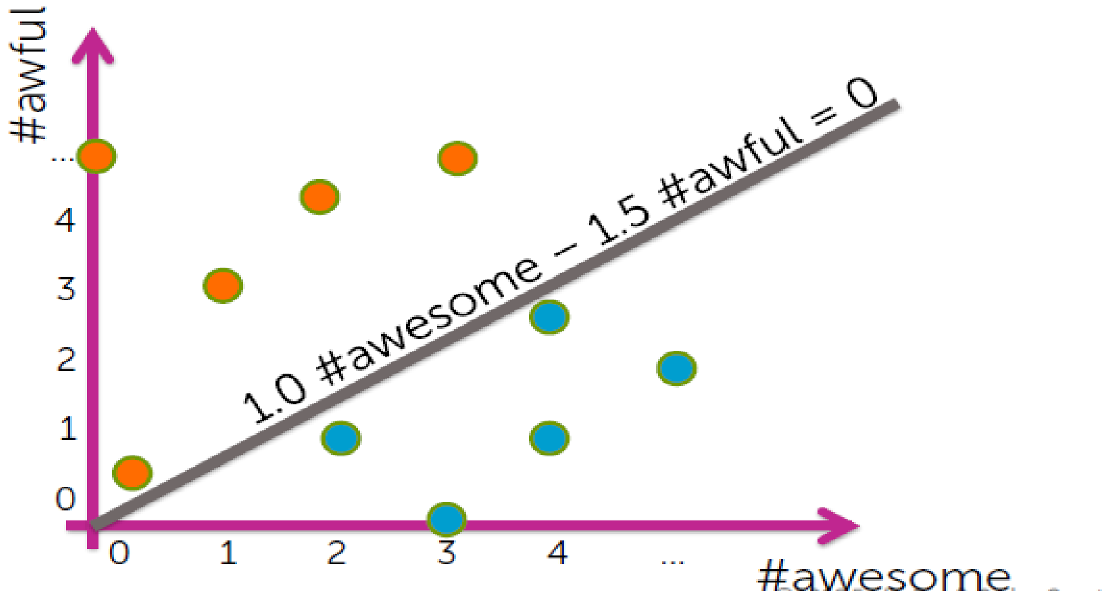
| Bin | 0 | 1 |
|---|---|---|
| List containing indices of datapoints: | {1,2,4,7,...} | {3,5,6,8,...} |

# Locality sensitive hashing



## How to define the line?

**Crazy idea:**
Define line randomly!

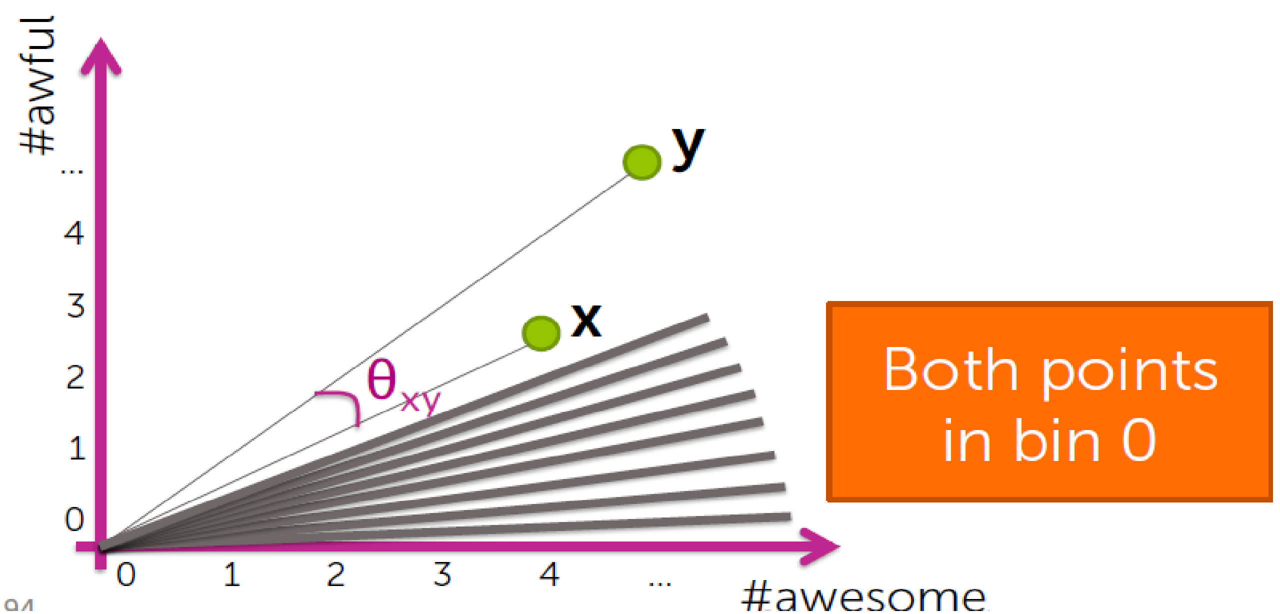


# Locality sensitive hashing



## How bad can a random line be?

**Goal:** If **x**,**y** are close (according to cosine similarity), want binned values to be the same.



# Locality sensitive hashing



## How bad can a random line be?

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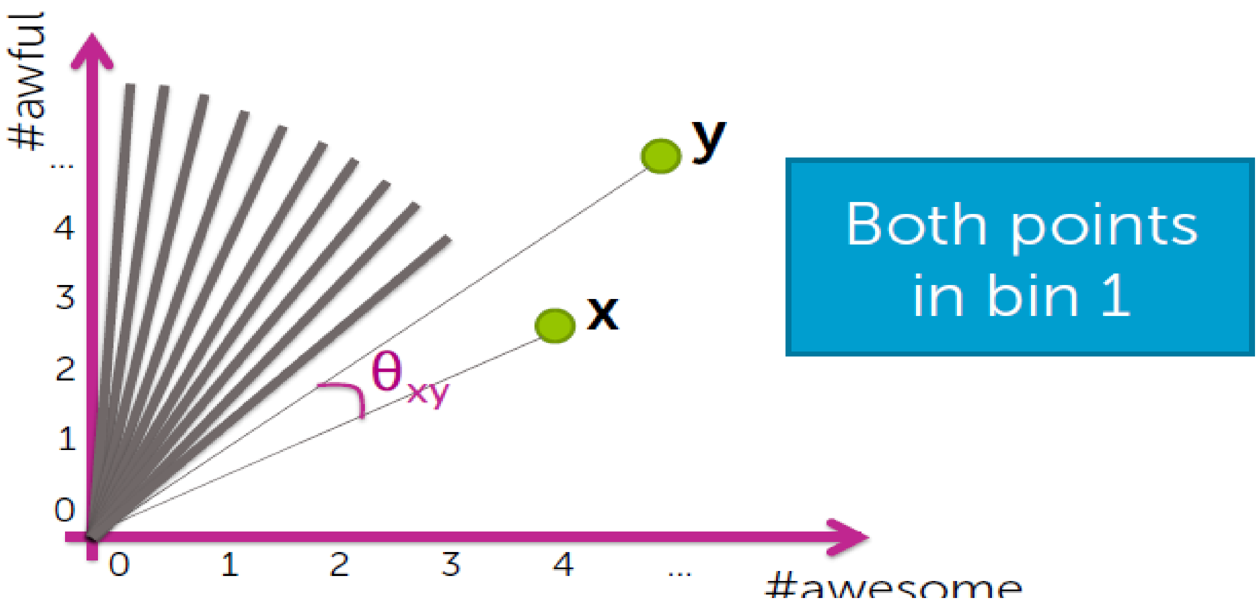
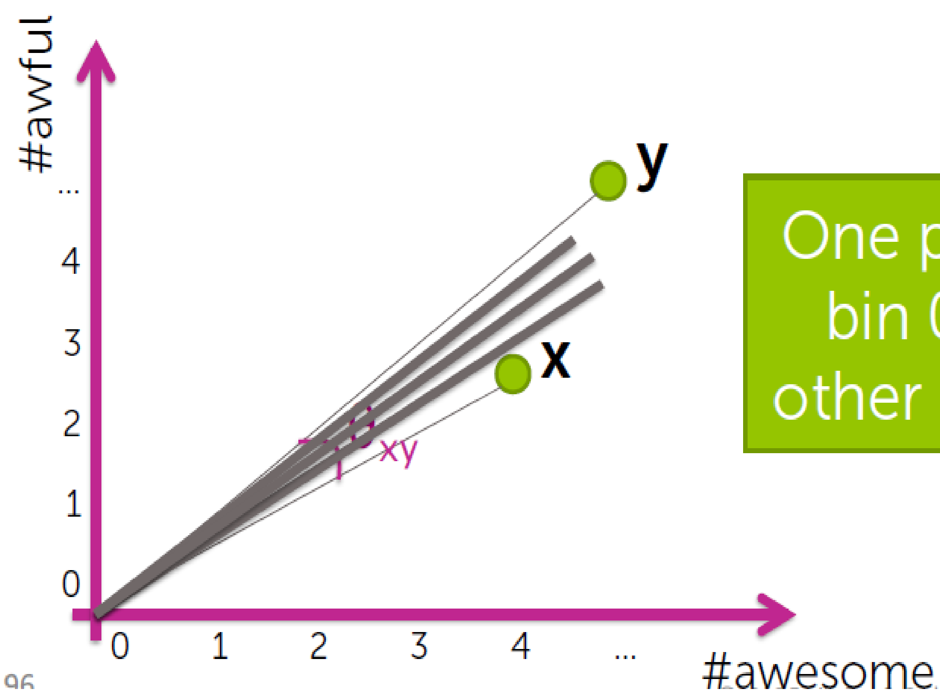


# Locality sensitive hashing



**Goal:** If **x**,**y** are close (according to cosine similarity), want binned values to be the same.

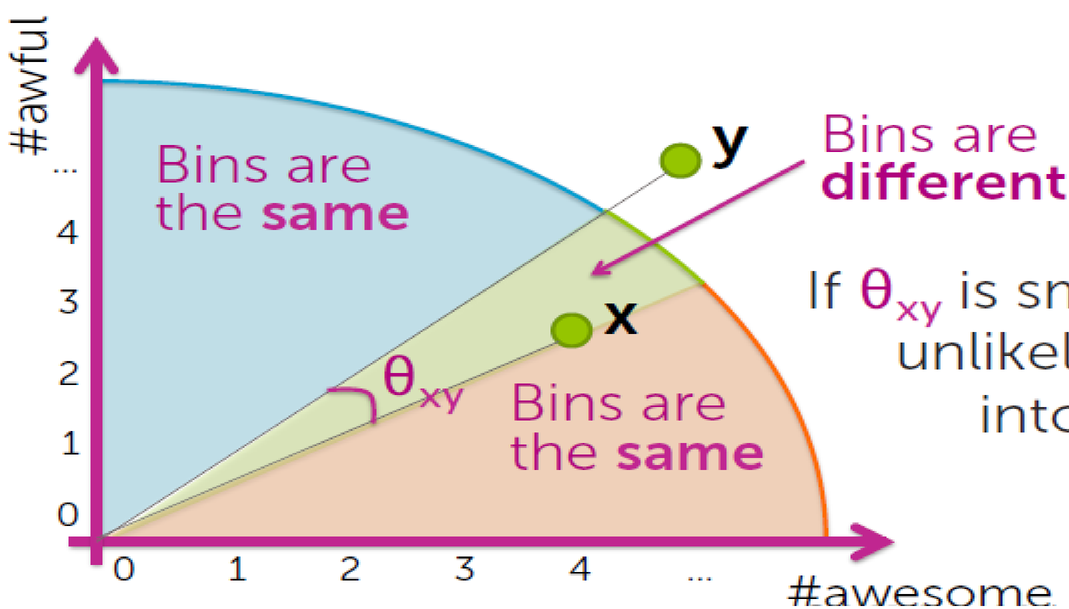



One point in bin 0 and other in bin 1

# Locality sensitive hashing

## How bad can a random line be?

**Goal:** If **x**,**y** are close (according to cosine similarity), want binned values to be the same.

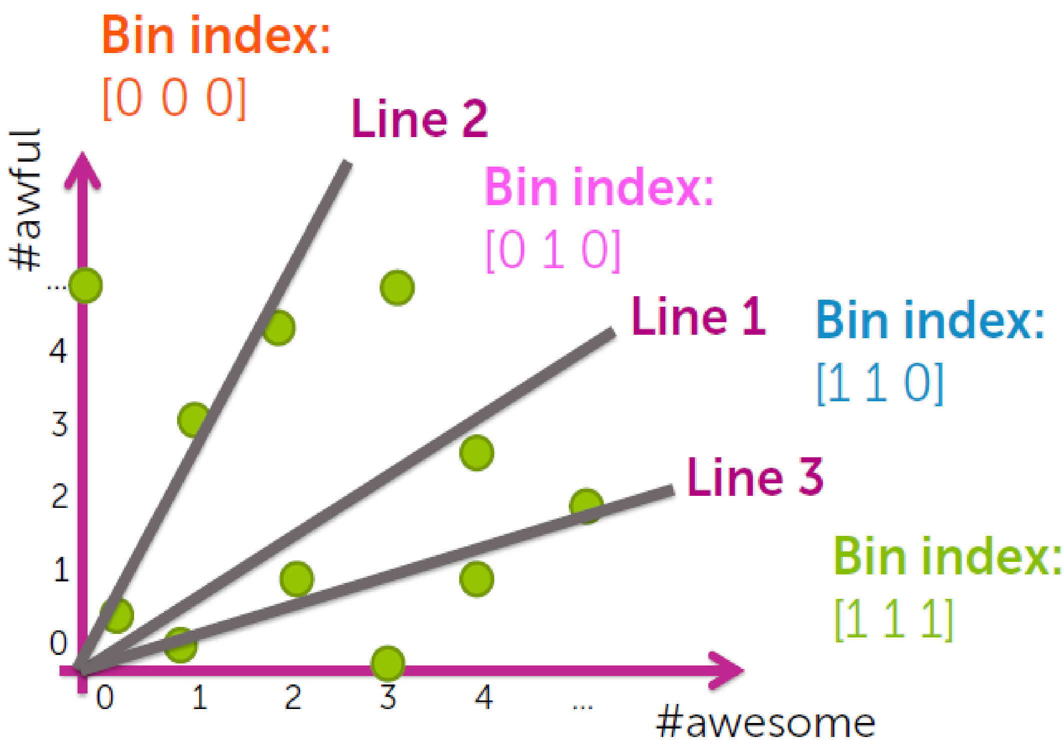



If $\theta_{xy}$ is small (**x**,**y** close), unlikely to be placed into separate bins

# LSH: improving efficiency



## Reducing search cost through more bins



# LSH: improving efficiency



## Using score for NN search

| 2D Data | Sign (Score$_1$) | Bin 1 index | Sign (Score$_2$) | Bin 2 index | Sign (Score$_3$) | Bin 3 index |
|---|---|---|---|---|---|---|
| $\mathbf{x}_1$ = [0, 5] | -1 | 0 | -1 | 0 | -1 | 0 |
| $\mathbf{x}_2$ = [1, 3] | -1 | 0 | -1 | 0 | -1 | 0 |
| $\mathbf{x}_3$ = [3, 0] | 1 | 1 | 1 | 1 | 1 | 1 |
| ... | ... | ... | ... | ... | ... | ... |

| Bin | [0 0 0] = 0 | [0 0 1] = 1 | [0 1 0] = 2 | [0 1 1] = 3 | [1 0 0] = 4 | [1 0 1] = 5 | [1 1 0] = 6 | [1 1 1] = 7 |
|---|---|---|---|---|---|---|---|---|
| Data indices: | {1,2} | -- | {4,8,11} | -- | -- | -- | {7,9,10} | {3,5,6} |

search for NN amongst this set

# LSH: improving efficiency



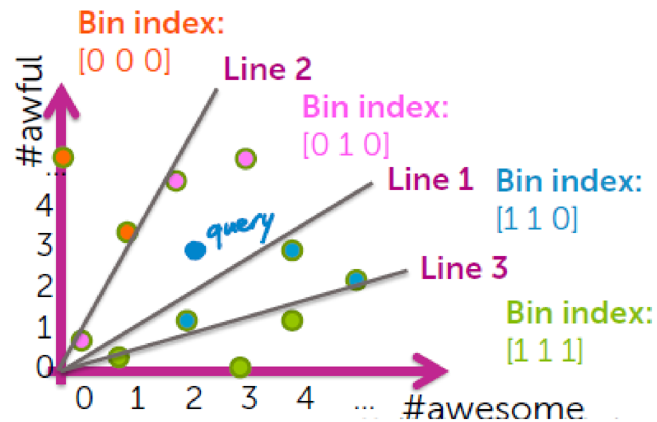
## Improving search quality by searching neighboring bins

| Bin | [0 0 0] = 0 | [0 0 1] = 1 | [0 1 0] = 2 | [0 1 1] = 3 | [1 0 0] = 4 | [1 0 1] = 5 | [1 1 0] = 6 | [1 1 1] = 7 |
|---|---|---|---|---|---|---|---|---|
| Data indices: | {1,2} | -- | {4,8,11} | -- | -- | -- | {7,9,10} | {3,5,6} |

Query point here, but is NN?

**Not necessarily**

Even worse than before...Each line can split pts.
Sacrificing accuracy for speed



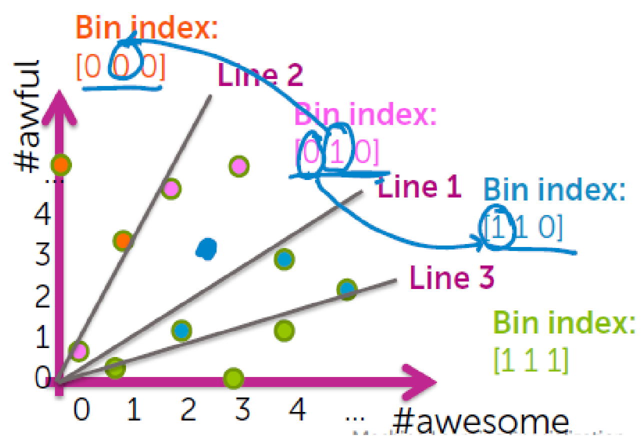
# LSH: improving efficiency



Improving search quality by
searching neighboring bins

| Bin | [0 0 0] = 0 | [0 0 1] = 1 | [0 1 0] = 2 | [0 1 1] = 3 | [1 0 0] = 4 | [1 0 1] = 5 | [1 1 0] = 6 | [1 1 1] = 7 |
|---|---|---|---|---|---|---|---|---|
| Data indices: | {1,2} | -- | {4,8,11} | -- | -- | -- | {7,9,10} | {3,5,6} |

Next closest bins
(flip 1 bit)



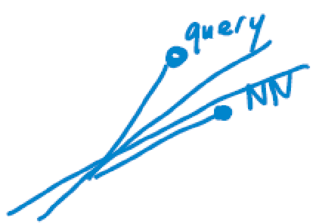
# LSH: improving efficiency

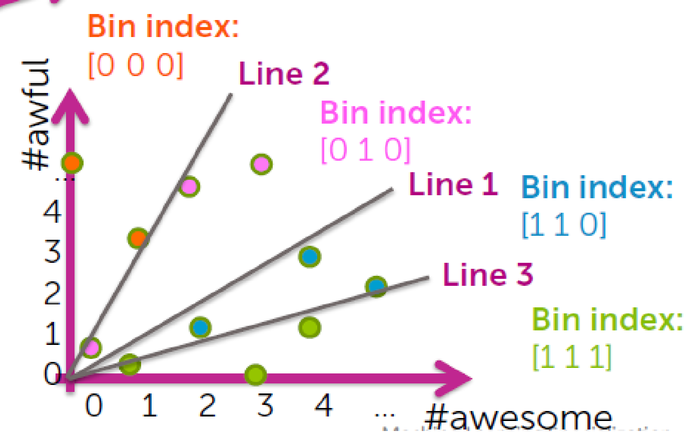


## Improving search quality by searching neighboring bins

| Bin | [0 0 0] = 0 | [0 0 1] = 1 | [0 1 0] = 2 | [0 1 1] = 3 | [1 0 0] = 4 | [1 0 1] = 5 | [1 1 0] = 6 | [1 1 1] = 7 |
|---|---|---|---|---|---|---|---|---|
| Data indices: | {1,2} | -- | {4,8,11} | -- | -- | -- | {7,9,10} | {3,5,6} |

Further bin
(flip 2 bits)



# LSH: improving efficiency



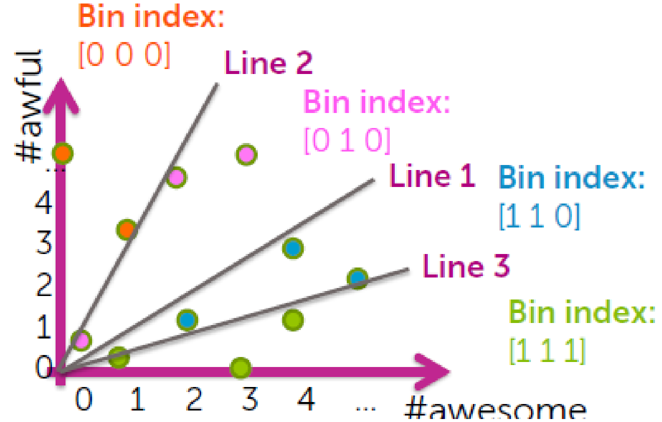
## Improving search quality by searching neighboring bins

| Bin | [0 0 0] = 0 | [0 0 1] = 1 | [0 1 0] = 2 | [0 1 1] = 3 | [1 0 0] = 4 | [1 0 1] = 5 | [1 1 0] = 6 | [1 1 1] = 7 |
|---|---|---|---|---|---|---|---|---|
| Data indices: | {1,2} | -- | {4,8,11} | -- | -- | -- | {7,9,10} | {3,5,6} |

Quality of retrieved NN can only improve with searching more bins

**Algorithm:**

Continue searching until computational budget is reached or quality of NN good enough



# LSH recap



kd-tree competitor data structure

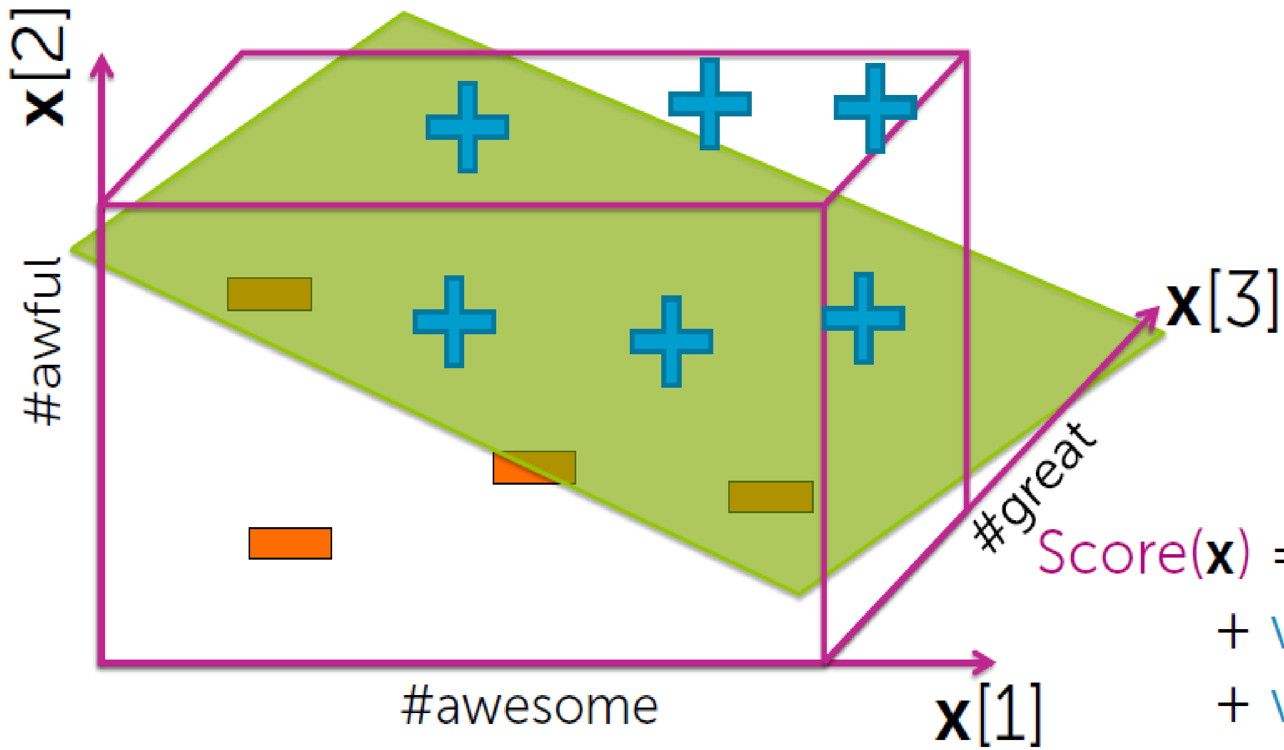
- Draw h random lines
- Compute "score" for each point under each line and translate to binary index
- Use h-bit binary vector per data point as bin index
- Create hash table

- For each query point **x**, search bin(**x**), then neighboring bins until time limit

# LSH: moving to higher dimmensions d



## Draw random *planes*




Score(**x**) = $v_1$ #awesome
+ $v_2$ #awful
+ $v_3$ #great

# Cost of binning points in d-dim

$$\mathrm{Score}_i(\mathbf{x}) = v_1^{(i)} \#awesome + v_2^{(i)} \#awfull + v_3^{(i)} \#great$$

$i^{th}$ hyperplane

Per data point, need d multiplies to determine bin index per plane

In high-dim, (and some applications) this is often a sparse mult.

One-time cost offset if many queries of fixed dataset

# What you can do now …



- Implement nearest neighbor search for retrieval tasks
- Contrast document representations (e.g., raw word counts, tf-idf,…)
  - Emphasize important words using tf-idf
- Contrast methods for measuring similarity between two documents
  - Euclidean vs. weighted Euclidean
  - Cosine similarity vs. similarity via unnormalized inner product
- Describe complexity of brute force search
- Implement KD-trees for nearest neighbor search
- Implement LSH for approximate nearest neighbor search
- Compare pros and cons of KD-trees and LSH, and decide which is more appropriate for given dataset

# Clustering:
# An unsupervised learning task

# Motivation

**Goal:** Structure documents by topic

Discover groups (*clusters*) of related articles

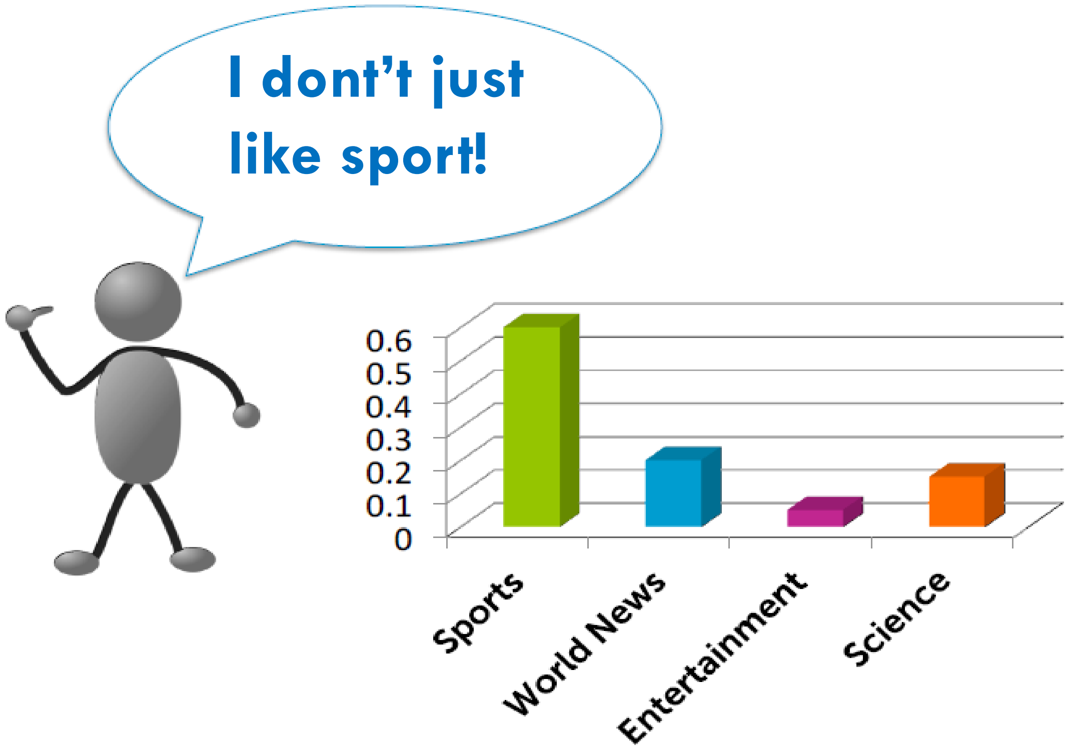
SPORTS


WORLD NEWS

# Motivation



Why might clustering be useful?

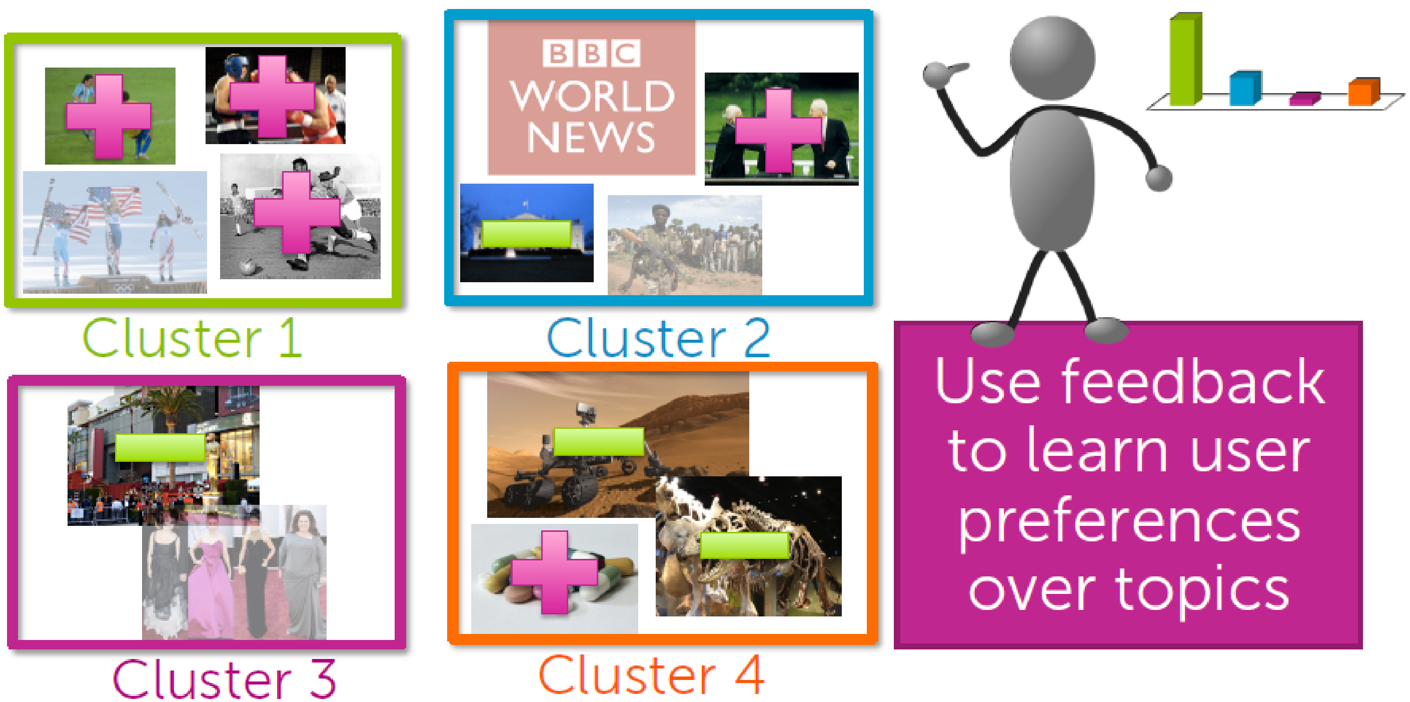


# Motivation



## Learn user preferences

Set of clustered documents read by user



# Clustering: a supervised learning

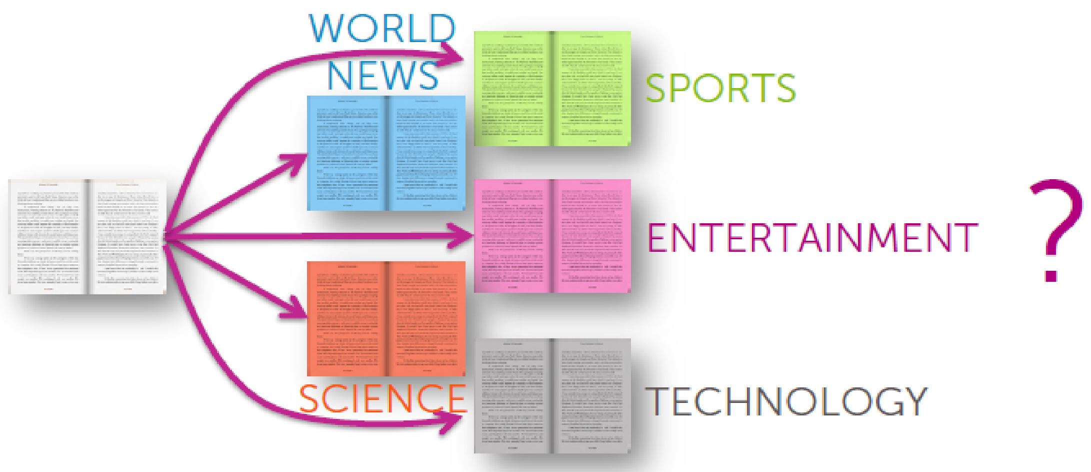


What if some of the labels are known?

# Custering: a supervised learning



## Multiclass classification problem




Example of
supervised learning

# Clustering: an unsupervised learning



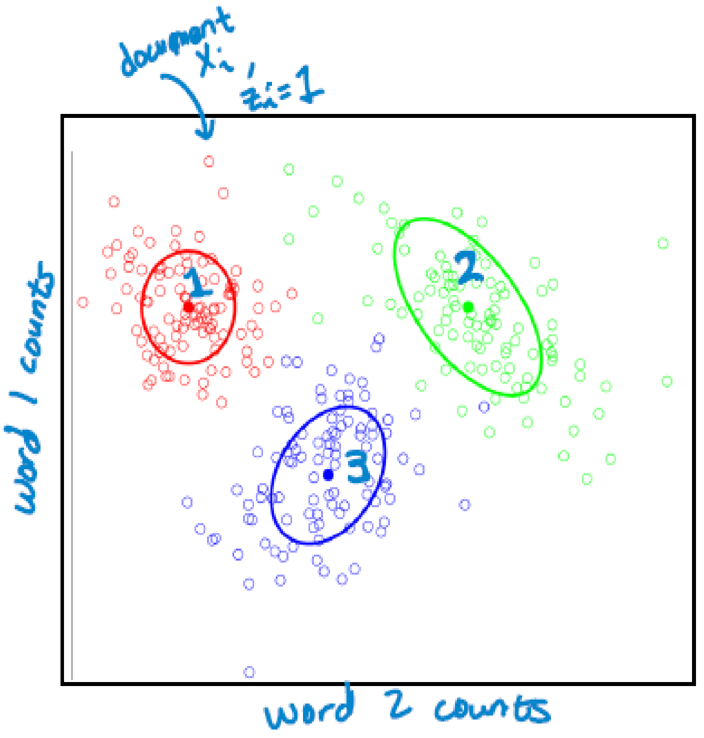
No labels provided

...uncover cluster structure from input alone

**Input:** docs as vectors $\mathbf{x}_i$

**Output:** cluster labels $z_i$

An unsupervised learning task



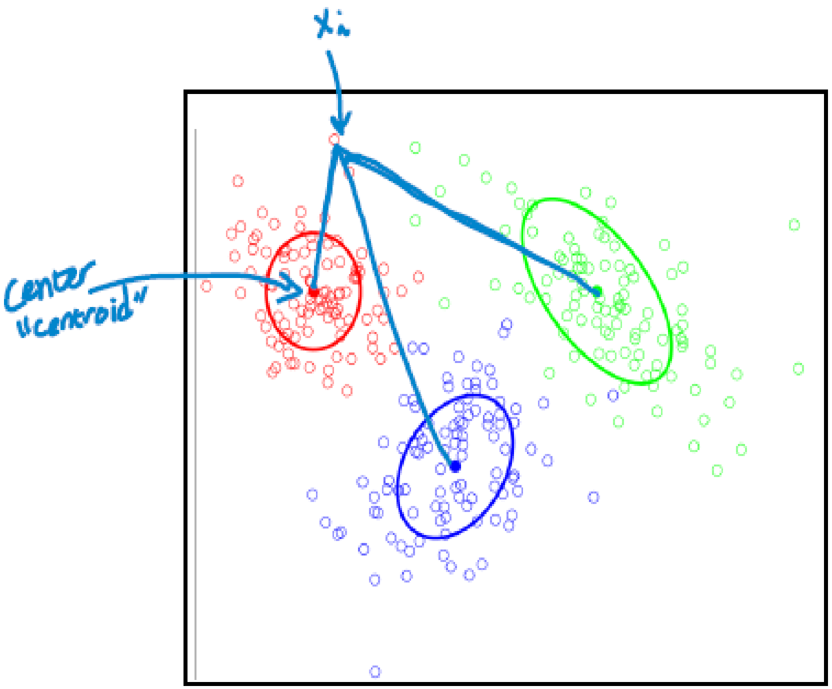
# What defines a cluster ?



Cluster defined by
center & shape/spread

Assign observation $\mathbf{x}_i$ (doc) to cluster k (topic label) if

- Score under cluster k is higher than under others
- For simplicity, often define score as distance to cluster center (ignoring shape)



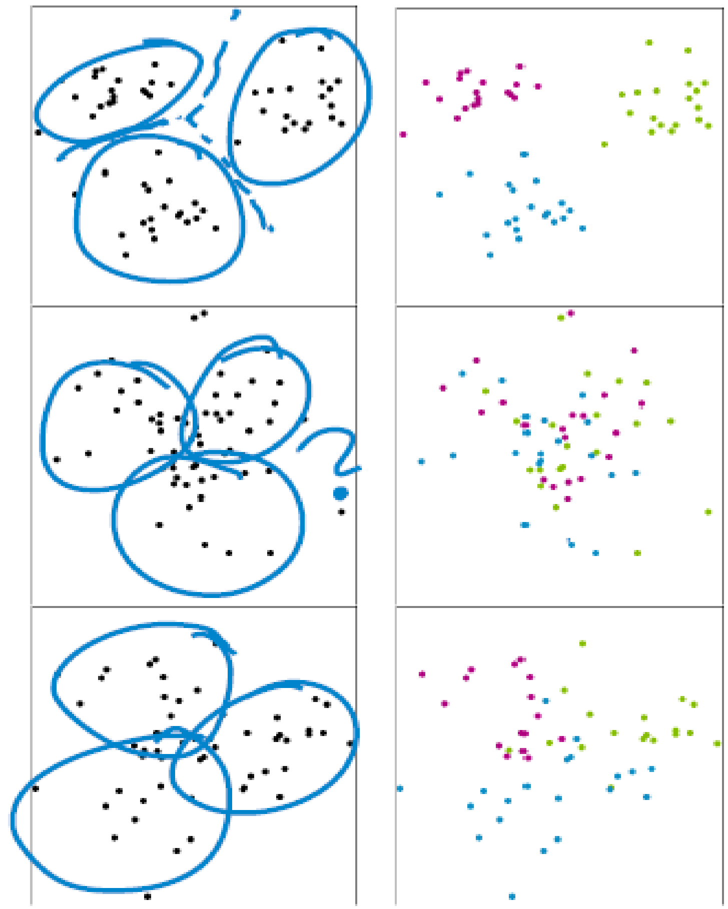
# Hope for unsupervised learning



Easy

Impossible

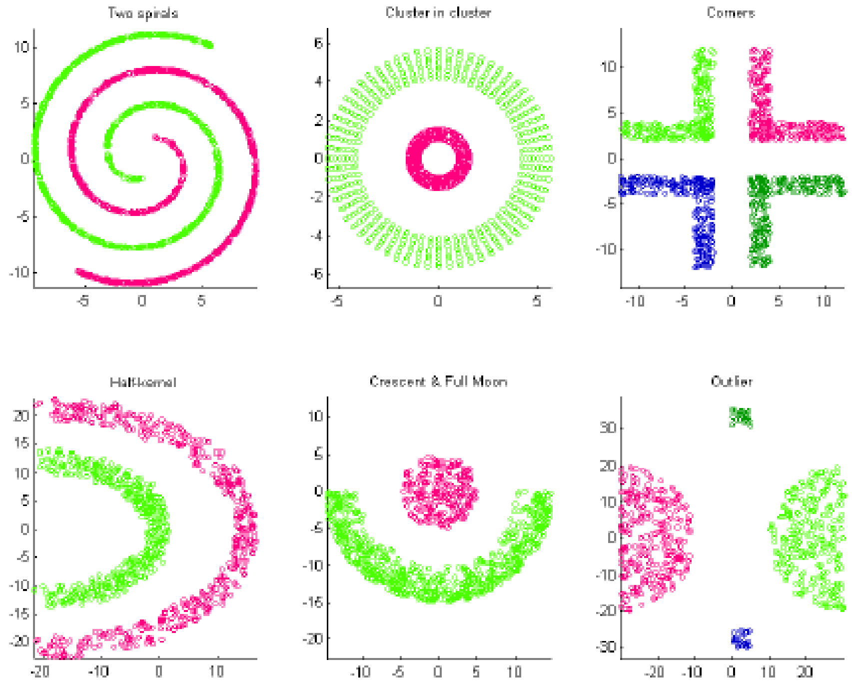
In between



# Other (challenging!) clusters to discover



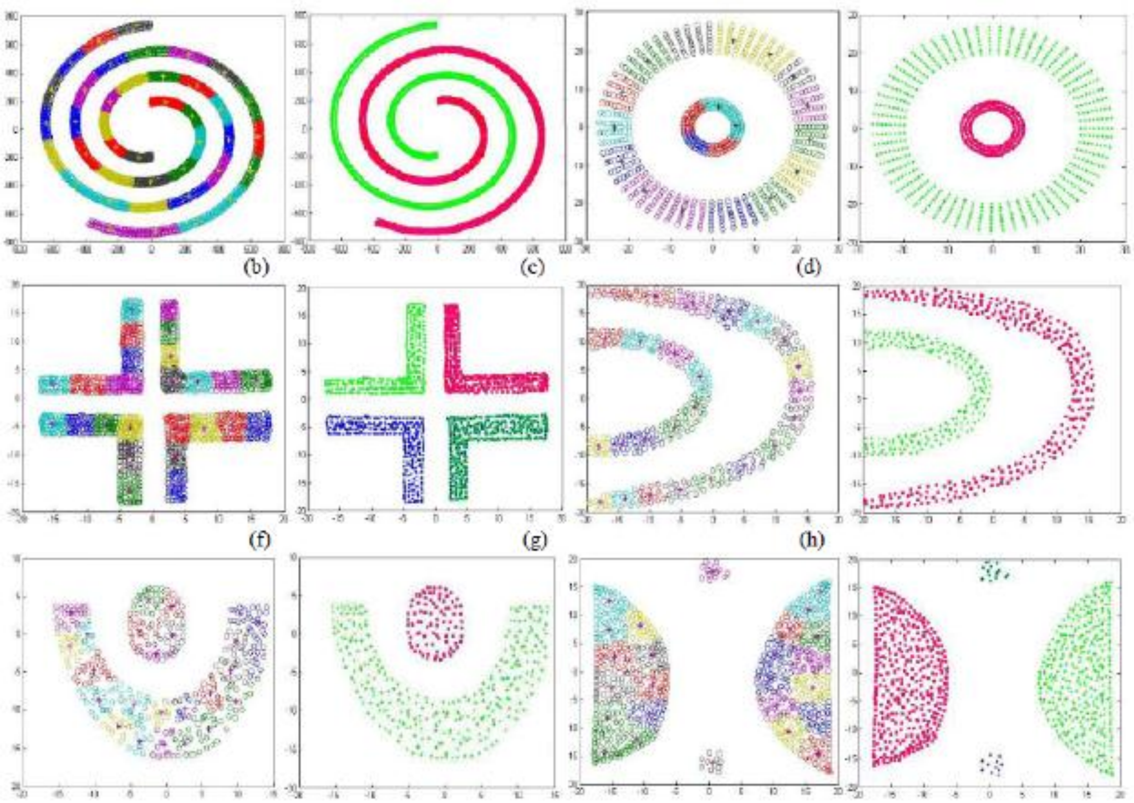
**Analysed by your eyes**



# Other (challenging!) clusters to discover



**Analysed by clustering algorithms**

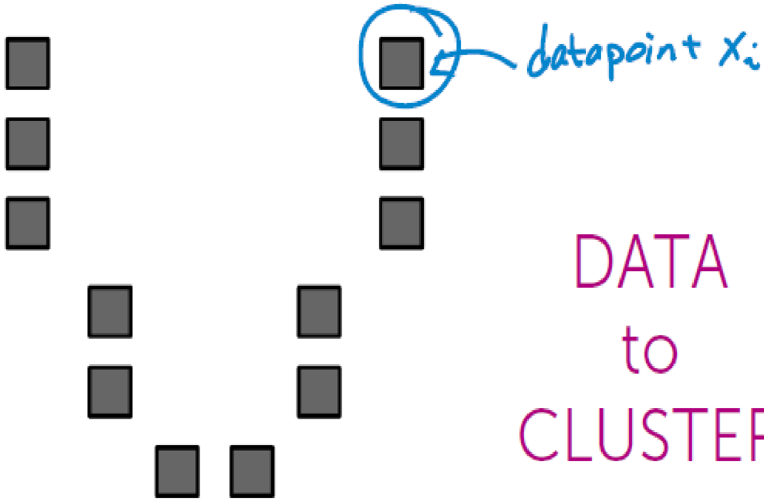


# k-means clustering algorithm

# k-means clustering algorithm

Assume

- Score= distance to cluster center (smaller better)



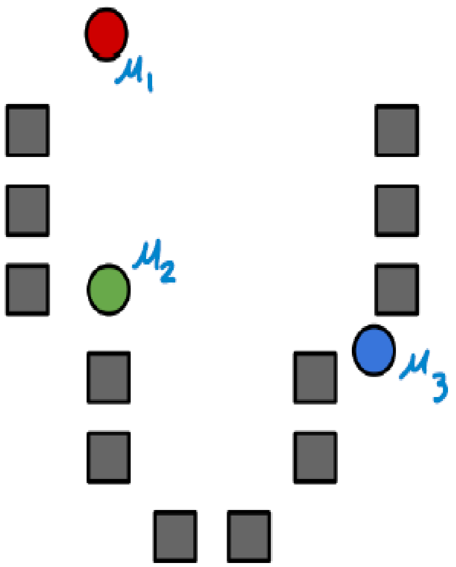

DATA
to
CLUSTER

# k-means clustering algorithm



0. Initialize cluster centers

$$\mu_1, \mu_2, \ldots, \mu_k$$




(k=3 clusters)

# k-means clustering algorithm

0. Initialize cluster centers
1. Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

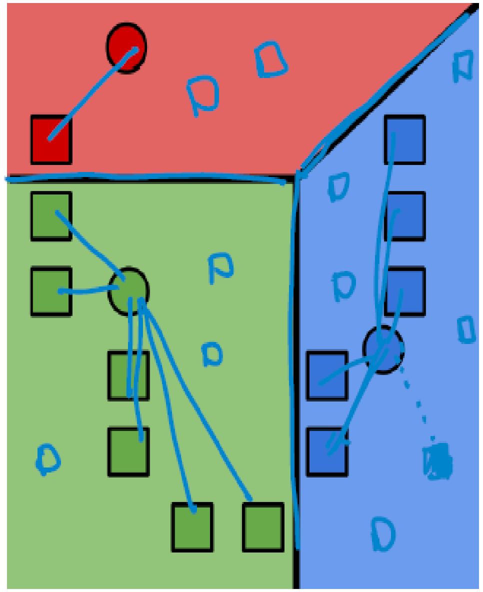
$j^{th}$ cluster center (varying)

$i^{th}$ obs. (fixed)

Inferred label for obs i, whereas supervised learning has given label $y_i$

return index j of the cluster whose center is closest to obs $x_i$

(whereas min returning minimum value of $\|\cdot\|_2^2$)



Voronoi tesselation

(for visualization only ... you don't need to compute this)

# k-means clustering algorithm

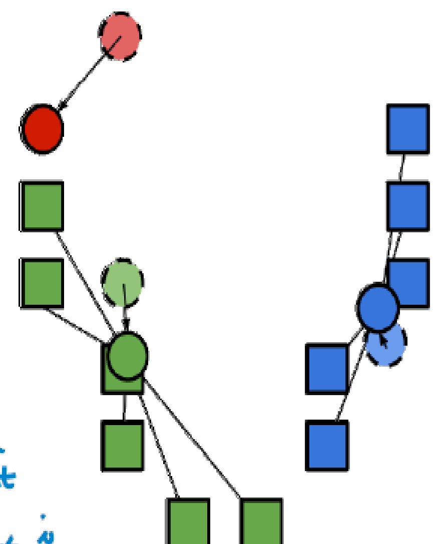


0. Initialize cluster centers
1. Assign observations to closest cluster center
2. Revise cluster centers as mean of assigned observations

$$\underline{\underline{\mu_j}} = \frac{1}{n_j} \sum_{i:z_i=j} \mathbf{x}_i$$

\# of obs. in cluster j

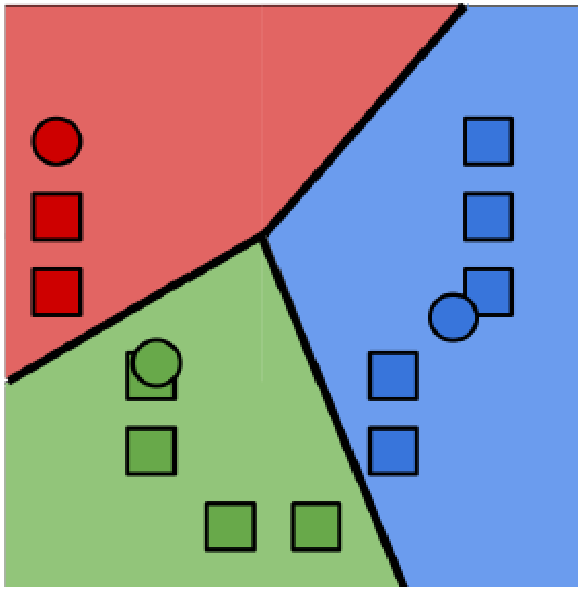
all obs. i such that $z_i = j$ (obs i is in cluster j)



# k-means clustering algorithm



0. Initialize cluster centers
1. Assign observations to closest cluster center
2. Revise cluster centers as mean of assigned observations
3. Repeat 1.+2. until convergence



# k-means as coordinate descent algorithm



1. Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

2. Revise cluster centers as mean of assigned observations

$$\mu_j = \frac{1}{n_j} \sum_{i:z_i=j} \mathbf{x}_i$$

equivalent to

$$\mu_j \leftarrow \arg\min_\mu \sum_{i:z_i=j} ||\mu - \mathbf{x}_i||_2^2$$

# K-means as coordinate descent algorithm



1. Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

2. Revise cluster centers as mean of assigned observations

$$\mu_j \leftarrow \arg\min_\mu \sum_{i:z_i=j} ||\mu - \mathbf{x}_i||_2^2$$

Alternating minimization
1. (z given μ) and 2. (μ given z)
= **coordinate descent**

# Convergence of k-means



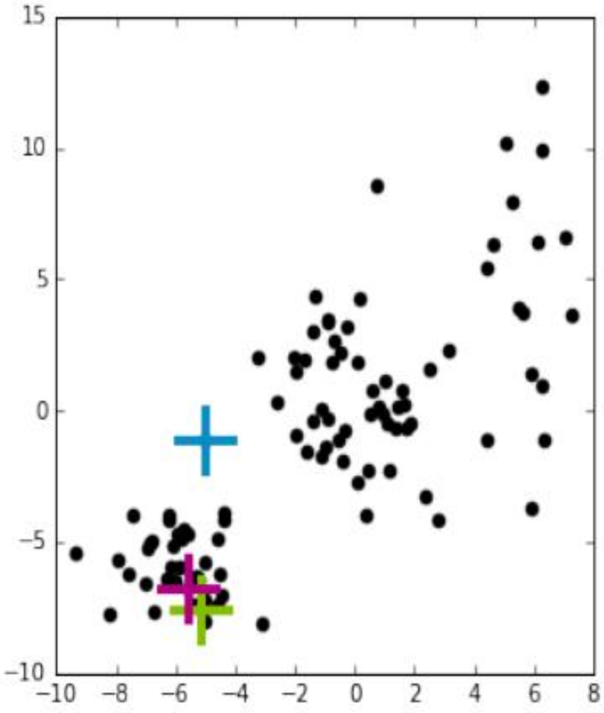
Converges to:

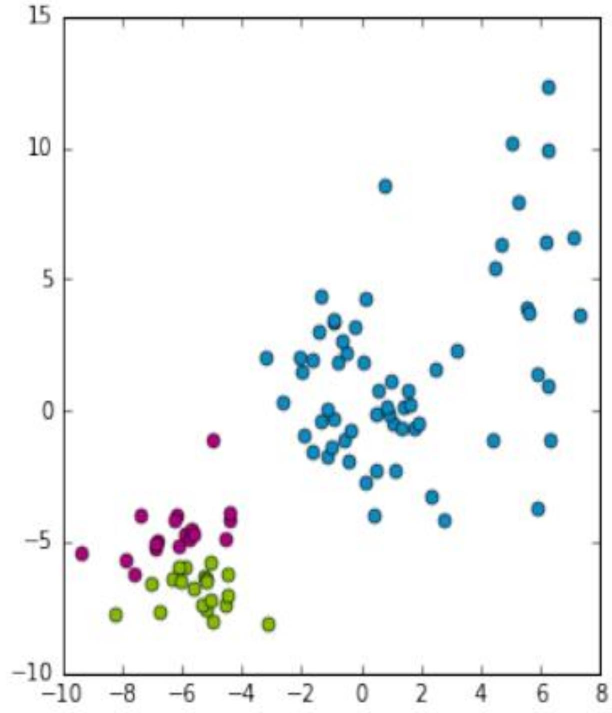
- ~~Global optimum~~
- $\boxed{\text{Local optimum}}$
- ~~neither~~

***Because we can cast k-means as coordinate descent algorithm we know that we are converging to local optimum***

# Convergence of k-mans to local mode



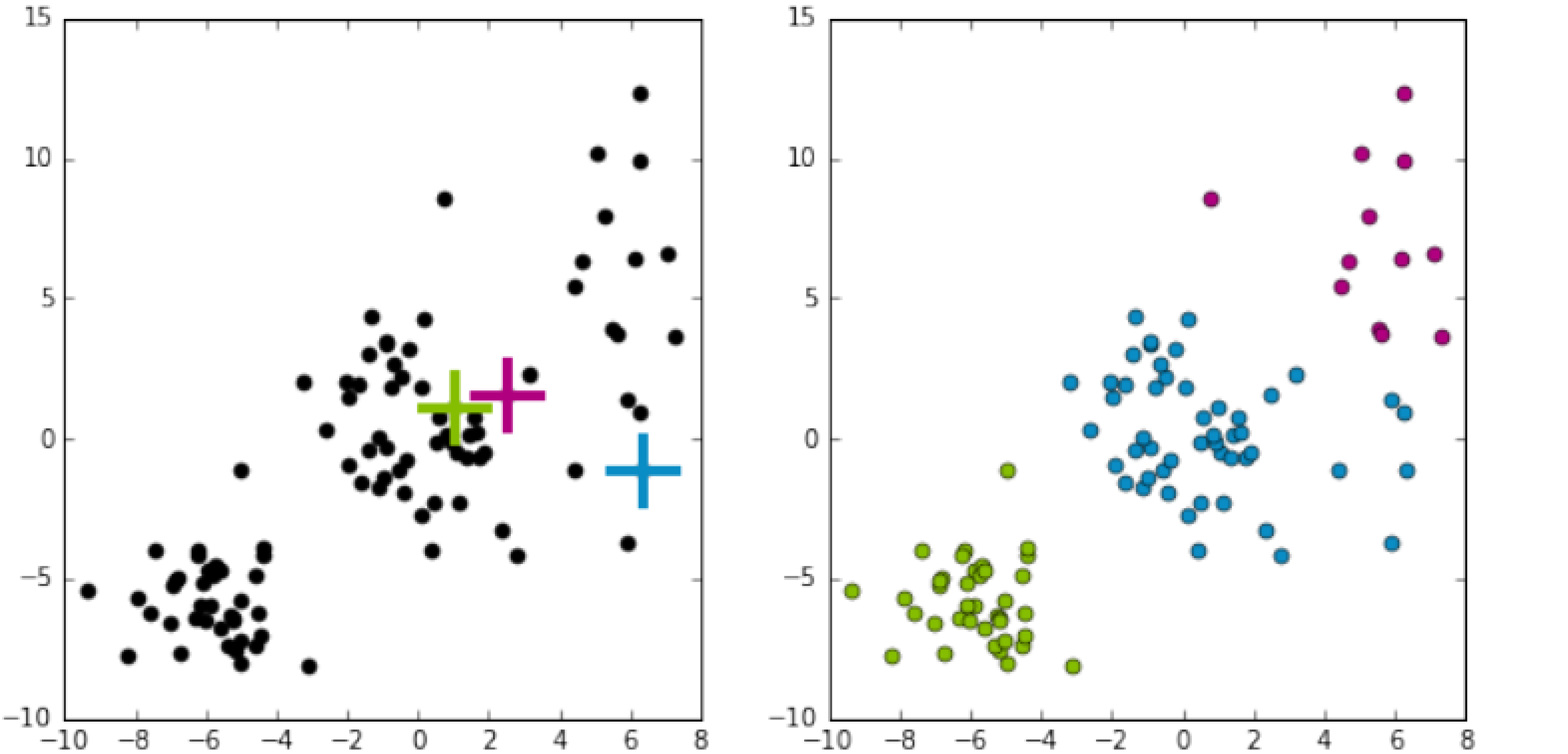



*Crosses: initialised centers*

# Convergence of k-mans to local mode

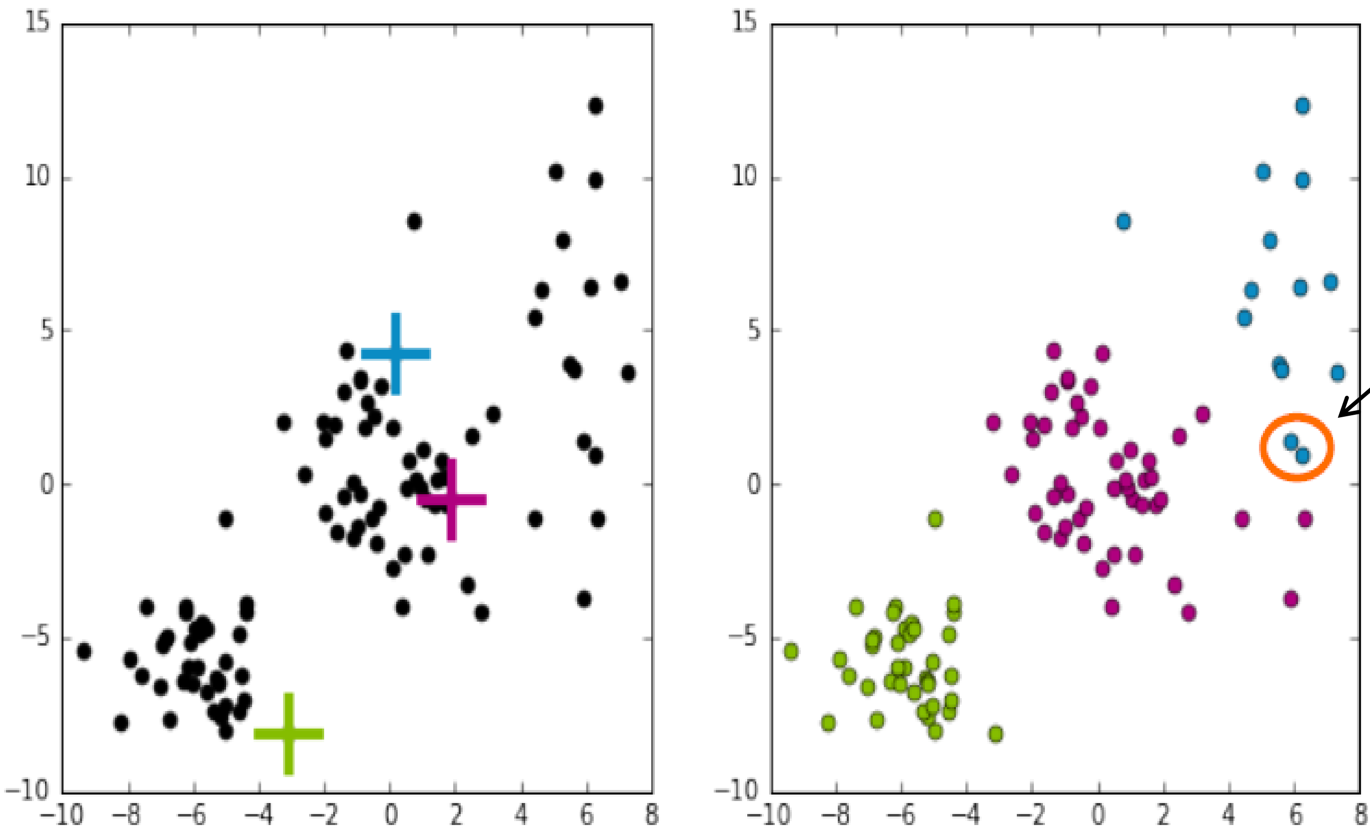





***Crosses: initialised centers***

# Convergence of k-mans to local mode






*Crosses: initialised centers*

***Assigment to which group has changed***

***k-means very sensitive to initiased centers***

# Smart initialisation: k-means++ overwiew



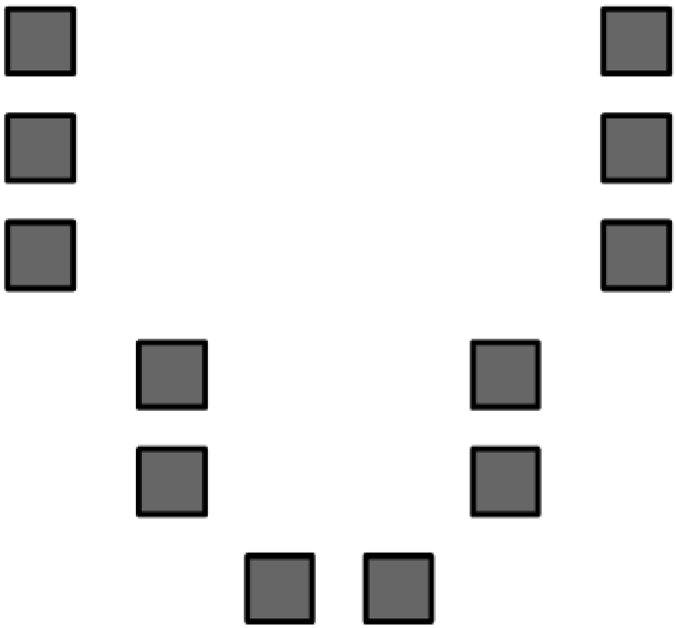
Initialization of k-means algorithm is critical to quality of local optima found

**Smart initialization:**

1. Choose first cluster center uniformly at random from data points
2. For each obs **x**, compute distance d(**x**) to nearest cluster center
3. Choose new cluster center from amongst data points, with probability of **x** being chosen proportional to $d(\mathbf{x})^2$
4. Repeat Steps 2 and 3 until k centers have been chosen

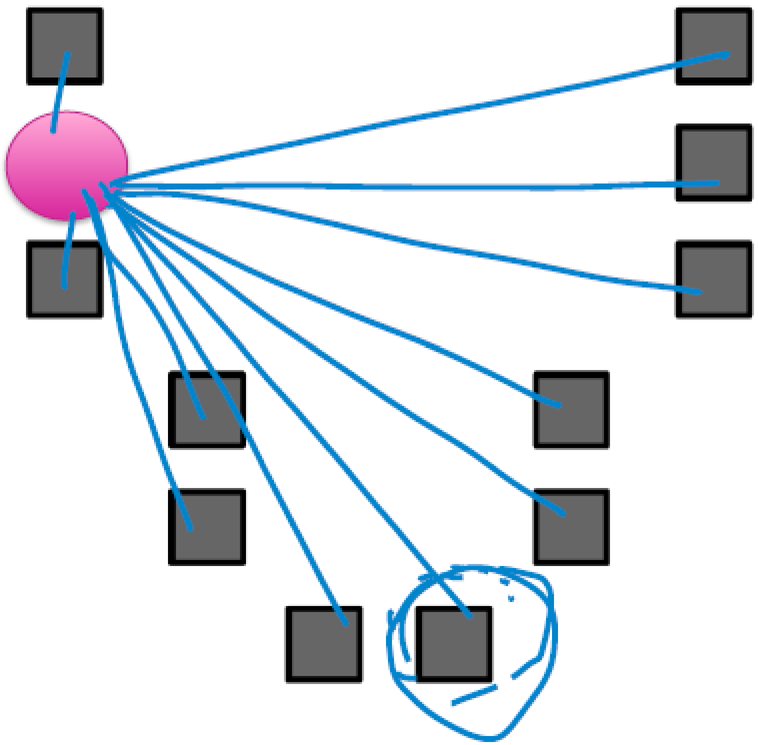
# k-means++ visualised





# k-means++ visualised

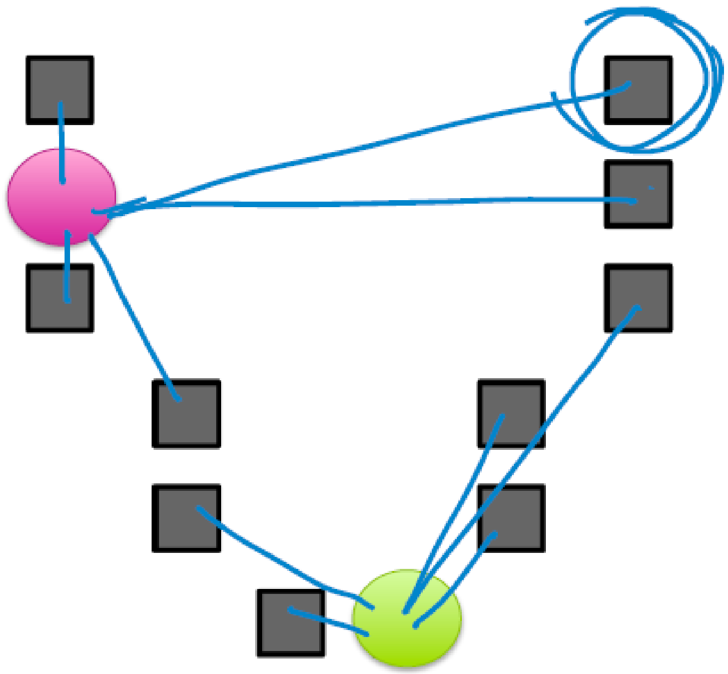




more likely to select a datapoint as a cluster center if that datapoint is far away (dist$^2$ increases this effect)

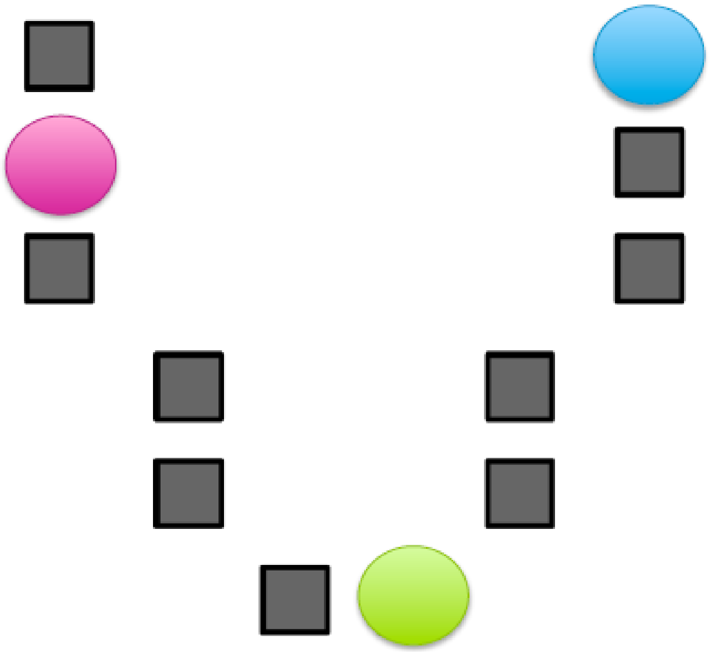
# k-means++ visualised





# k-means++ visualised





# k-means++ pros/cons

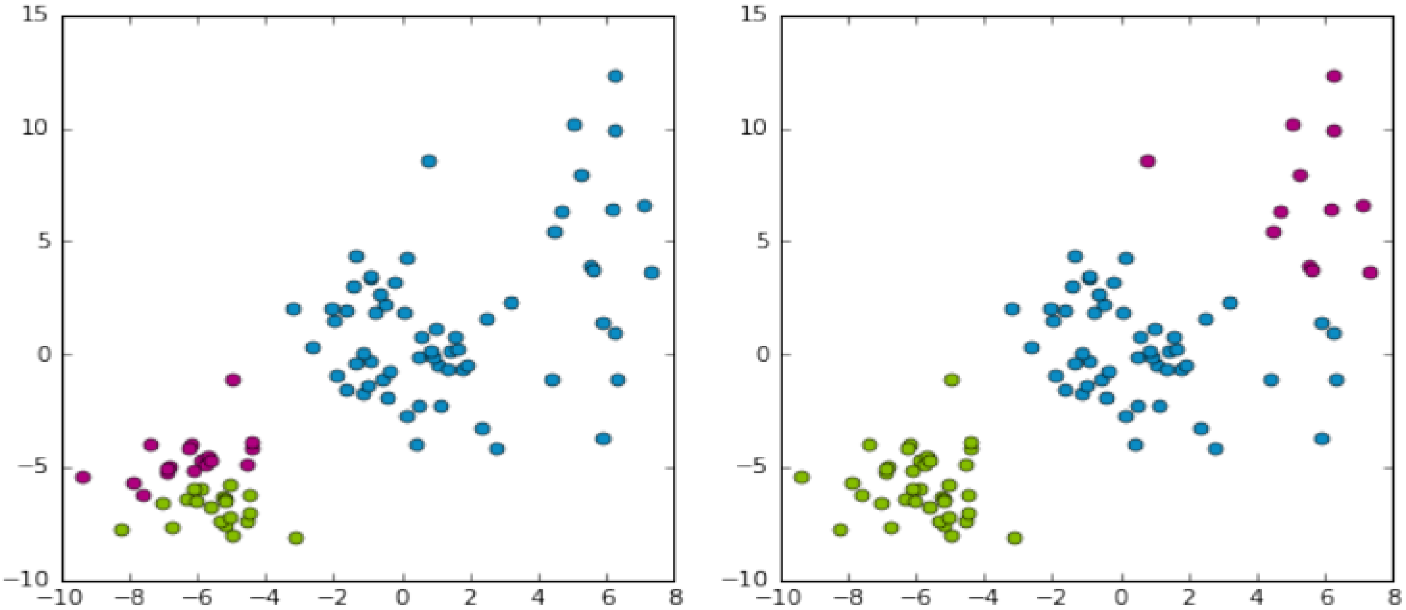
Computationally costly relative to random initialization, but the subsequent k-means often converges more rapidly

Tends to improve quality of local optimum and lower runtime

# Assessing quality of the clustering

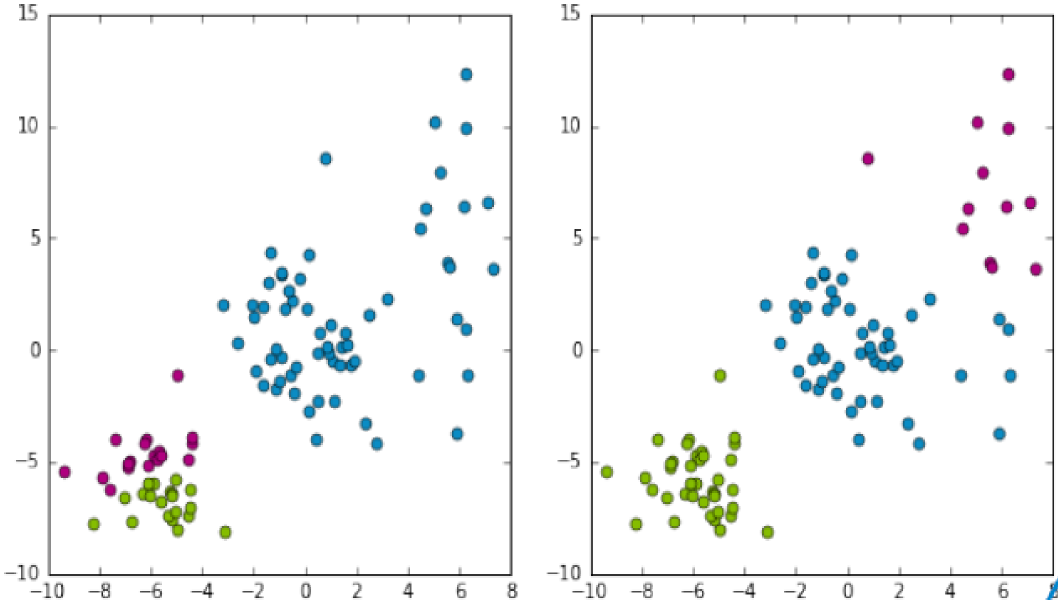


Which clustering do I prefer?



# k-means objective





**k-means** is trying to minimize the sum of squared distances:

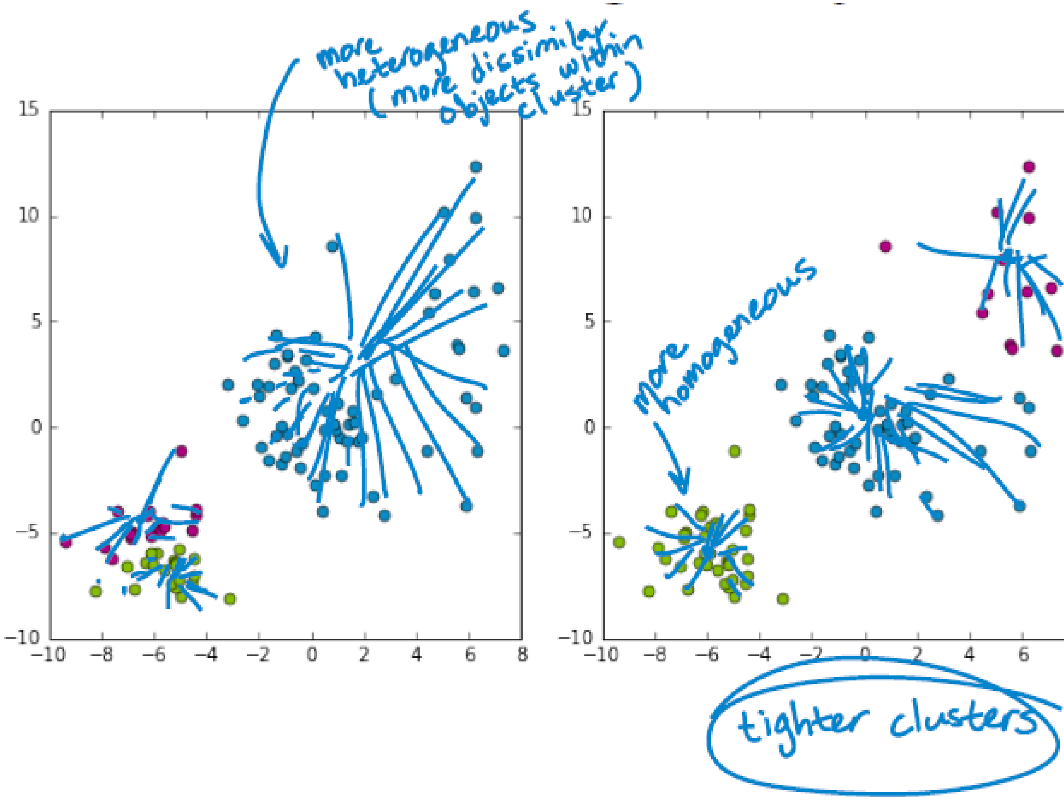
sum over all clusters

sum of squared distances in cluster j

$$\min_{\{z_i\},\{\mu_j\}} \sum_{j=1}^{k} \sum_{i:z_i=j} ||\mu_j - \mathbf{x}_i||_2^2$$

# Cluster heterogeneity






Measure of quality of given clustering:

$$\sum_{j=1}^{k} \sum_{i:z_i=j} ||\mu_j - \mathbf{x}_i||_2^2$$

Lower is better!

# What happens to heterogeneity as k increases?



Can refine clusters more and more to the data

→ overfitting!

\# of observations

**Extreme case** of k=N:

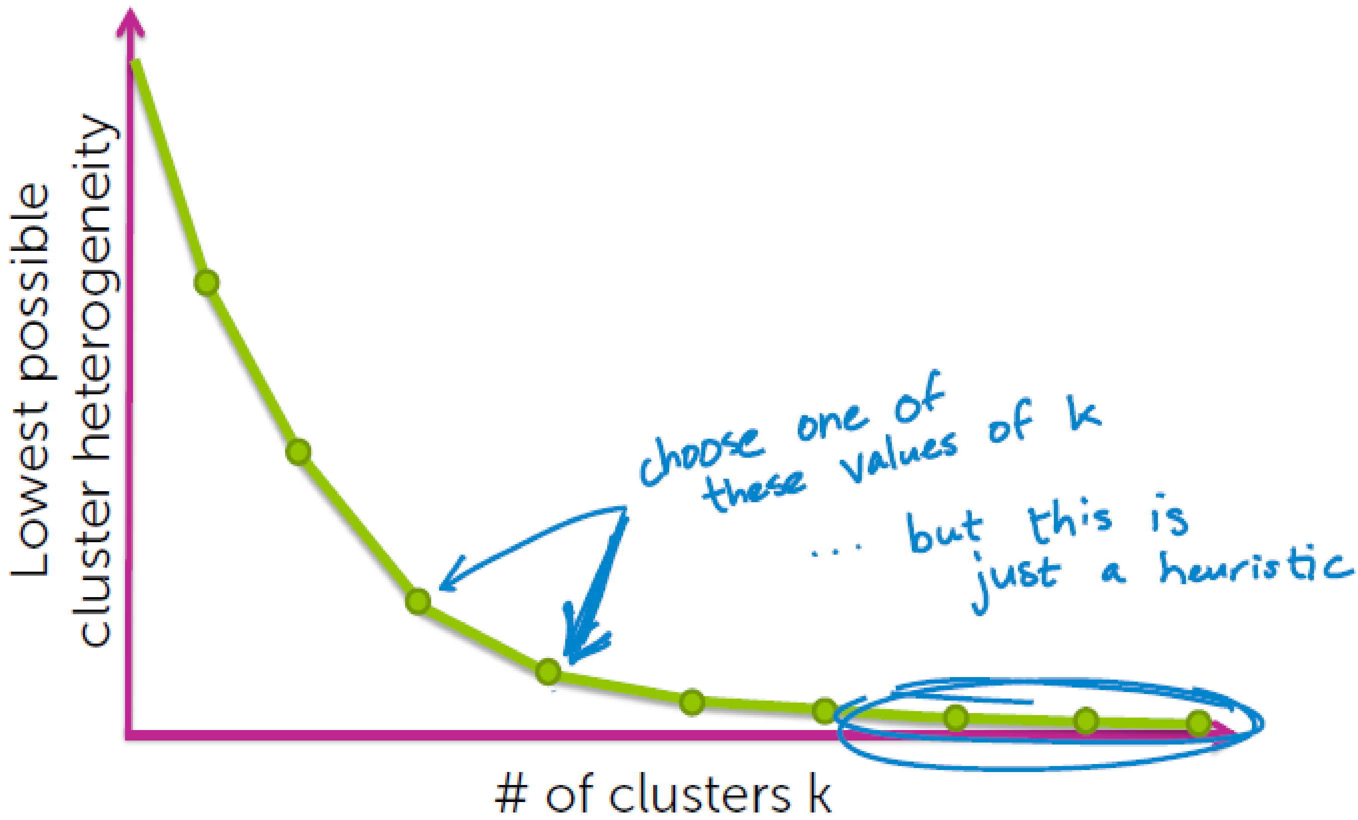
– can set each cluster center equal to datapoint

– heterogeneity = 0 ! (all distances to cluster centers are 0)

Lowest possible cluster heterogeneity decreases with increasing k

# How to choose k?





# MapReduce

# Counting words on a single processor



(The "Hello World!" of MapReduce)

Suppose you have 10B documents and 1 machine and want to count the # of occurrences of each word in the corpus

Code:

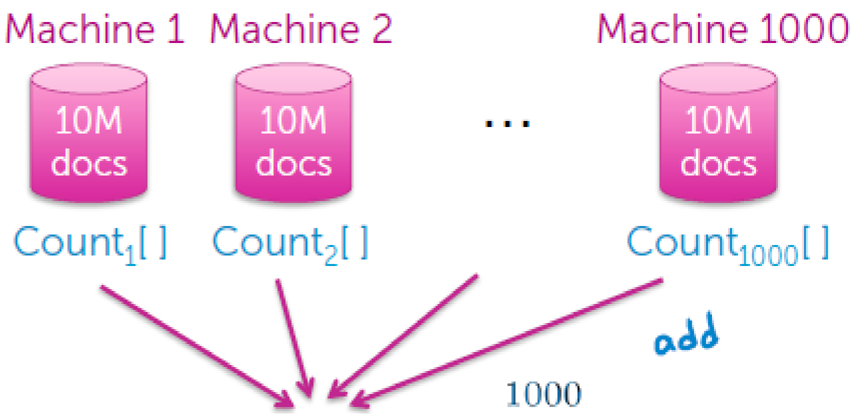
```
count[ ] ← init hash table
  for d in documents
    for word in d
      count[word] += 1
```

# Naive parallel word counting



- Word counts are independent across documents $\boxed{\text{(data parallel)}}$
- Count occurrences in sets of documents separately, then merge

evenly distribute data




add

combine local hash tables:

$$\text{Count[word]} = \sum_{i=1}^{1000} \text{Count}_i\text{[word]}$$

How do we do this for all words in vocab?

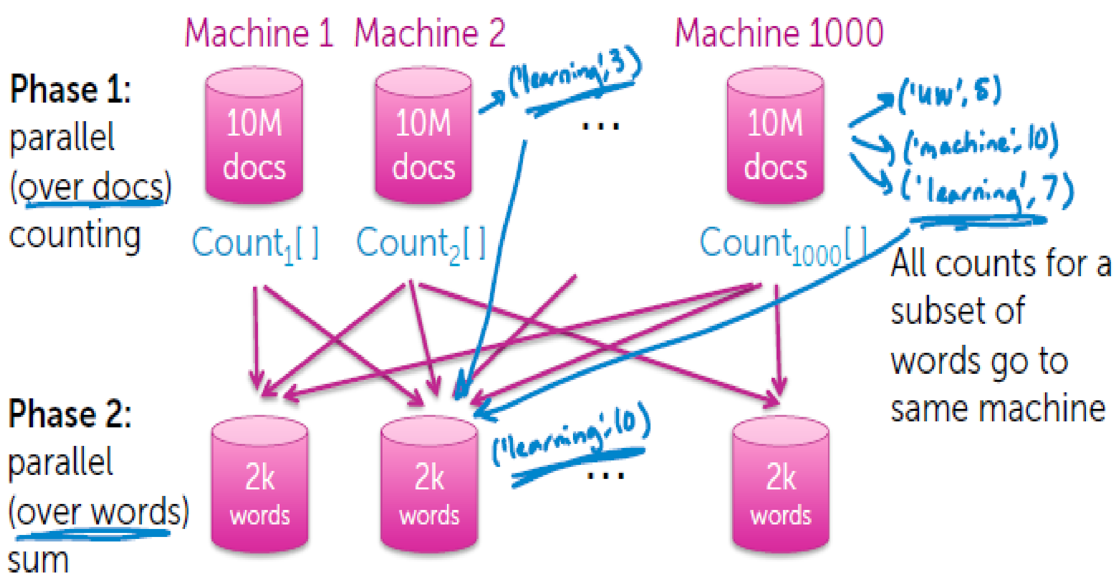
Back to sequential problem to merge counts…

have to cycle through all words in vocab… ugh.

# Counting words & merging tabels



1. Generate pairs (word,count) in parallel
2. Merge counts for each word in parallel




How to map words to machines? Use a hash function!

h(word index) → machine index

Which words go to machine $i$?

$h: \underset{\text{vocab}}{V} \to [1, 2, \dots, \#\text{machines}]$

Send counts of 'learning' to machine h['learning']

# MapReduce abstraction



**Map:**
- Data-parallel over elements, e.g., documents
- Generate (key,value) pairs
  - "value" can be any data type

('uw', 1)
('machine', 1)
('uw', 1)
('learning', 1) . . .

**Reduce:**
- Aggregate values for each key
- Must be commutative-associative operation

a+b = b+a    (a+b)+c = a+(b+c)

- Data-parallel over keys
- Generate (key,value) pairs

reduce ('uw', [1,17,0,0,12,2])
emit ('uw', 32)

**Word count example:**

```
map(doc)
    for word in doc
    emit(word,1)
```

key    value

key    list of values

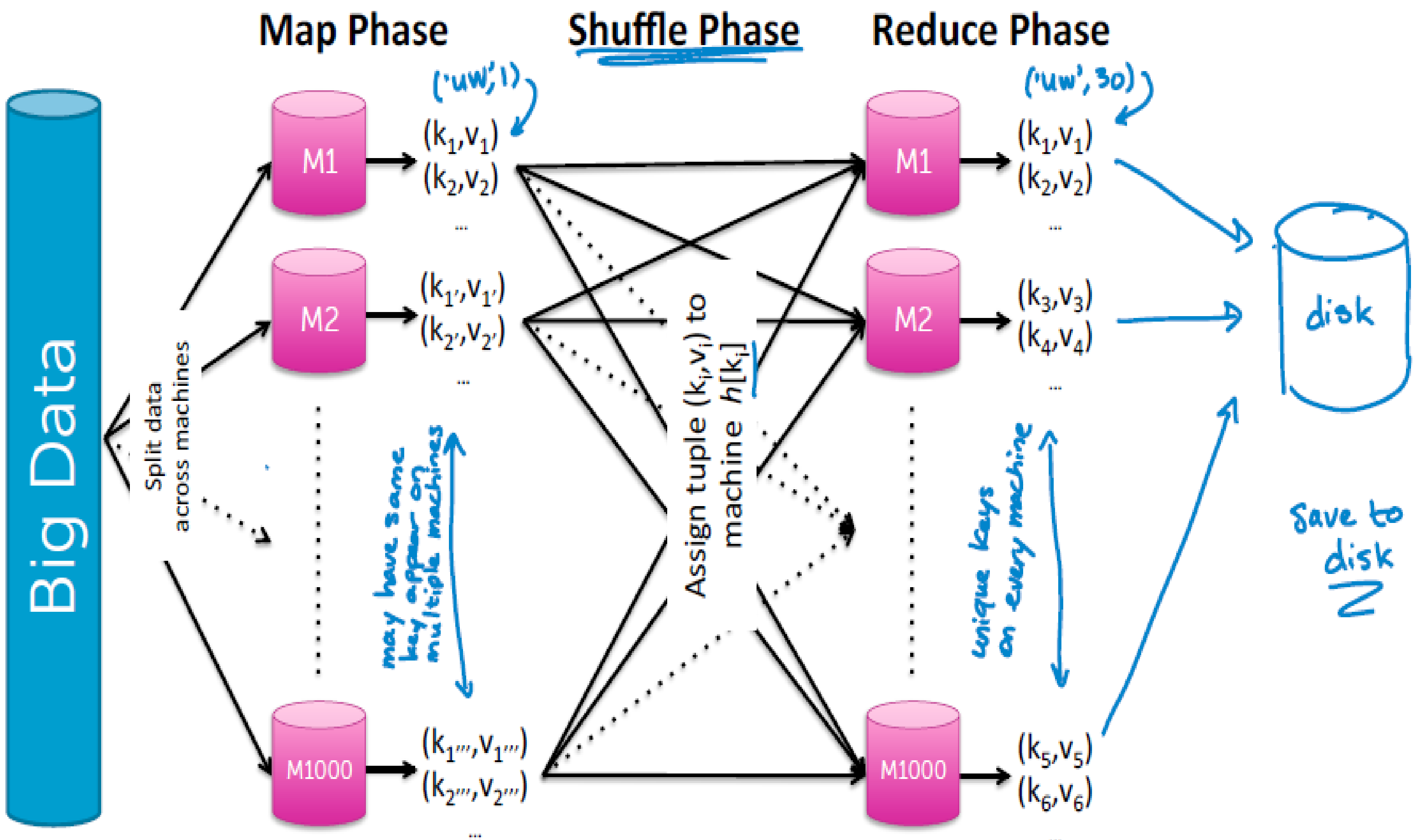
```
reduce(word, counts_list)
    c = 0
    for i in counts_list
    c += counts_list[i]
    emit(word, c)
```

key    value

MapReduce has long history in functional programming
- Popularized by Google, and subsequently by open-source Hadoop implementation from Yahoo!

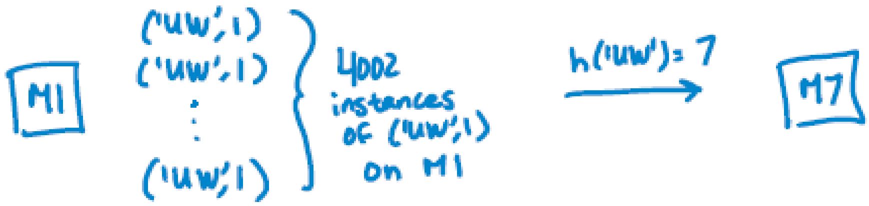
# MapReduce – Execution overwiew



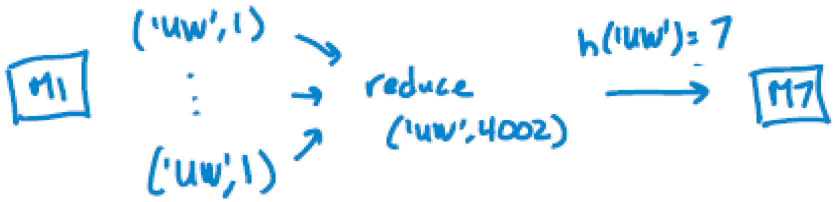


## Combiners

- Naïve implementation of MapReduce is very wasteful in communication during shuffle:




- Combiner: Simple solution…Perform reduce locally before communicating for global reduce
  - Works because reduce is commutative-associative



# Scaling up k-means via MapReduce



## MapReducing 1 iteration of k-means

**Classify:** Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

**Map:** For each data point, given ($\{\mu_j\}$,$\mathbf{x}_i$), emit($z_i$,$\mathbf{x}_i$)

**Recenter:** Revise cluster centers as mean of assigned observations

$$\mu_j = \frac{1}{n_j} \sum_{i:z_i=k} \mathbf{x}_i$$

**Reduce:** Average over all points in cluster j ($z_i$=k)

## Classification step as Map

**Classify:** Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

set of cluster centers

a datapoint

map([$\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$,..., $\boldsymbol{\mu}_k$], $\mathbf{x}_i$)

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

emit($z_i$,$\mathbf{x}_i$)

datapoint

cluster label

$z_i=2$ (assigned to cluster 2)

datapoint $x_i$

e.g. emit (2, [17, 0, 1, 7, 0, 0, 5])

# Scaling up k-means via MapReduce



## Recenter step as Reduce

**Recenter:** Revise cluster centers as mean of assigned observations

$$\mu_j = \frac{1}{n_j} \sum_{i:z_i=k} \mathbf{x}_i$$

cluster label (key)

datapoints assigned to cluster j (have key j)

reduce(j, x_in_clusterj : [$\mathbf{x}_1$, $\mathbf{x}_3$,..., ])

    sum = 0 ← total mass in cluster

    count = 0 ← total # of obs. in cluster

    for **x** in x_in_clusterj

        sum += **x**

        count += 1

    emit(j, sum/count)

cluster label

$\frac{\text{total mass}}{\text{total \# obs}}$

## Some practical considerations

k-means needs an iterative version of MapReduce

- Not standard formulation

Mapper needs to get data point and all centers

- A lot of data!
- Better implementation:
  mapper gets many data points

# Parallel k-means via MapReduce



Map: classification step;
data parallel over data points

Reduce: recompute means;
data parallel over centers

# What you can do now …



- Describe potential applications of clustering
- Describe the input (unlabeled observations) and output (labels) of a clustering algorithm
- Determine whether a task is supervised or unsupervised
- Cluster documents using k-means
- Interpret k-means as a coordinate descent algorithm
- Define data parallel problems
- Explain Map and Reduce steps of MapReduce framework
- Use existing MapReduce implementations to parallelize k-means, understanding what's being done under the hood

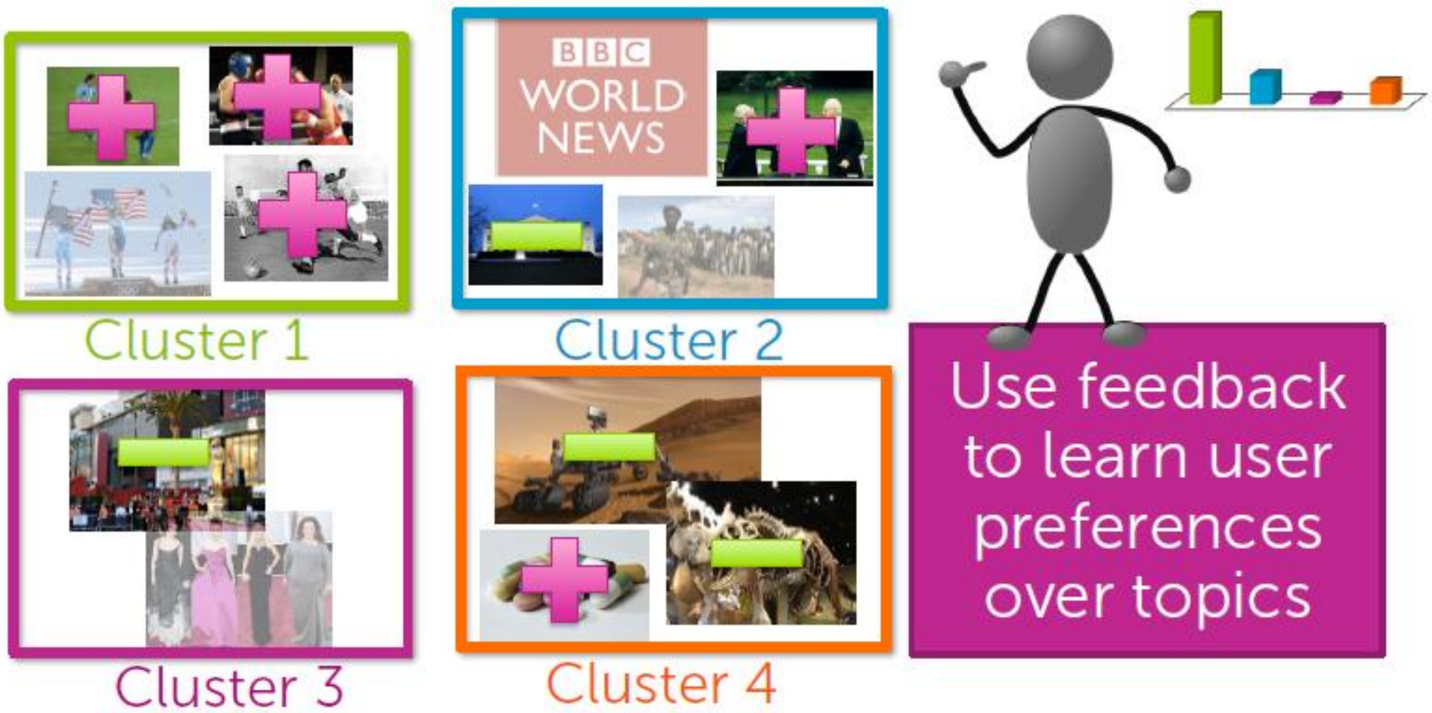
# Probabilistic approach: mixture model

# Why probabilistic approach?



## Learn user preferences

Set of clustered documents read by user



# Why probabilistic approach?



## Uncertainty in cluster assignments

# Why probabilistic approach?



## Other limitations of k-means

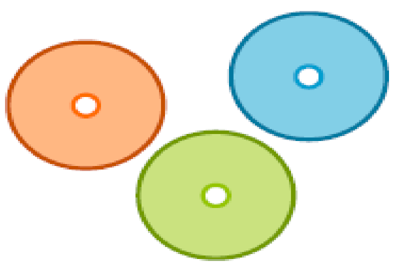
Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

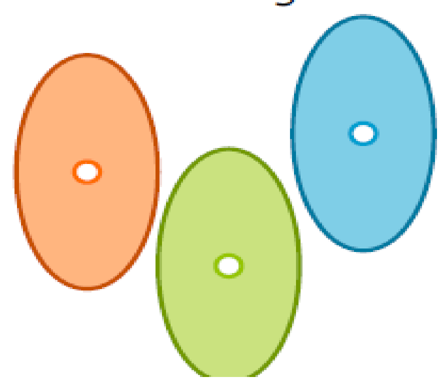
Can use weighted Euclidean, but requires *known* weights

Only center matters

Equivalent to assuming spherically symmetric clusters



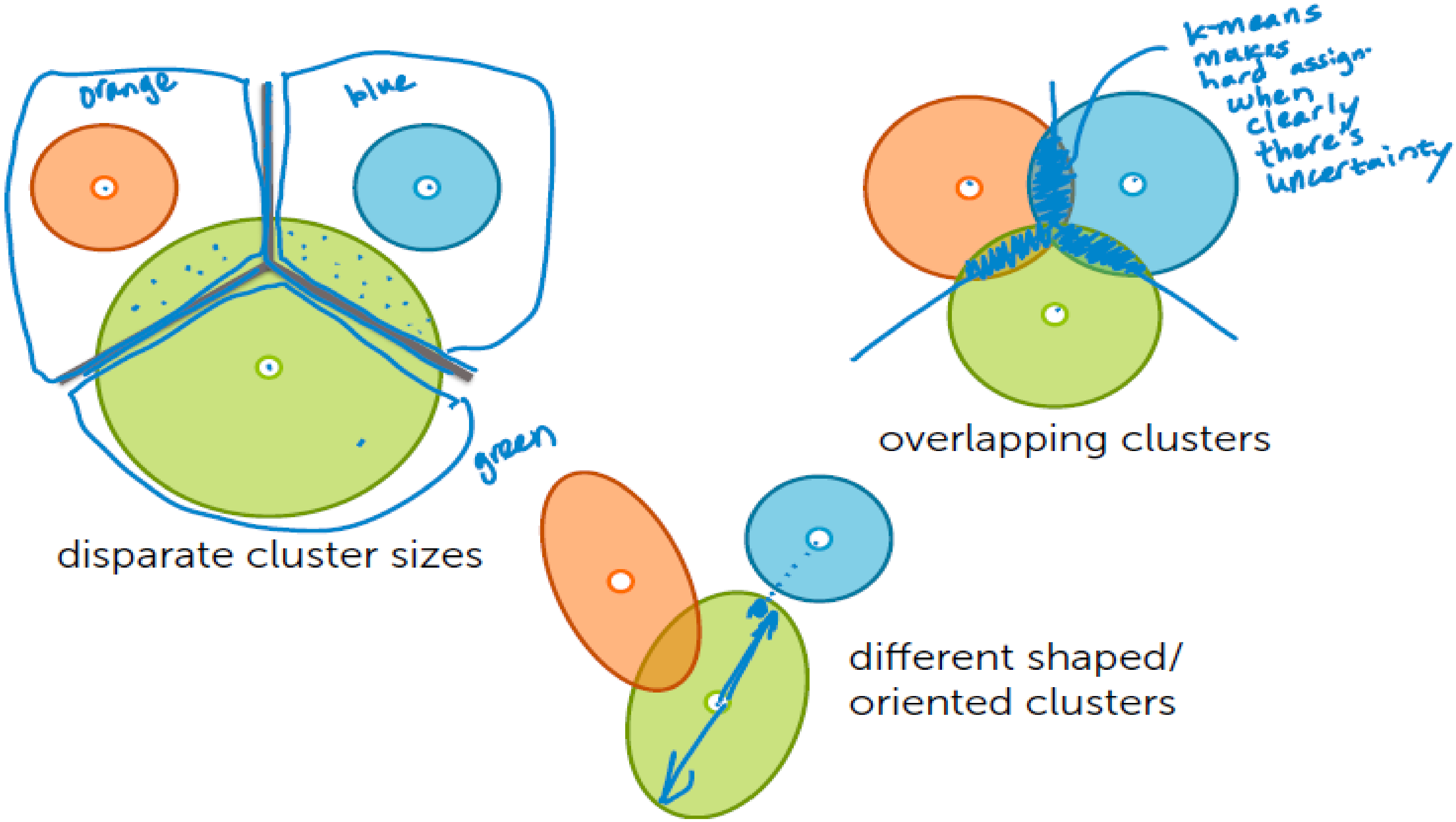
Still assumes all clusters have the same axis-aligned ellipses



# Why probabilistic approach?



## Failure modes of k-means



# Mixture models



- Provides **soft assignments** of observations to clusters (uncertainty in assignment)
  - e.g., 54% chance document is world news, 45% science, 1% sports, and 0% entertainment
- Accounts for cluster shapes not just centers
- Enables learning weightings of dimensions
  - e.g., how much to weight each word in the vocabulary when computing cluster assignment

# Application: clustering images



Discover groups of similar images

- Ocean
- Pink flower
- Dog
- Sunset
- Clouds
- ...

# Application: clustering images



## Simple image representation

Consider average red, green, blue pixel intensities

[R = 0.05, G = 0.7, B = 0.9]

[R = 0.85, G = 0.05, B = 0.35]

[R = 0.02, G = 0.95, B = 0.4]

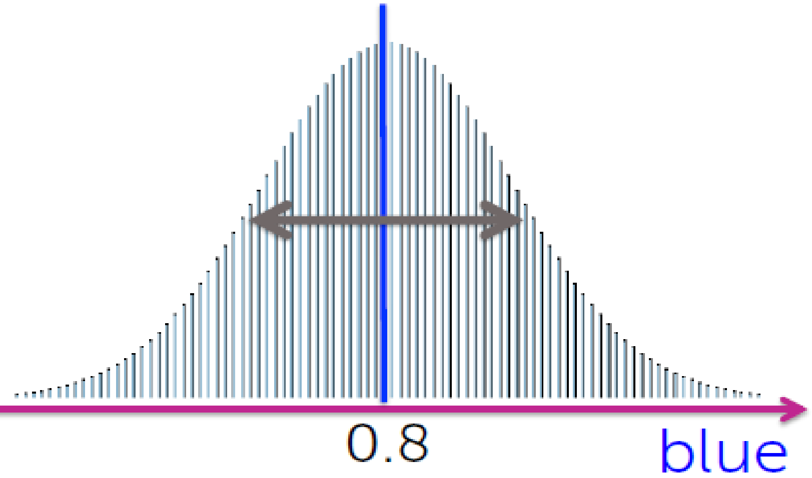
**Single RGB vector per image**

# Application: clustering images



## Distribution over all cloud images

Let's look at just the blue dimension

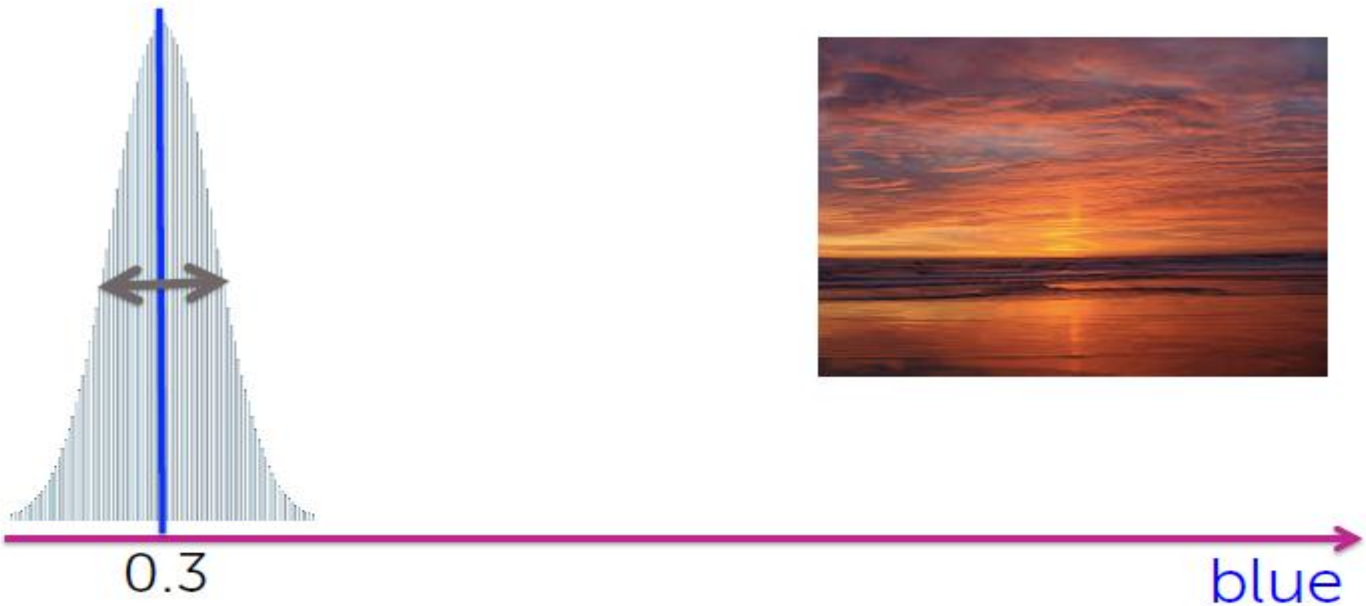


# Application: clustering images



## Distribution over all sunset images

Let's look at just the blue dimension

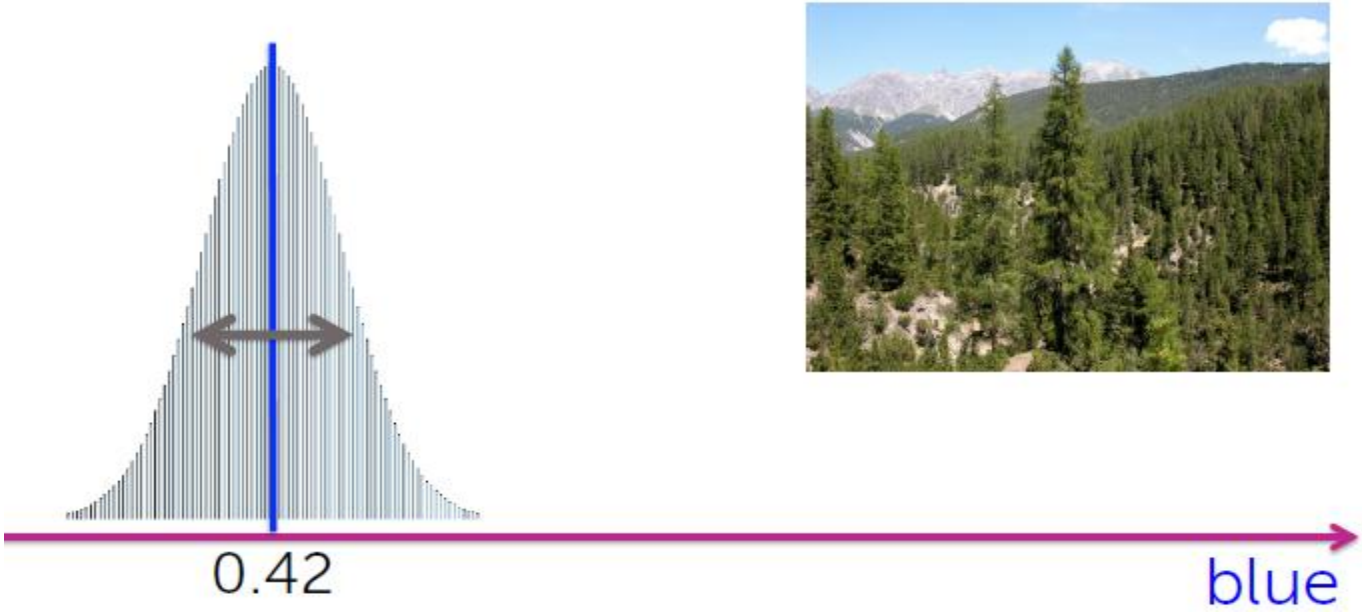


# Application: clustering images



## Distribution over all forest images

Let's look at just the blue dimension



# Application: clustering images



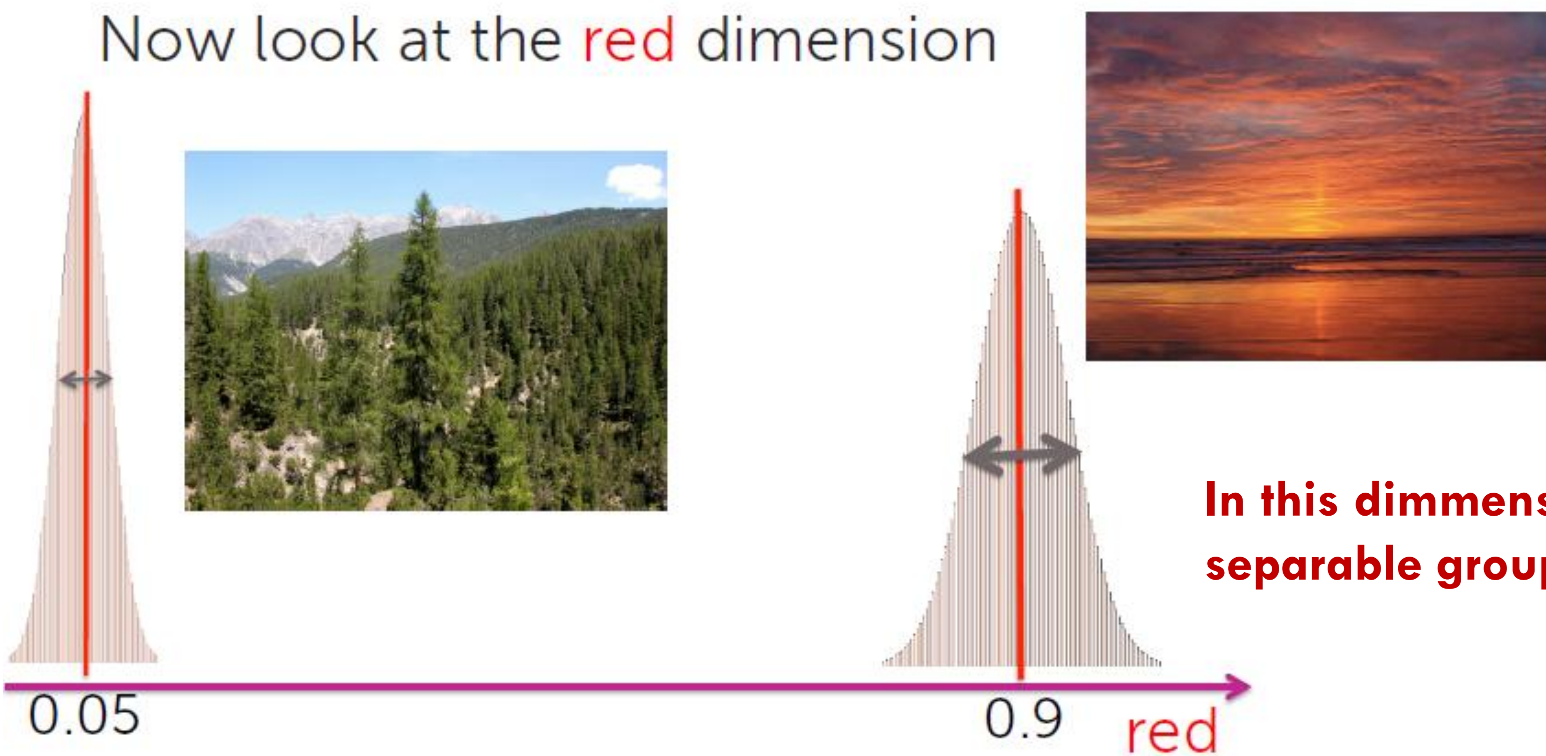
## Distribution over all images

**We see that they are grouping!**
**But not easy to distinguish between groups**

# Application: clustering images



## Can be distinguished along other dim

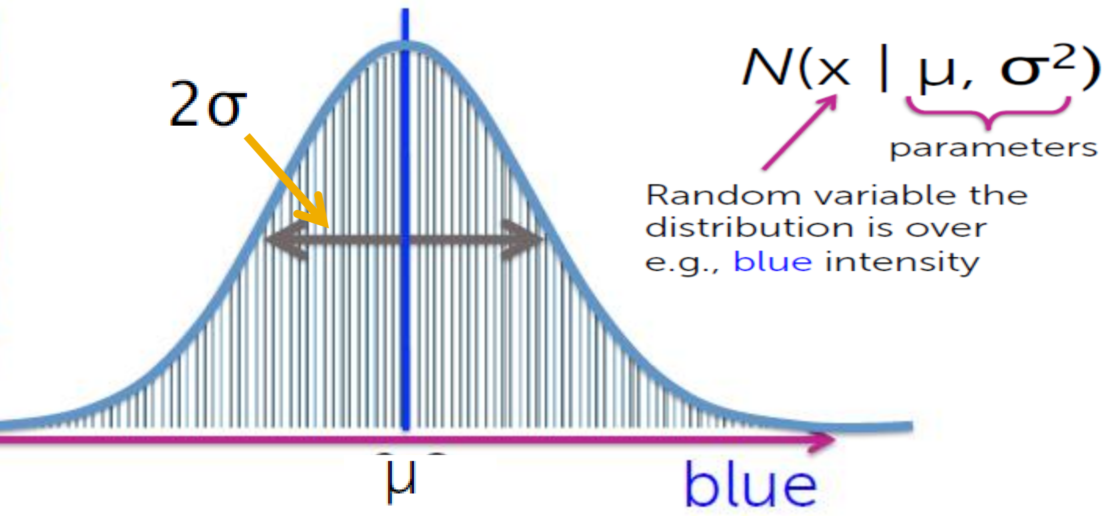



**In this dimmension separable groups!**

# Model for a given image type



For **each dimension** of the [R, G, B] vector, and **each image type**, assume a Gaussian distribution over color intensity

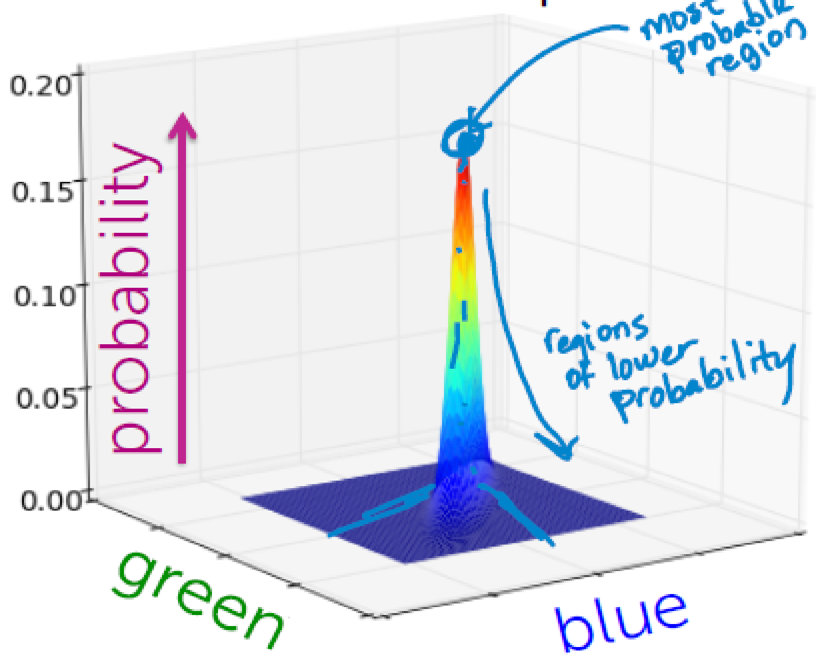


# Model for a given image type

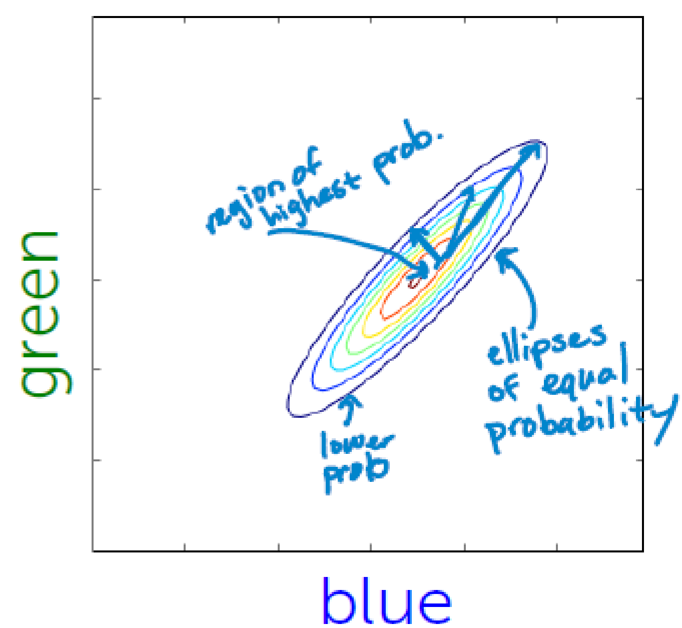


## 2D Gaussians – Bird's eye view

3D mesh plot




Contour plot



# Application: clustering images

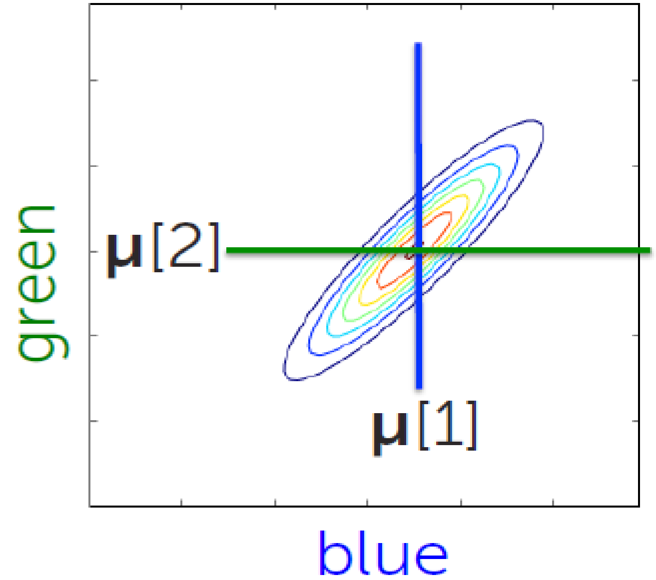


## 2D Gaussians – Parameters

Fully specified by **mean μ** and **covariance Σ**

$\boldsymbol{\mu} = [\mu_{blue} \, , \, \mu_{green}]$

mean centers the distribution in 2D



# Application: clustering images



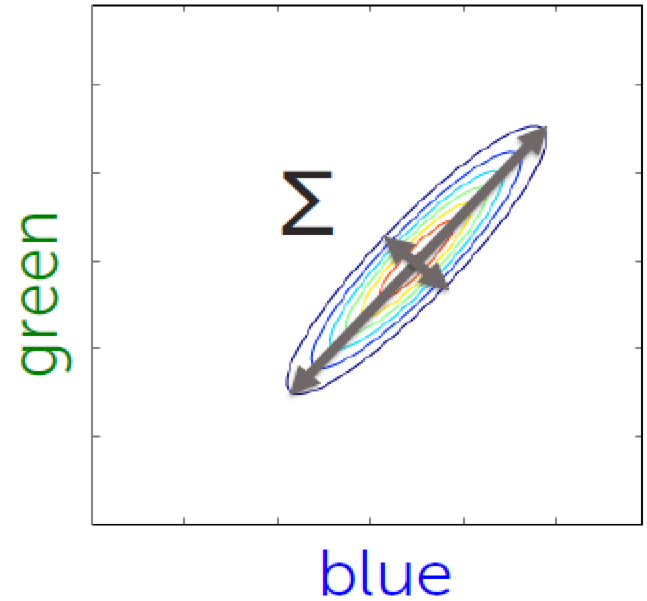
## 2D Gaussians – Parameters

Fully specified by **mean** μ and **covariance** Σ

$$\boldsymbol{\mu} = [\mu_{blue}, \mu_{green}]$$

$$\Sigma = \begin{pmatrix} \sigma_{blue}^2 & \sigma_{blue,green} \\ \sigma_{green,blue} & \sigma_{green}^2 \end{pmatrix}$$

covariance determines
orientation + spread

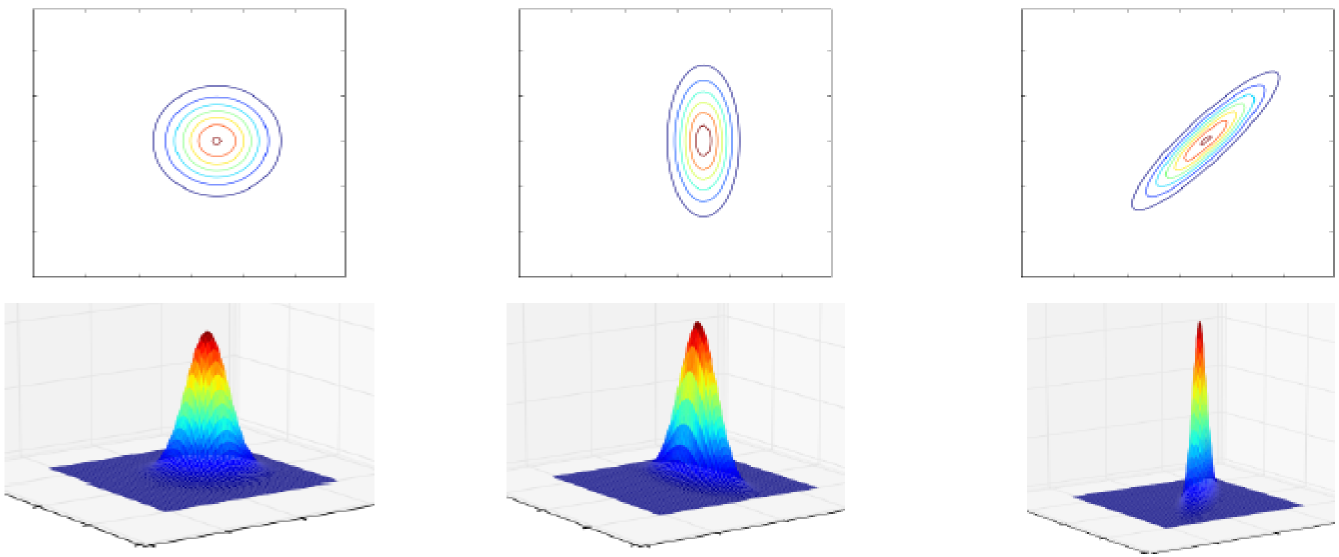


# Application: clustering images



## Covariance structures

$$\Sigma = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_B{}^2 & 0 \\ 0 & \sigma_G{}^2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \sigma_B{}^2 & \sigma_{B,G} \\ \sigma_{G,B} & \sigma_G{}^2 \end{pmatrix}$$



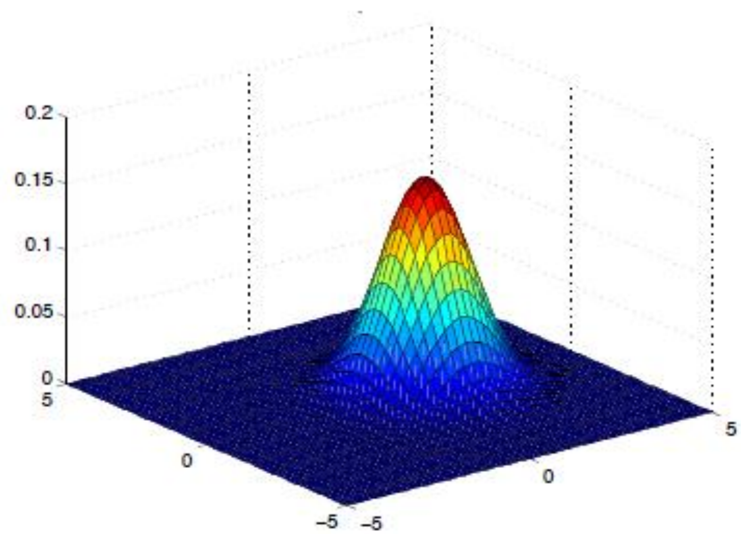
# Application: clustering images



## Notating a multivariate Gaussian

$$N(\mathbf{x} \mid \underbrace{\boldsymbol{\mu}, \Sigma}_{\text{parameters}})$$

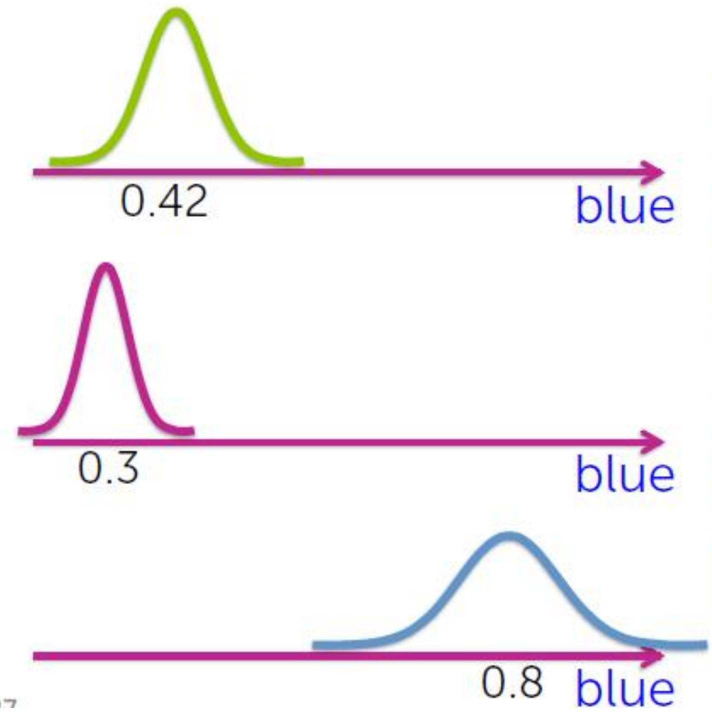
Random vector
e.g., [R, G, B] intensities



# Mixture of Gaussians



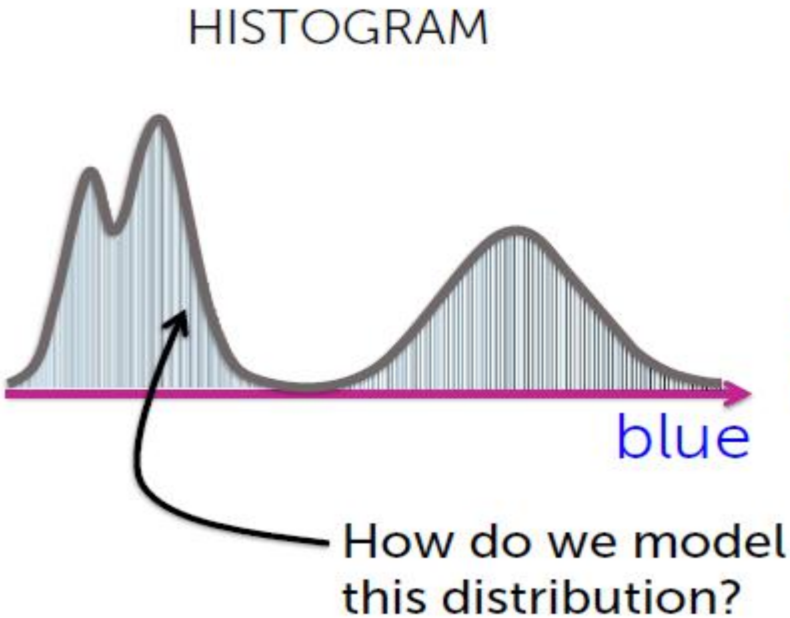
Model as Gaussian per category/cluster




# Mixture of Gaussians



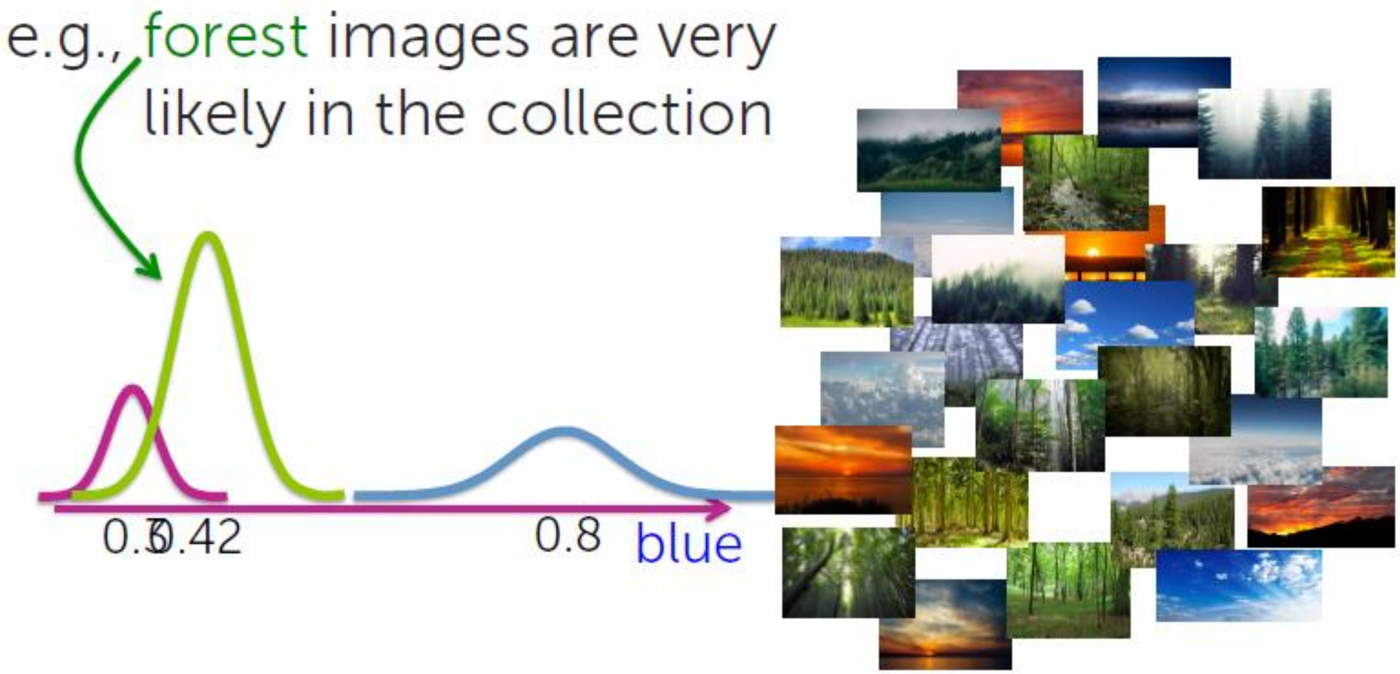
## Jumble of unlabeled images




# Mixture of Gaussians



What if image types not equally represented?

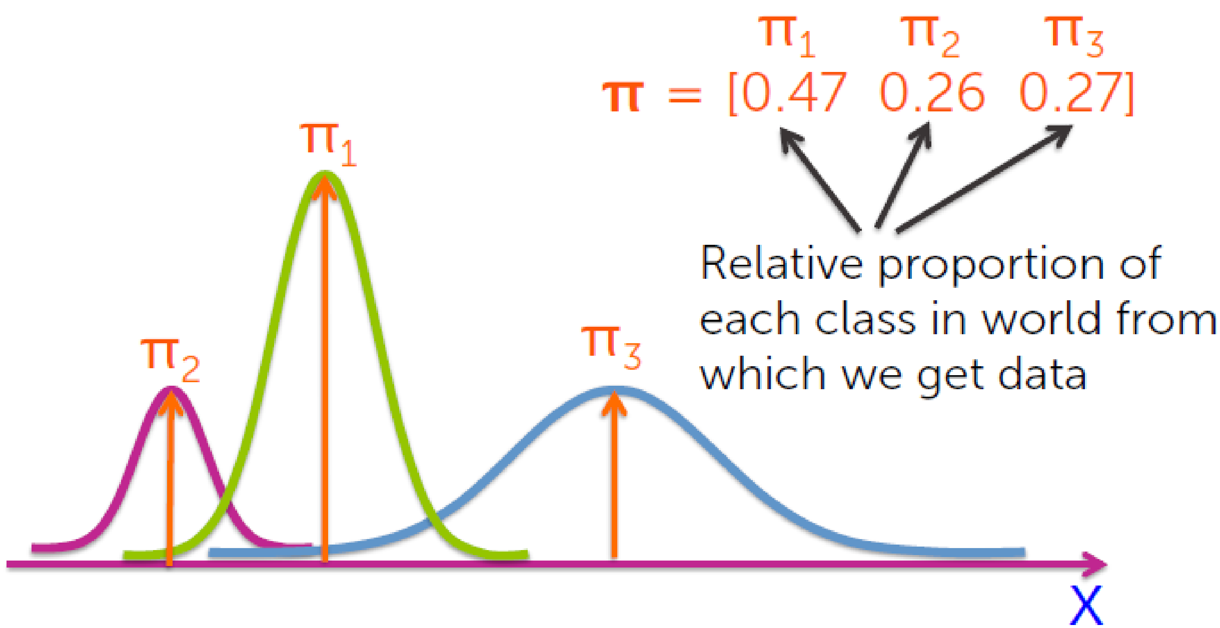


# Mixture of Gaussians



## Combination of weighted Gaussians

Associate a weight $\pi_k$ with each Gaussian component



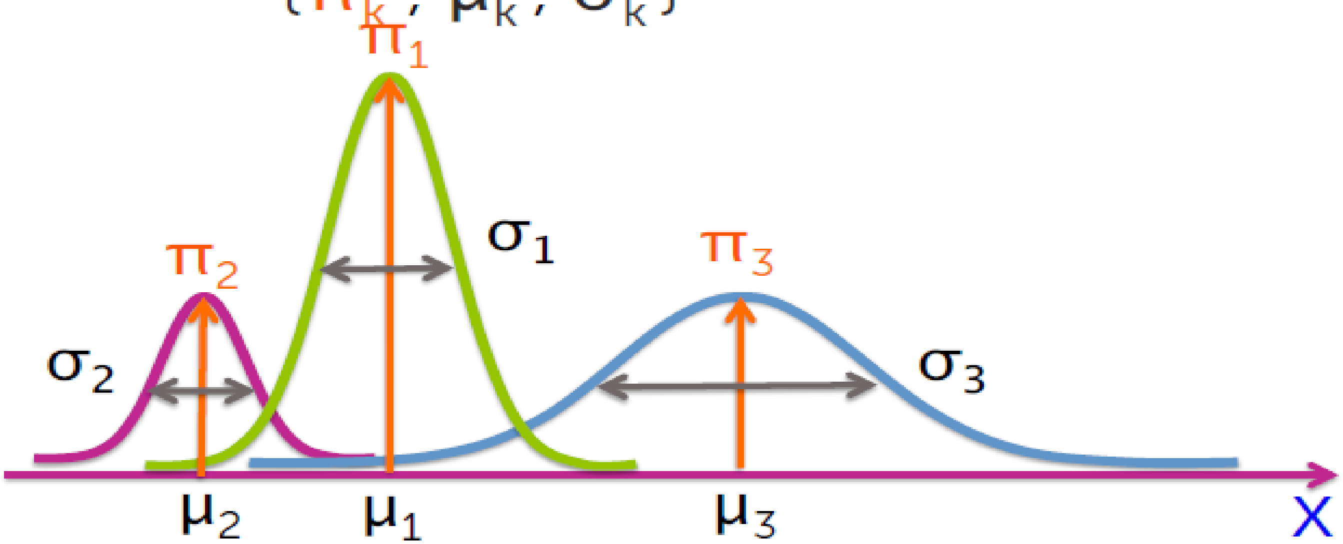

$$0 \leq \pi_k \leq 1$$

$$\sum_{k=1}^{K} \pi_k = 1$$

## Mixture of Gaussians (1D)

Each mixture component represents a unique cluster specified by:

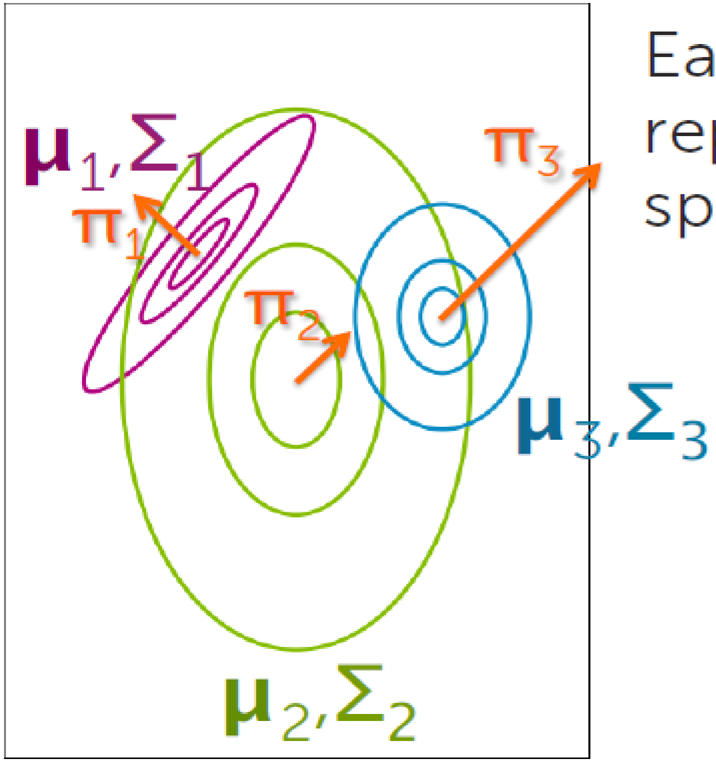
$\{\pi_k, \mu_k, \sigma_k^2\}$



# Mixture of Gaussians



## Mixture of Gaussians (general)




Each mixture component represents a unique cluster specified by:

$$\{\pi_k , \boldsymbol{\mu}_k , \Sigma_k\}$$

# Mixture of Gaussians



## According to the model...

Without observing the image content, what's the probability it's from cluster k? (e.g., prob. of seeing "clouds" image)

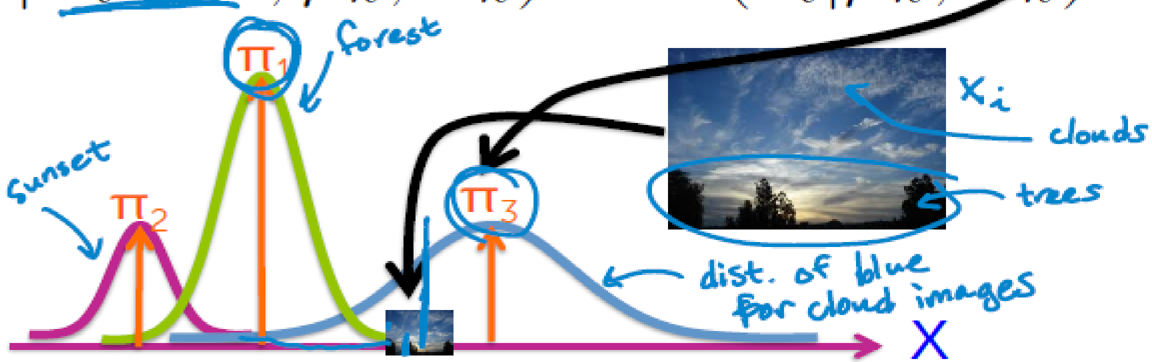
cluster assignment for obs. $x_i$

$$p(z_i = k) = \pi_k$$ prior

Given observation $\mathbf{x}_i$ is from cluster k, what's the likelihood of seeing $\mathbf{x}_i$? (e.g., just look at distribution for "clouds")

$$p(x_i \mid z_i = k, \mu_k, \Sigma_k) = N(x_i \mid \mu_k, \Sigma_k)$$ likelihood

$[RGB]_i$



# Application: clustering documents



Discover groups of related documents

# Application: clustering documents



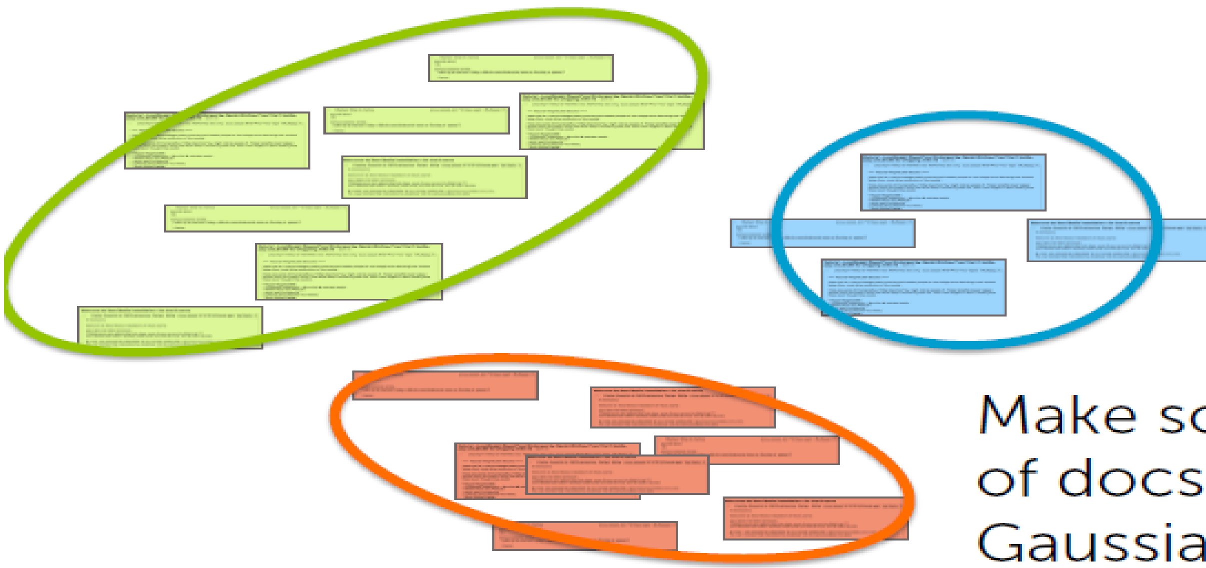
## Document representation

# Application: clustering documents



## Mixture of Gaussians for clustering documents

Space of all documents
(really lives in $\mathbf{R}^V$ for vocab size V)



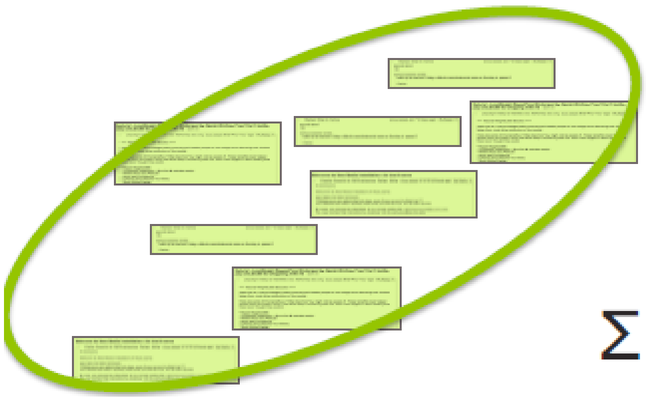
Make soft assignments of docs to each Gaussian

# Application: clustering documents



## Counting parameters

Each cluster has $\{\pi_k , \boldsymbol{\mu}_k , \Sigma_k\}$



In 2D:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} \\ \sigma_{2,1} & \sigma_2^2 \end{pmatrix}$$

# Application: clustering documents



## Counting parameters

Each cluster has $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$

In V (vocab size) dims:

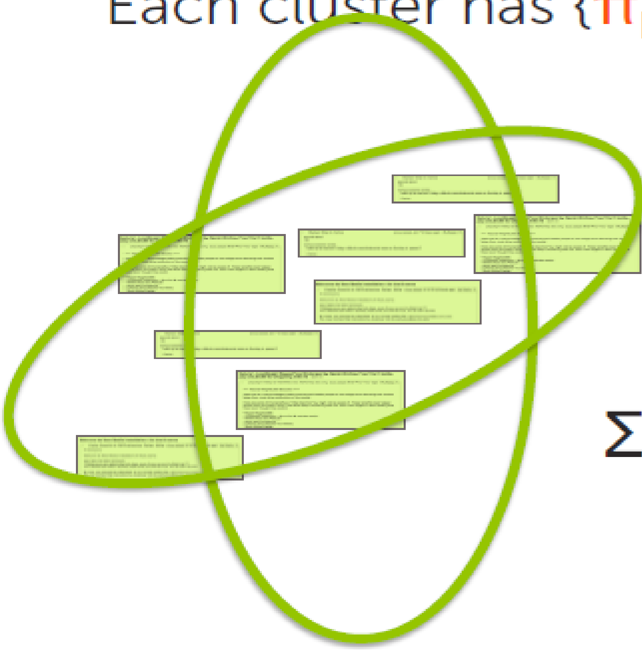
$$\Sigma = \frac{V(V+1)}{2}$$

# Application: clustering documents



## Restricting to diagonal covariance

Each cluster has $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k$ diagonal $\}$



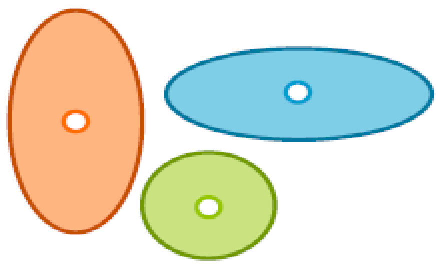
V params

$$\Sigma = \begin{pmatrix} \sigma_1^2 & & & & 0 \\ & \sigma_2^2 & & & \\ & & \sigma_3^2 & & \\ & 0 & & \ddots & \\ & & & & \sigma_V^2 \end{pmatrix}$$

# Application: clustering documents



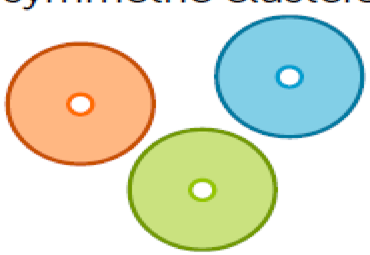
## Restrictive assumption, but…

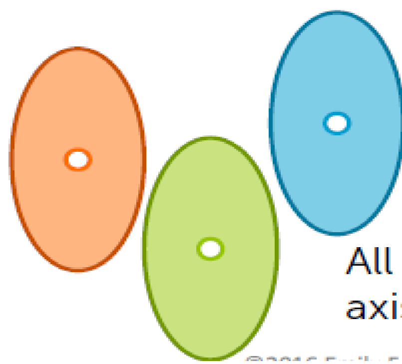


- Can **learn** weights on dimensions (e.g., weights on words in vocab)
- Can learn **cluster-specific** weights on dimensions

**Still more flexible than k-means**

Spherically symmetric clusters





**Specify weights…**

All clusters have same axis-aligned ellipses

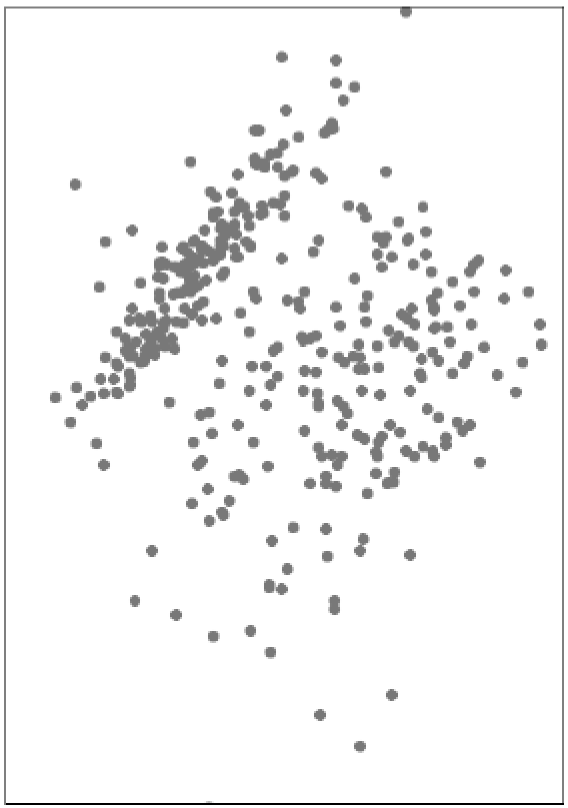
44

# Inferring soft assignments with expectation maximization (EM)

# Inferring cluster labels



## Data

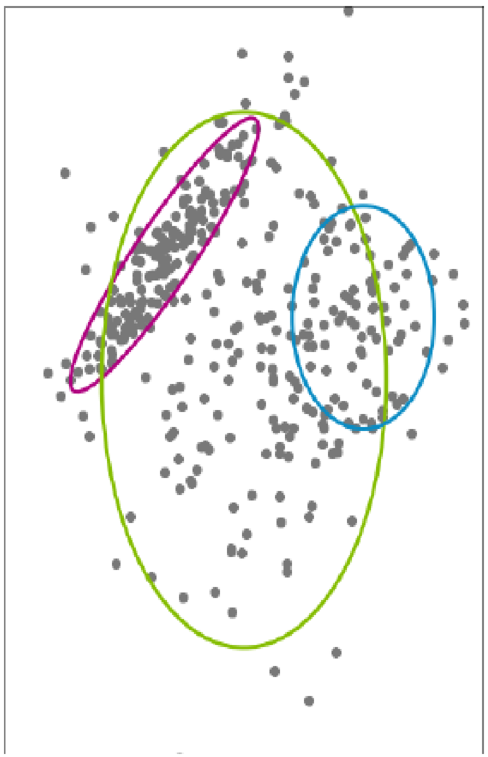


## Desired soft assignments

# What if we knew the cluster parameters $\{\pi_k , \boldsymbol{\mu}_k , \Sigma_k\}$?



## Compute responsibilities



$r_i = [r_{i1}\ r_{i2} \dots r_{iK}]$ # clusters

fixed values defining the distribution

Responsibility cluster k takes for observation i

"given"

$$r_{ik} = p(z_i = k \mid \{\pi_j , \mu_j , \Sigma_j\}_{j=1}^{K} , x_i)$$

random variable

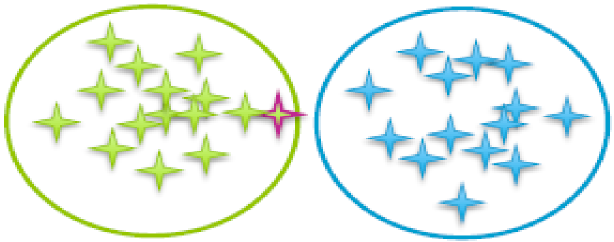
probability of assignment to cluster k

given model parameters and observed value

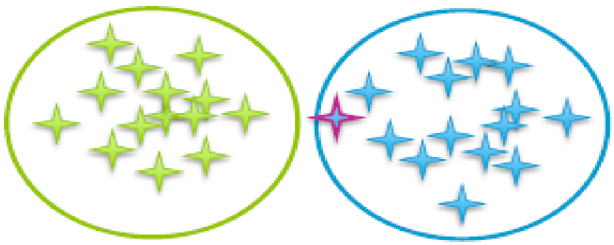
# What if we knew the cluster parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$?



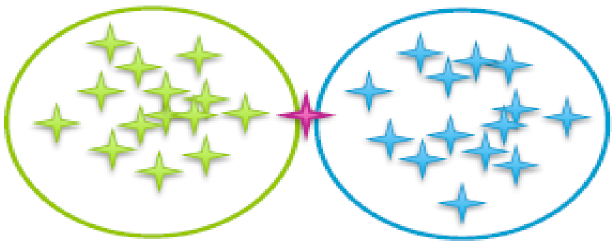
## Responsibilities in pictures



Green cluster takes more responsibility



Blue cluster takes more responsibility



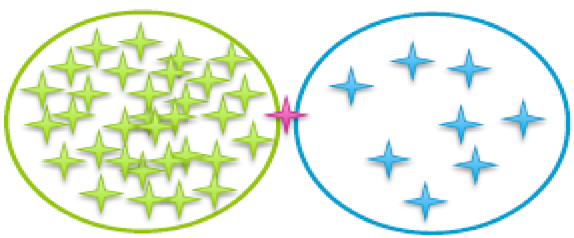
Uncertain… split responsibility

# What if we knew the cluster parameters $\{\pi_k, \mu_k, \Sigma_k\}$?



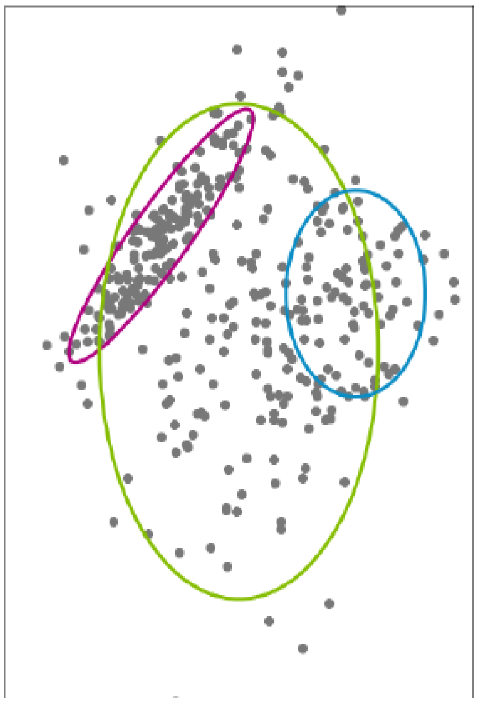
## Responsibilities in pictures

Need to weight by cluster probabilities,
not just cluster shapes



Still uncertain,
but green cluster seems
more probable…
takes more responsibility

# Responsibilities in equations

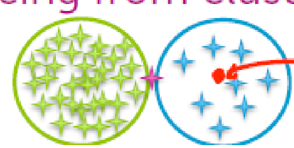


Responsibility cluster k takes for observation i

$$r_{ik} = \pi_k \, N(x_i \mid \mu_k, \Sigma_k)$$

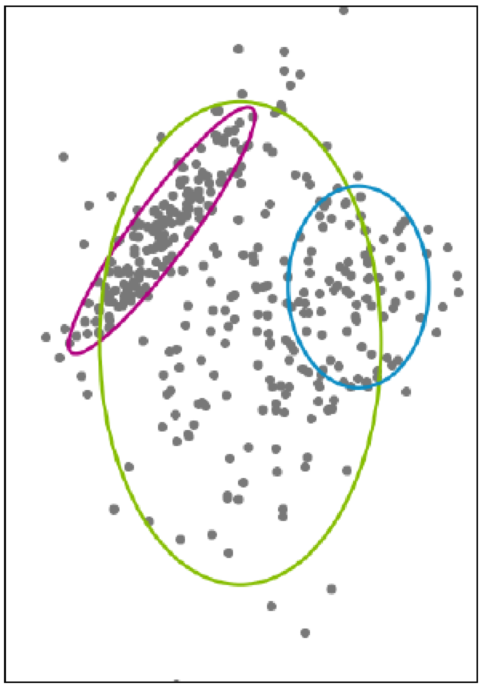
Initial probability of being from cluster k

How likely is the observed value $\mathbf{x}_i$ under this cluster assignment?



very unlikely under the green cluster, even though the prior on green is higher

# Responsibilities in equations



Responsibility cluster k takes for observation i

$$r_{ik} = \frac{\pi_k \, N(x_i \mid \mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j N(x_i \mid \mu_j, \Sigma_j)}$$

Normalized over all possible cluster assignments

# What if we knew the cluster parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$?



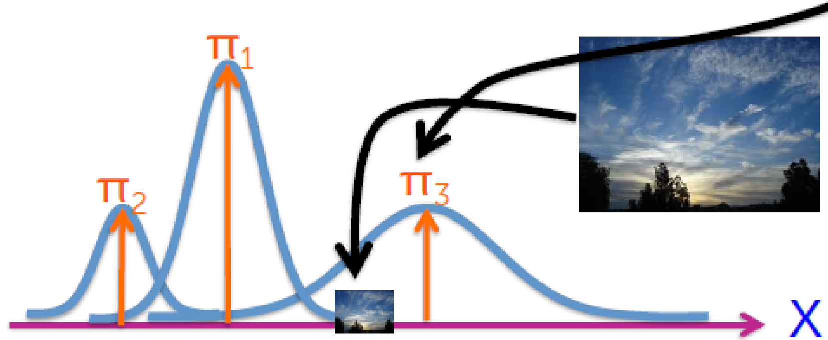
## Recall: According to the model...

Without observing the image content, what's the probability it's from cluster k? (e.g., prob. of seeing "clouds" image)

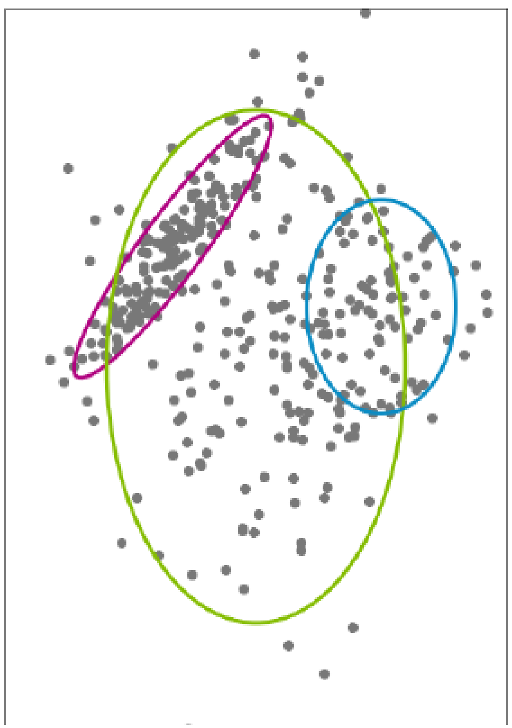
$$p(z_i = k) = \pi_k$$

Given observation $\mathbf{x}_i$ is from cluster k, what's the likelihood of seeing $\mathbf{x}_i$? (e.g., just look at distribution for "clouds")

$$p(x_i \mid z_i = k, \mu_k, \Sigma_k) = N(x_i \mid \mu_k, \Sigma_k)$$



# Part 1: Summary



Desired soft assignments (responsibilities) are **easy** to compute when cluster parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$ are known

**But, we don't know these!**

# Imagine we knew the cluster (hard) assignments $z_i$



## Estimating cluster parameters

Imagine we know the cluster assignments

**Estimation problem decouples across clusters**

Is green point informative of fuchsia cluster parameters?

**NO!**

# Imagine we knew the cluster (hard) assignments $z_i$



## Data table decoupling over clusters

| R | G | B | Cluster |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 3 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 3 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 3 |
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 1 |
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 2 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 2 |

**Then split into separate tables and consider them independently.**

# Imagine we knew the cluster (hard) assignments $z_i$



## Maximum likelihood estimation

| R | G | B | Cluster |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 3 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 3 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 3 |

Estimate $\{\pi_k , \boldsymbol{\mu}_k , \Sigma_k\}$ given data assigned to cluster k

maximum likelihood estimation (MLE)

Find parameters that maximize the score, or *likelihood*, of data

# Imagine we knew the cluster (hard) assignments $z_i$



## Mean/covariance MLE

sum these vectors

| R | G | B | Cluster |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 3 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 3 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 3 |

divide by 3 (the total # of obs.)

denotes "estimate"

$$\hat{\mu}_k = \frac{1}{N_k} \sum_{i \text{ in } k} x_i$$

← average data points in cluster k

# of obs. in cluster

$$\hat{\Sigma}_k = \frac{1}{N_k} \sum_{\underline{i \text{ in } k}} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

Scalar case: $\hat{\sigma}_k^2 = \frac{1}{N_k} \sum_{i \text{ in } k} (x_i - \hat{\mu}_k)^2$

# Imagine we knew the cluster (hard) assignments $z_i$



## Cluster proportion MLE

| R | G | B | Cluster |
|---|---|---|---|
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 1 |

| R | G | B | Cluster |
|---|---|---|---|
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 2 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 2 |

| R | G | B | Cluster |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 3 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 3 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 3 |

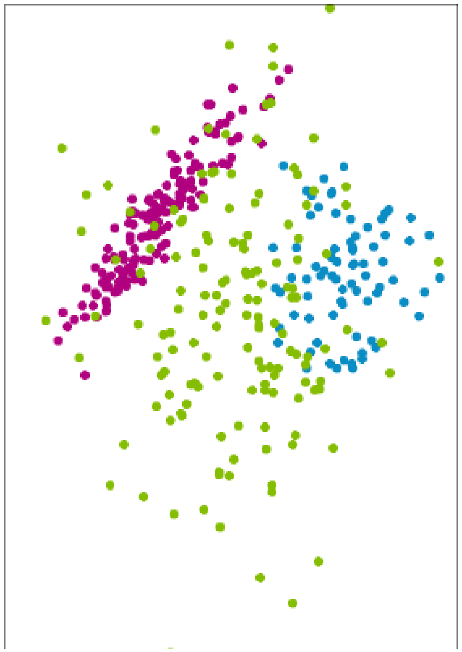
# obs in cluster k

$$\hat{\pi}_k = \frac{N_k}{N}$$

total # of obs

True for general mixtures of i.i.d. data, not just Gaussian clusters

# Part 2a : Summary

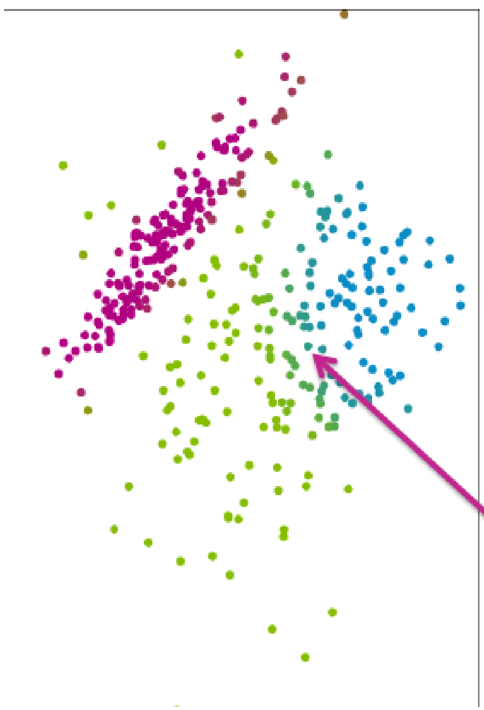


needed to compute soft assignments

Cluster parameters are simple to compute if we know the cluster assignments

**But, we don't know these!**

# Estimating cluster parameters from soft assignments



Instead of having a full observation $\mathbf{x}_i$ in cluster k, just allocate a portion $r_{ik}$

$\mathbf{x}_i$ divided across all clusters, as determined by $r_{ik}$

# Maximum likelihood estimation from soft assignments

Just like in boosting with weighted observations...

| R | G | B | $r_{i1}$ | $r_{i2}$ | $r_{i3}$ |
|---|---|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0.30 | 0.18 | 0.52 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 0.01 | 0.26 | 0.73 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 0.002 | 0.008 | 0.99 |
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 0.75 | 0.10 | 0.15 |
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 0.05 | 0.93 | 0.02 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 0.13 | 0.86 | 0.01 |

52% chance this obs is in cluster 3

| Total weight in cluster: (effective # of obs) | | | |
|---|---|---|---|
| | **1.242** | **2.8** | **2.42** |

# What can we do with just soft assignments $r_{ij}$?



## Maximum likelihood estimation from soft assignments

| R | G | B | Cluster 1 weights |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0.30 |
| $x_2[1]$ | | | |
| $x_3[1]$ | | | |
| $x_4[1]$ | | | |
| $x_5[1]$ | | | |
| $x_6[1]$ | | | |

| R | G | B | Cluster 2 weights |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0.18 |
| $x_2[1]$ | | | |
| $x_3[1]$ | | | |
| $x_4[1]$ | | | |
| $x_5[1]$ | | | |
| $x_6[1]$ | | | |

| R | G | B | Cluster 3 weights |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0.52 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 0.73 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 0.99 |
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 0.15 |
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 0.02 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 0.01 |

# What can we do with just soft assignments $r_{ij}$?



## Cluster-specific location/shape MLE

| R | G | B | Cluster 1 weights |
|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0.30 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 0.01 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 0.002 |
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 0.75 |
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 0.05 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 0.13 |

$$\hat{\mu}_k = \frac{1}{N_k^{\text{soft}}} \sum_{i=1}^{N} \boxed{r_{ik}} x_i$$

$$\hat{\Sigma}_k = \frac{1}{N_k^{\text{soft}}} \sum_{i=1}^{N} \boxed{r_{ik}} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

$$\boxed{N_k^{\text{soft}} = \sum_{i=1}^{N} r_{ik}}$$

Total weight in cluster k
= effective # obs

Compute cluster parameter estimates with weights on each row operation

# What can we do with just soft assignments $r_{ij}$?



## MLE of cluster proportions $\hat{\pi}_k$

| $r_{i1}$ | $r_{i2}$ | $r_{i3}$ |
|---|---|---|
| 0.30 | 0.18 | 0.52 |
| 0.01 | 0.26 | 0.73 |
| 0.002 | 0.008 | 0.99 |
| 0.75 | 0.10 | 0.15 |
| 0.05 | 0.93 | 0.02 |
| 0.13 | 0.86 | 0.01 |

Total weight in cluster:

| | | |
|---|---|---|
| 1.242 | 2.8 | 2.42 |

Total weight in dataset: 6

# datapoints N

$$\hat{\pi}_k = \frac{N_k^{\text{soft}}}{N}$$

$$N_k^{\text{soft}} = \sum_{i=1}^{N} r_{ik}$$

Total weight in cluster k = effective # obs

Estimate cluster proportions from relative weights

# What can we do with just soft assignments $r_{ij}$?



## Defaults to hard assignment case when $r_{ij}$ in {0,1}

Hard assignments have:

$$r_{ik} = \begin{cases} 1 & i \text{ in } k \\ 0 & \text{otherwise} \end{cases}$$

| R | G | B | $r_{i1}$ | $r_{i2}$ | $r_{i3}$ |
|---|---|---|---|---|---|
| $x_1[1]$ | $x_1[2]$ | $x_1[3]$ | 0 | 0 | 1 |
| $x_2[1]$ | $x_2[2]$ | $x_2[3]$ | 0 | 0 | 1 |
| $x_3[1]$ | $x_3[2]$ | $x_3[3]$ | 0 | 0 | 1 |
| $x_4[1]$ | $x_4[2]$ | $x_4[3]$ | 1 | 0 | 0 |
| $x_5[1]$ | $x_5[2]$ | $x_5[3]$ | 0 | 1 | 0 |
| $x_6[1]$ | $x_6[2]$ | $x_6[3]$ | 0 | 1 | 0 |
| Total weight in cluster: | | | **1** | **2** | **3** |

One-hot encoding of cluster assignment

# What can we do with just soft assignments $r_{ij}$?



## Equating the estimates...

$$\hat{\pi}_k = \frac{N_k^{\text{soft}}}{N} \longleftarrow \boxed{N_k^{\text{soft}} = \sum_{i=1}^{N} r_{ik}}$$

if {0,1}
just count
obs i in cluster
k if $r_{ik}=1$
$= N_k$ ✓

$$\hat{\mu}_k = \frac{1}{N_k^{\text{soft}}} \sum_{i=1}^{N} r_{ik} x_i$$

only add $x_i$ if i in k ($r_{ik}=1$)

$\rightarrow \frac{1}{N_k} \sum_{i \text{ in } k} x_i$ ✓

$$\hat{\Sigma}_k = \frac{1}{N_k^{\text{soft}}} \sum_{i=1}^{N} r_{ik} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$ ✓

same as above

$= \frac{1}{N_k} \sum_{i \text{ in } k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$

# Part 2b: Summary

Still straightforward to compute cluster parameter estimates from soft assignments

# Expectation maximization (ME)



## An iterative algorithm

Motivates an iterative algorithm:

1. **E-step:** estimate cluster responsibilities given current parameter estimates

$$\hat{r}_{ik} = \frac{\hat{\pi}_k N(x_i \mid \hat{\mu}_k, \hat{\Sigma}_k)}{\sum_{j=1}^{K} \hat{\pi}_j N(x_i \mid \hat{\mu}_j, \hat{\Sigma}_j)}$$

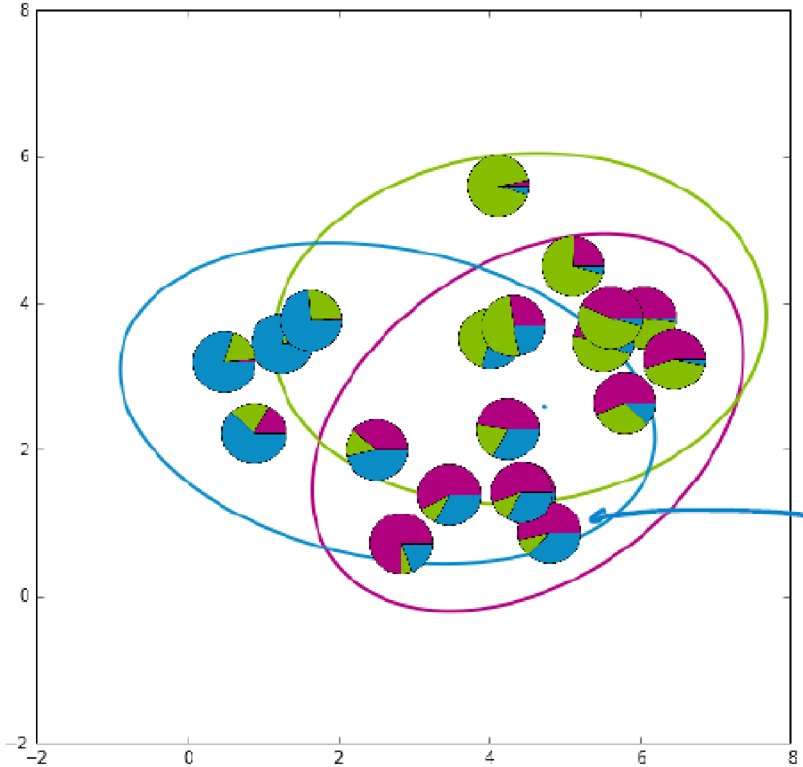
2. **M-step:** maximize likelihood over parameters given current responsibilities

$$\hat{\pi}_k, \hat{\mu}_k, \hat{\Sigma}_k \mid \{\hat{r}_{ik}, x_i\}$$

# Expectation maximization (ME)



## EM for mixtures of Gaussians in pictures – initialization




Initialize

iter counter

$\{\pi_k^{(0)}, \hat{\mu}_k^{(0)}, \hat{\Sigma}_k^{(0)}\}$

Then compute

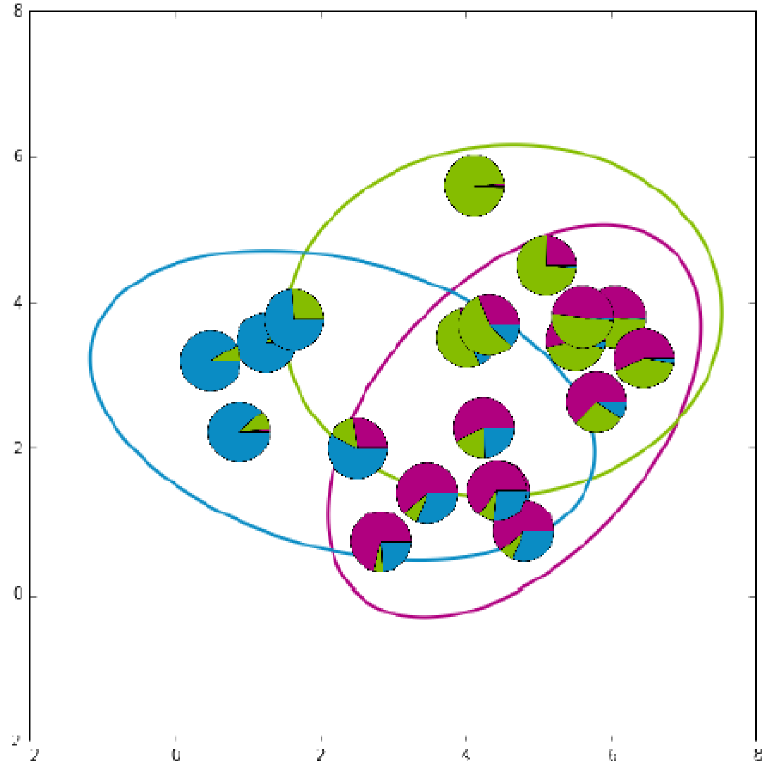
$\hat{r}_{ik}^{(1)}$

$$\hat{r}_i^{(1)} = \begin{array}{ccc} \text{fuchsia} & \text{blue} & \text{green} \\ \end{array}$$
$$[0.52 \quad 0.4 \quad 0.08]$$

# Expectation maximization (ME)



EM for mixtures of Gaussians
in pictures – after 1st iteration




Maximize likelihood given soft assign. $r_{ik}^{(1)}$

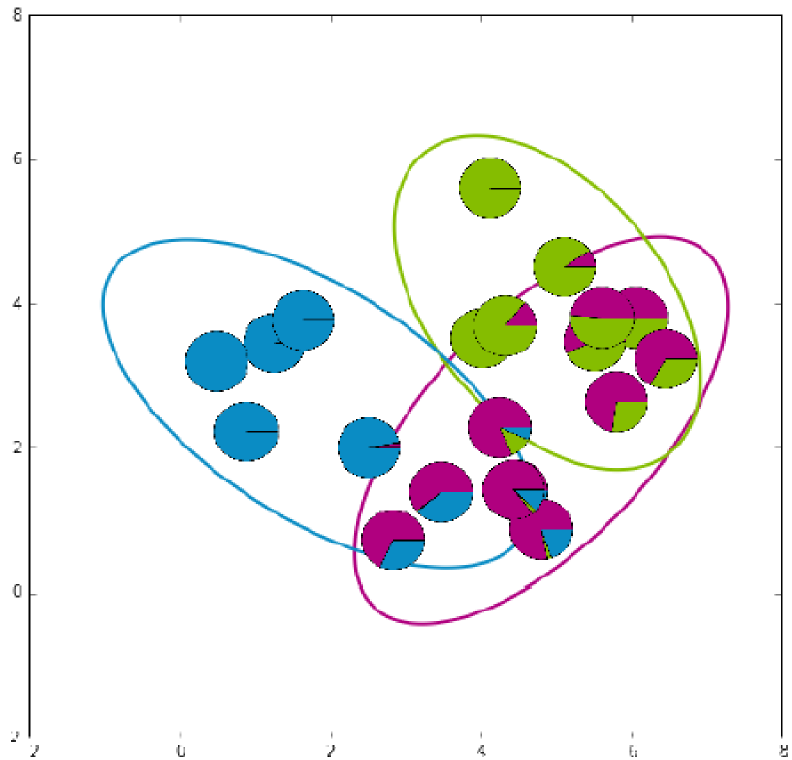
$\rightarrow \{\hat{\pi}_k^{(1)}, \hat{\mu}_k^{(1)}, \hat{\Sigma}_k^{(1)}\}$

Then recompute responsibilities $\hat{r}_{ik}^{(2)}$

# Expectation maximization (ME)



EM for mixtures of Gaussians
in pictures – after 2nd iteration

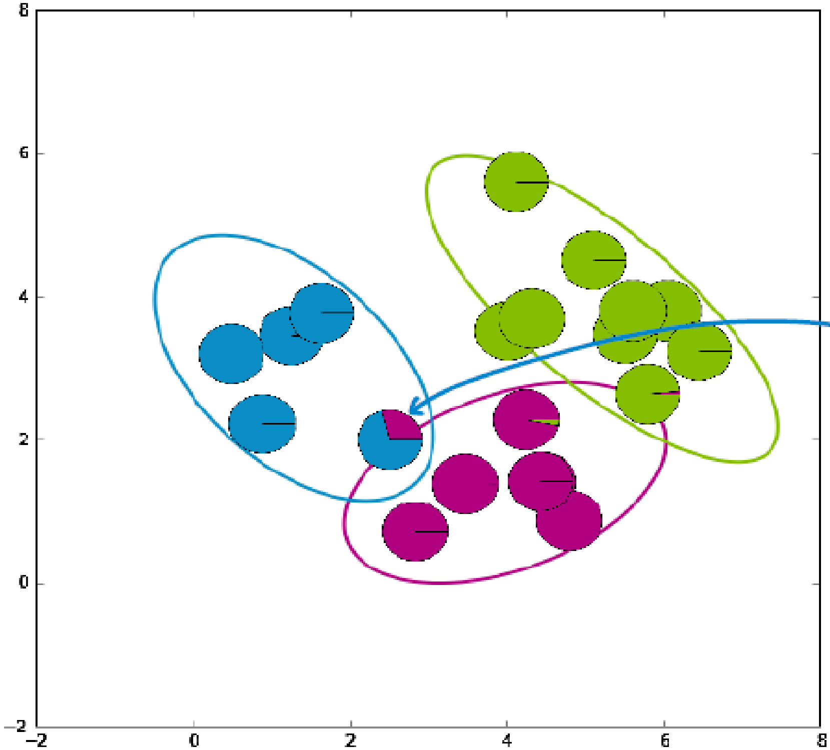



rinse
+
repeat
until convergence

# Expectation maximization (ME)



## EM for mixtures of Gaussians in pictures – converged solution

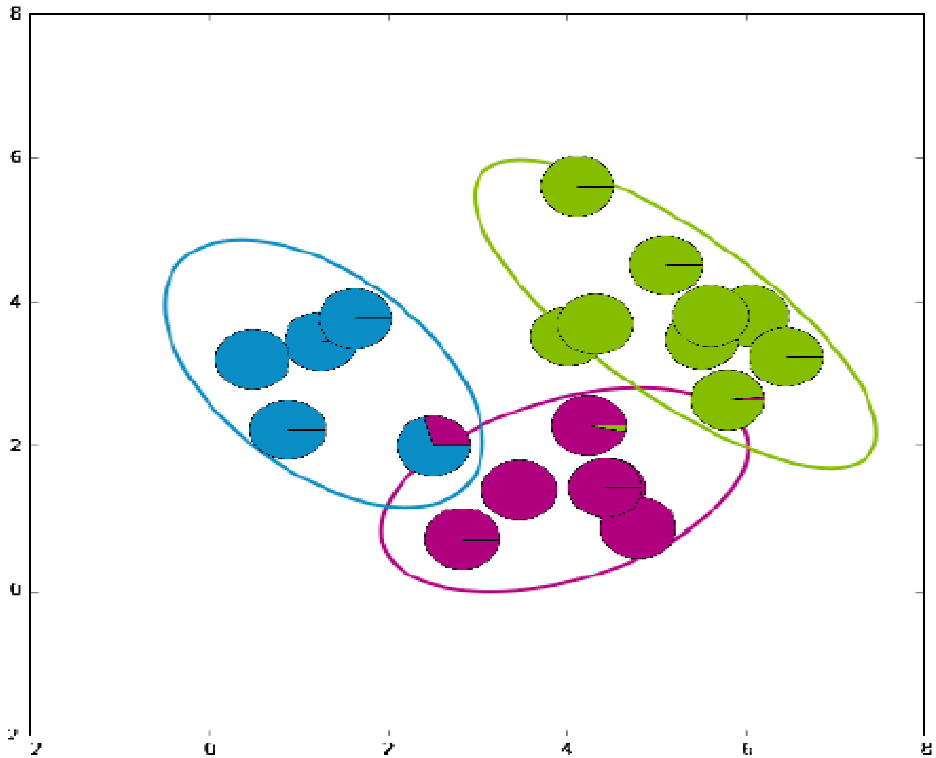



Clearly see uncertainty in assignment of obs. to blue or fuchsia cluster, even in final assignments.

# Expectation maximization (ME)



EM for mixtures of Gaussians
in pictures - replay



# Expectation maximization (ME)



## Convergence of EM

- EM is a coordinate-ascent algorithm
  - Can equate E-and M-steps with alternating maximizations of an objective function
- Convergences to a local mode

- We will assess via (log) likelihood of data under current parameter and responsibility estimates

# Expectation maximization (ME)



## Initialization

- Many ways to initialize the EM algorithm
- Important for convergence rates and quality of local mode found
- Examples:
  - Choose K observations at random to define K "centroids". Assign other observations to nearest centriod to form initial parameter estimates.
  - Pick centers sequentially to provide good coverage of data like in k-means++
  - Initialize from k-means solution
  - Grow mixture model by splitting (and sometimes removing) clusters until K clusters are formed

# Expectation maximization (ME)

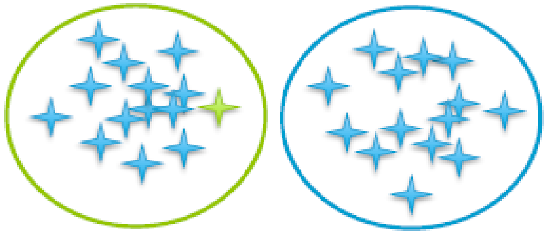


## Overfitting of MLE

Maximizing likelihood can overfit to data

Imagine at K=2 example with one obs assigned to cluster 1 and others assigned to cluster 2

- What parameter values maximize likelihood?



Set center equal to point and shrink variance to 0

Likelihood goes to ∞ !

# Expectation maximization (ME)



## Overfitting in high dims

**Doc-clustering example:**
Imagine only 1 doc assigned to cluster k has word w
(or all docs in cluster agree on count of word w)

Likelihood maximized by setting $\boldsymbol{\mu}_k[w] = \mathbf{x}_i[w]$ and $\sigma^2_{w,k} = 0$

Likelihood of any doc with different count on word w being in cluster k is 0!

# Expectation maximization (ME)



## Simple regularization of M-step for mixtures of Gaussians

Simple fix: Don’t let variances → 0!

Add small amount to diagonal of covariance estimate

Alternatively, take Bayesian approach and place prior on parameters.

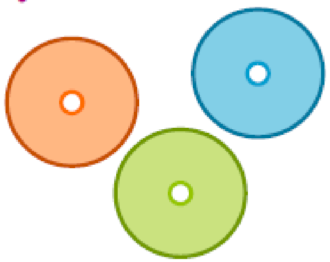
Similar idea, but all parameter estimates are “smoothed” via cluster pseudo-observations.

## Relationship to k-means

Consider Gaussian mixture model with

$$\Sigma = \begin{pmatrix} \sigma^2 & & & \\ & \sigma^2 & & \\ & & \sigma^2 & \\ & & & \ddots \end{pmatrix}$$

Spherically symmetric clusters



and let the variance parameter $\sigma \rightarrow 0$

**Datapoint gets fully assigned to nearest center, just as in k-means**

- Spherical clusters with equal variances, so relative likelihoods just function of distance to cluster center
- As variances→0, likelihood ratio becomes 0 or 1
- Responsibilities weigh in cluster proportions, but dominated by likelihood disparity

$$\hat{r}_{ik} = \frac{\hat{\pi}_k N(x_i \mid \hat{\mu}_k, \sigma^2 I)}{\sum_{j=1}^{K} \hat{\pi}_j N(x_i \mid \hat{\mu}_j, \sigma^2 I)}$$

# Expectation maximization (ME)



## Infinitesimally small variance EM = k-means

1. **E-step:** estimate cluster responsibilities given current parameter estimates

$$\hat{r}_{ik} = \frac{\hat{\pi}_k N(x_i \mid \hat{\mu}_k, \sigma^2 I)}{\sum_{j=1}^{K} \hat{\pi}_j N(x_i \mid \hat{\mu}_j, \sigma^2 I)} \in \{0, 1\}$$

Infinitesimally small

Decision based on distance to nearest cluster center

2. **M-step:** maximize likelihood over parameters given current responsibilities (hard assignments!)

$$\hat{\pi}_k, \hat{\mu}_k \mid \{\hat{r}_{ik}, x_i\}$$

# What you can do now …



- Interpret a probabilistic model-based approach to clustering using mixture models
- Describe model parameters
- Motivate the utility of soft assignments and describe what they represent
- Discuss issues related to how the number of parameters grow with the number of dimensions
  - Interpret diagonal covariance versions of mixtures of Gaussians
- Compare and contrast mixtures of Gaussians and k-means
- Implement an EM algorithm for inferring soft assignments and cluster parameters
  - Determine an initialization strategy
  - Implement a variant that helps avoid overfitting issues

# Mixed membership models for documents

# Clustering model



So far, clustered articles into groups


Doc labeled with a topic assignment

**Clustering goal:** discover groups of related docs

# Clustering model



## Are documents about just one thing?

# Clustering model



## Soft assignments capture uncertainty


Soft assignment $r_{ik}$ tells us this doc could be about world news **or** science

**But,** clustering model still specifies each doc belongs to **1 topic**

# Soft assignments




Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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[a]Department of Bioengineering, University of Pennsylvania, Philadelphia, PA
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**Abstract**

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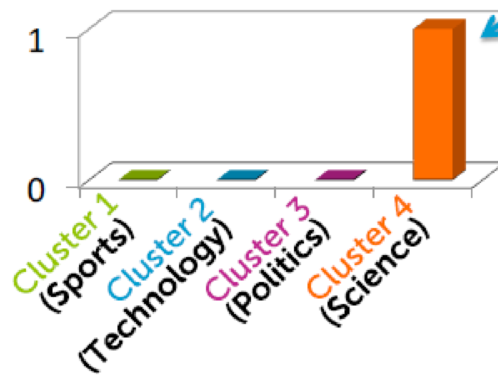
*Keywords:* Bayesian nonparametric, EEG, factorial hidden Markov model, graphical model, time series

**1. Introduction**

Despite over three decades of research, we still have very little idea of what defines a seizure. This ignorance stems both from the complexity of epilepsy as a disease and a paucity of quantitative tools that are flexible

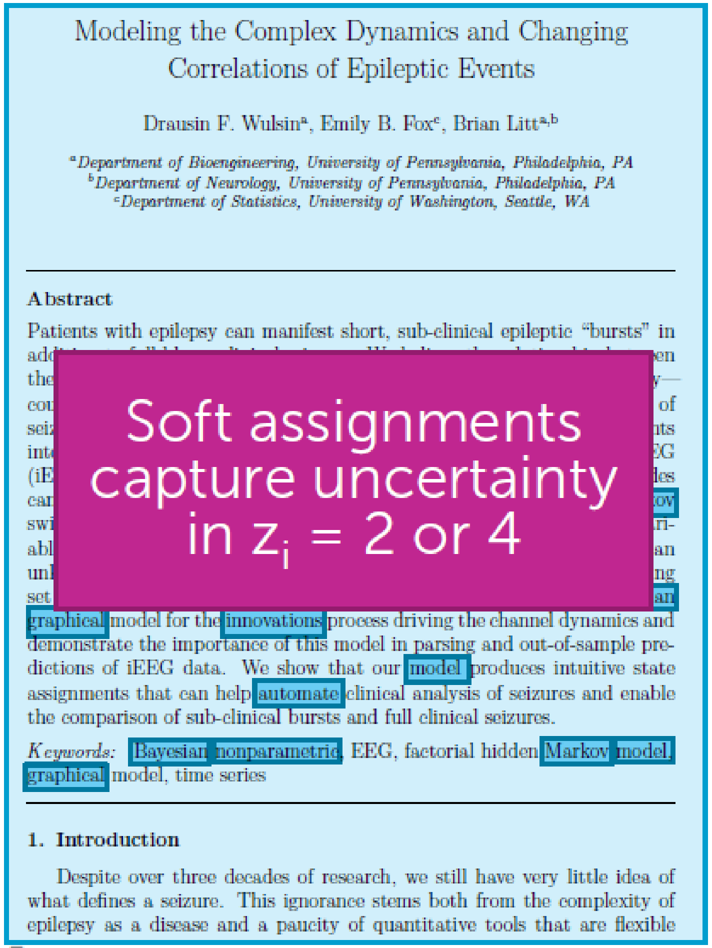
Encoding of cluster membership $z_i = 4$

Based on science related words, maybe doc in cluster 4



# Soft assignments





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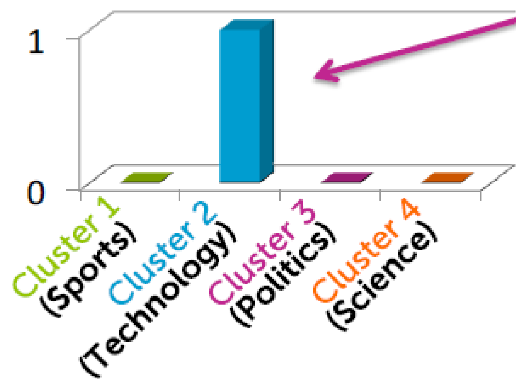
Soft assignments capture uncertainty in $z_i$ = 2 or 4

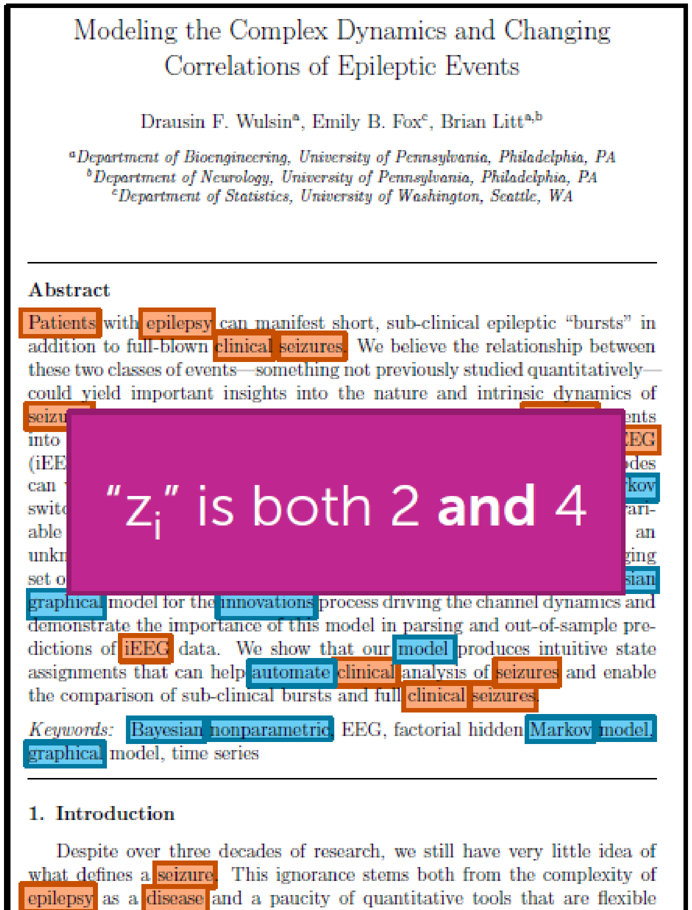
Encoding of cluster membership $z_i$ = 2

Or maybe cluster 2 (technology) is a better fit



# Soft assignments

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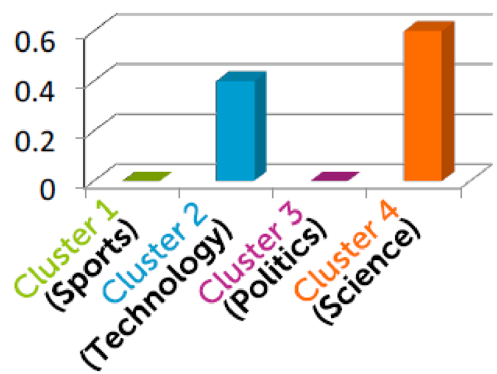
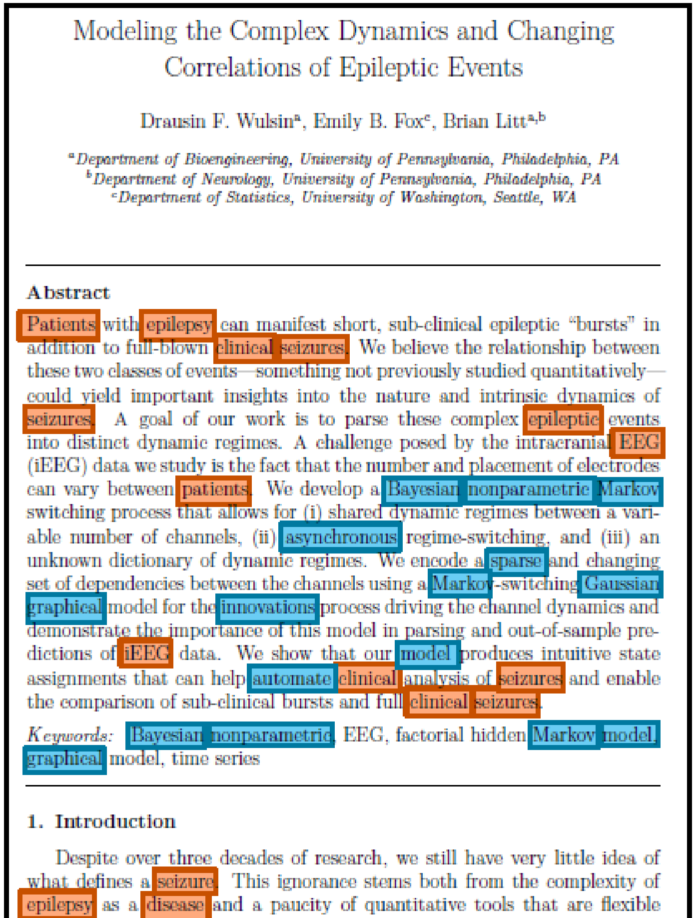
"$z_i$" is both 2 **and** 4

Really, it's about science **and** technology



# Mixed membershio models





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## Mixed membership models

Want to discover a **set** of memberships

(In contrast, cluster models aim at discovering a single membership)

# Building alternative model



## An alternative document clustering model


(Back to clustering, not mixed membership modeling)

# Building an alternative model



## So far, we have considered...

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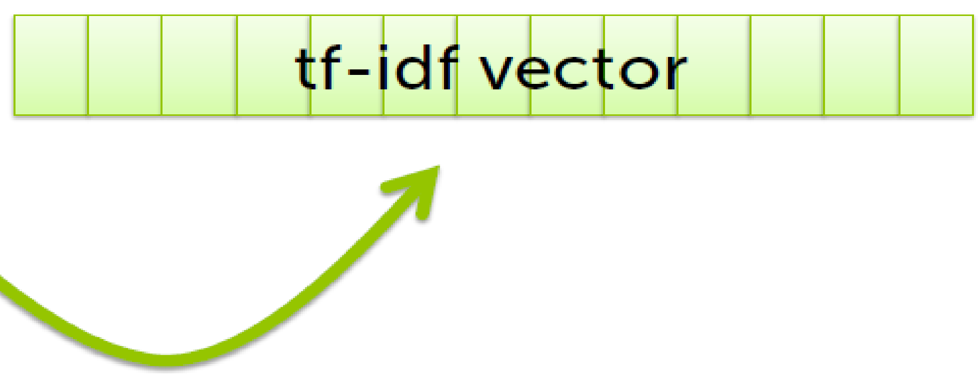
$\mathbf{x}_i =$



# Building an alternative model



## Bag-of-words representation

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# Building an alternative model



## Bag-of-words representation

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$\mathbf{x}_i$ = {modeling, complex, epilepsy, modeling, Bayesian, clinical, epilepsy, EEG, data, dynamic…}

multiset

= unordered set of words with duplication of unique elements mattering

# Model for „bag-of-words”



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## A model for bag-of-words representation

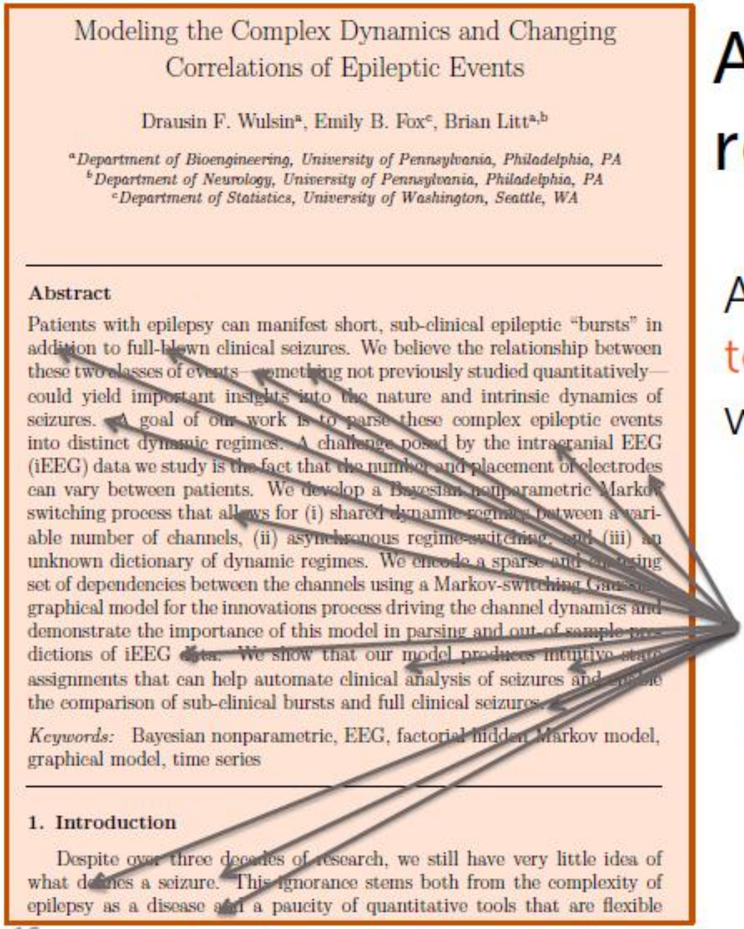
As before, the “prior” probability that doc i is from topic k is:

$$p(z_i = k) = \pi_k$$

$\boldsymbol{\pi} = [\pi_1 \ \ \pi_2 \ldots \pi_K]$
represents corpus-wide topic prevalence

# Model for „bag-of-words”





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## A model for bag-of-words representation

Assuming doc i **is** from topic k, words occur with probabilities:

| SCIENCE | |
|---|---|
| patients | 0.05 |
| clinical | 0.01 |
| epilepsy | 0.002 |
| seizures | 0.0015 |
| EEG | 0.001 |
| ... | ... |

words in vocab

20/11, 27/11 2024

# Model for „bag-of-words"



## Topic-specific word probabilities

Distribution on words in vocab for **each topic**

| SCIENCE | | TECH | | SPORTS | |
|---|---|---|---|---|---|
| experiment | 0.1 | develop | 0.18 | player | 0.15 |
| test | 0.08 | computer | 0.09 | score | 0.07 |
| discover | 0.05 | processor | 0.032 | team | 0.06 |
| hypothesize | 0.03 | user | 0.027 | goal | 0.03 |
| climate | 0.01 | internet | 0.02 | injury | 0.01 |
| ... | ... | ... | ... | ... | ... |

...

(table now organized by decreasing probabilities
showing top words in each category)

# Model for „bag-of-words”

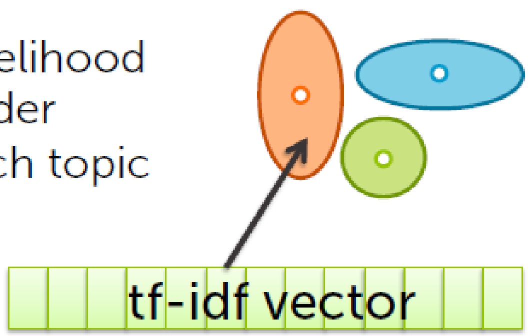


## Comparing and contrasting

**Previously**

Prior topic probabilities $p(z_i = k) = \pi_k$

Likelihood under each topic




compute likelihood of **tf-idf** vector under each **Gaussian**

**Now**

$p(z_i = k) = \pi_k$

| SCIENCE | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TECH | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| SPORTS | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

...

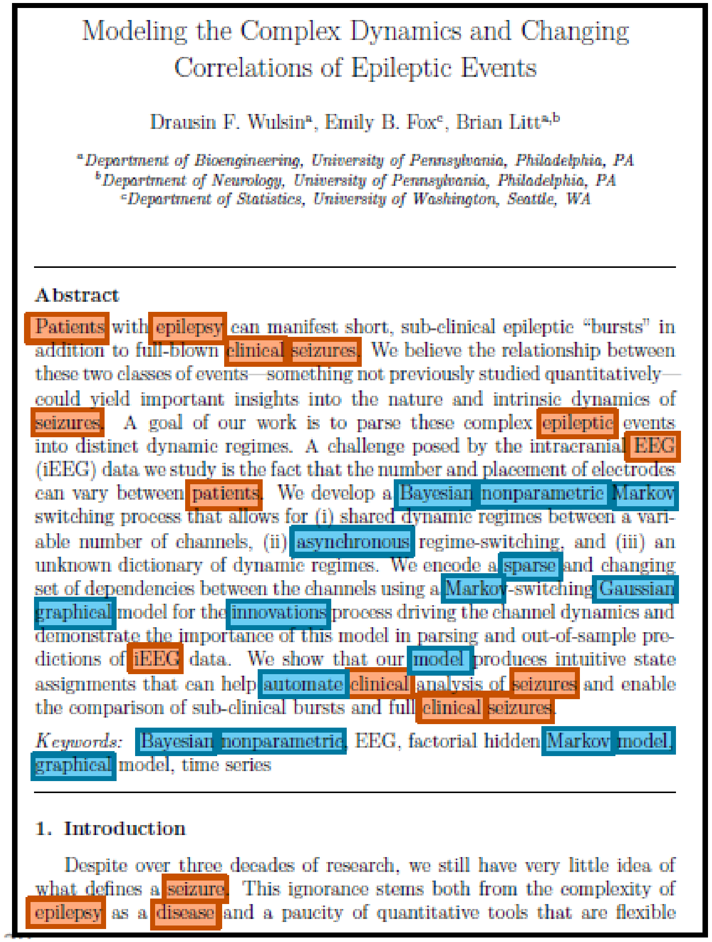
{modeling, complex, epilepsy, modeling, Bayesian, clinical, epilepsy, EEG, data, dynamic...}

compute likelihood of the **collection of words** in doc under each **topic distribution**

# Latent Dirichlet allocation (LDA)

# Latent Dirichlet allocation





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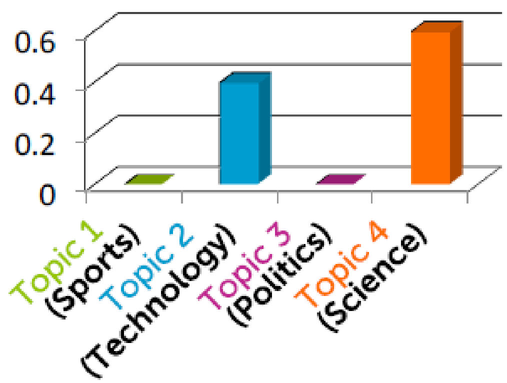
## LDA is a mixed membership model

Want to discover a **set** of topics



# Latent Dirichlet allocation



**Topic vocab distributions:**

| SCIENCE | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TECH | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| SPORTS | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
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| ... | ... |

⋮


Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

Drausin F. Wulsin[a], Emily B. Fox[c], Brian Litt[a,b]

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## Clustering:

One topic indicator $z_i$ per **document** i

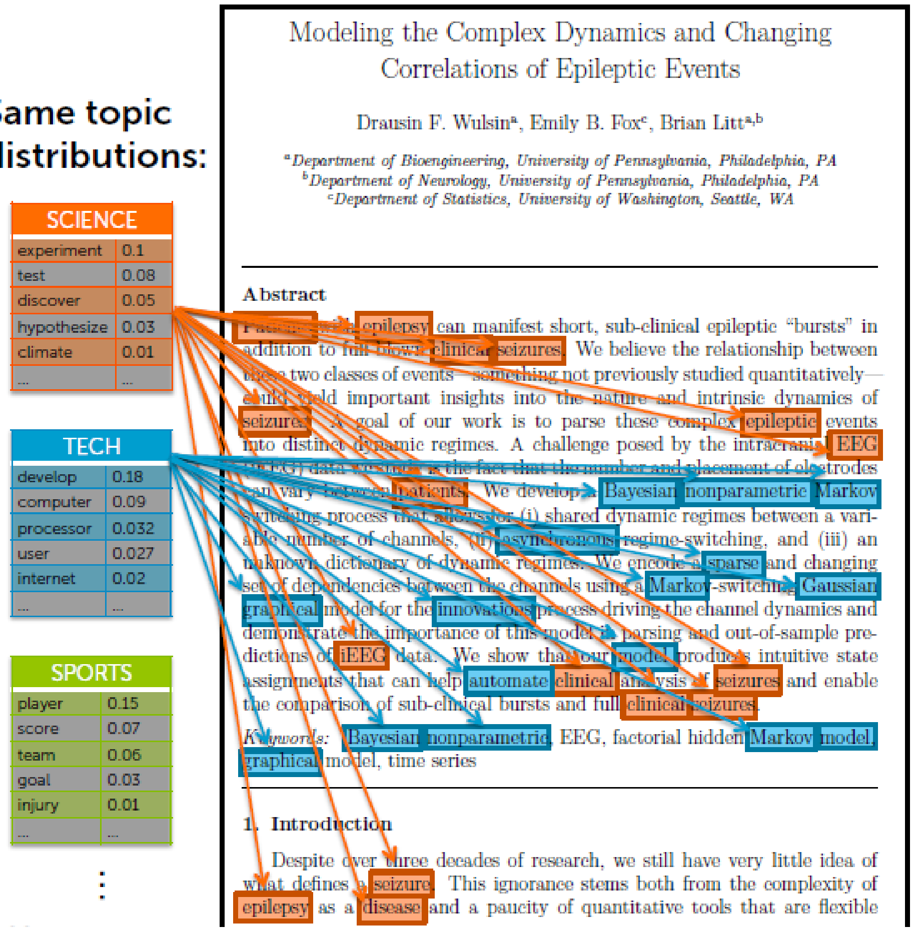
**All words** come from (get scored under) same topic $z_i$

Distribution on prevalence of topics in **corpus**
$\boldsymbol{\pi} = [\pi_1 \ \pi_2 \ \dots \ \pi_K]$

# Latent Dirichlet allocation



**Same topic distributions:**




## In LDA:

One topic indicator $z_{iw}$ per **word** in doc i

**Each word** gets scored under its topic $z_{iw}$

Distribution on prevalence of topics in **document**
$\boldsymbol{\pi}_i = [\pi_{i1} \ \pi_{i2} \ldots \pi_{iK}]$

# Inference in LDA models



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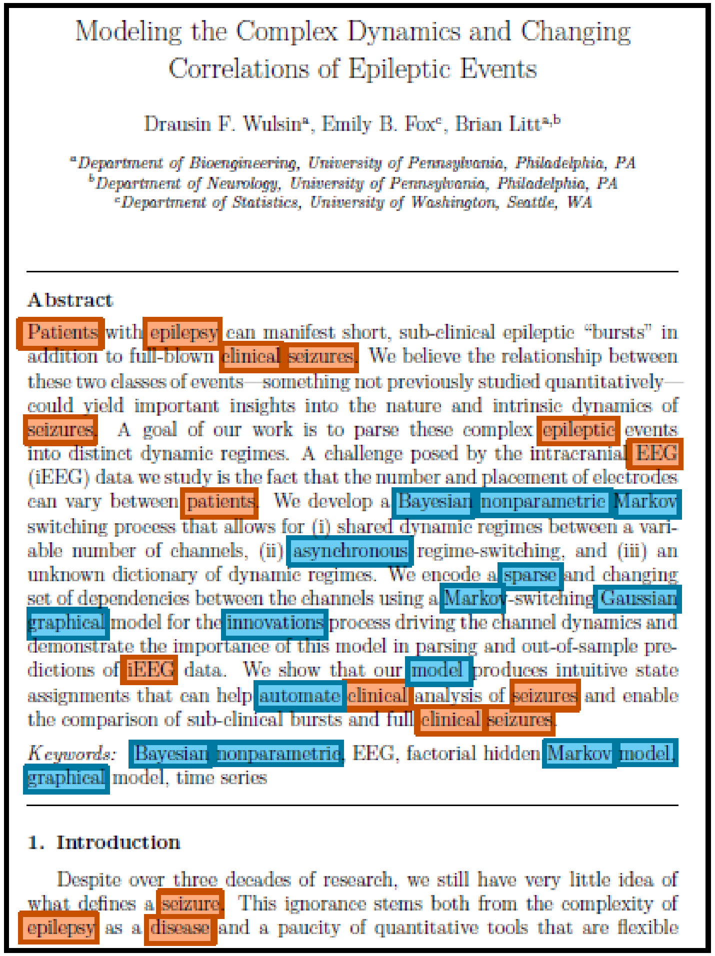

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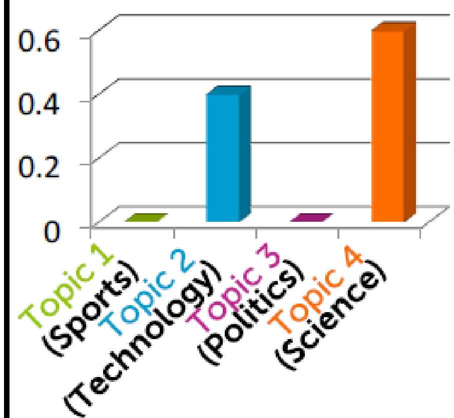

# Inference in LDA models



**Topic vocab distributions:**

| TOPIC 1 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| … | … |

| TOPIC 2 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| … | … |

| TOPIC 3 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| … | … |

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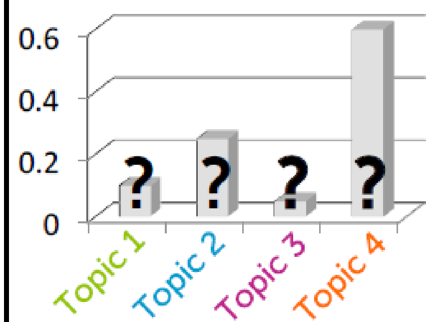

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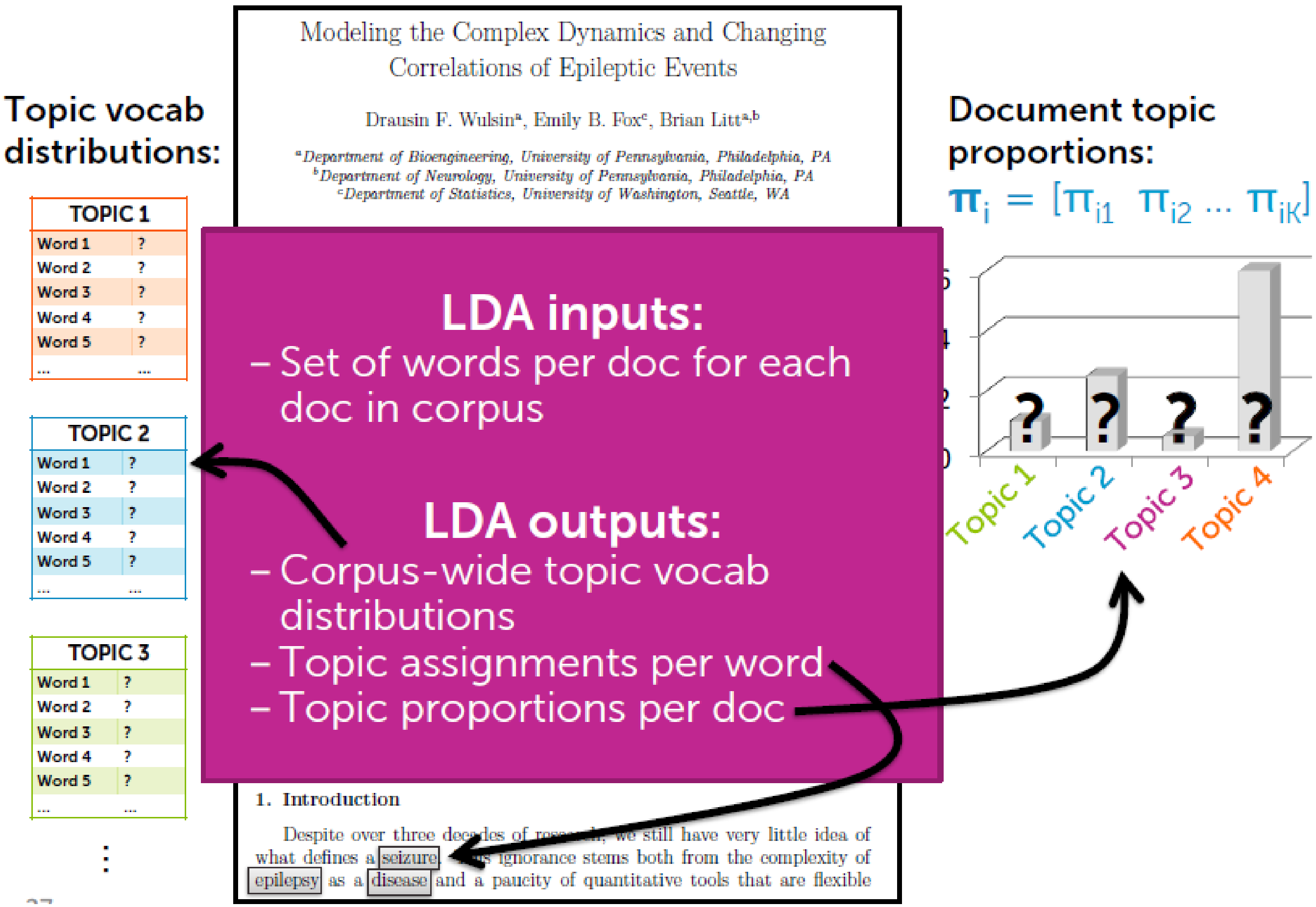

# Inference in LDA models



## Interpreting LDA outputs

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
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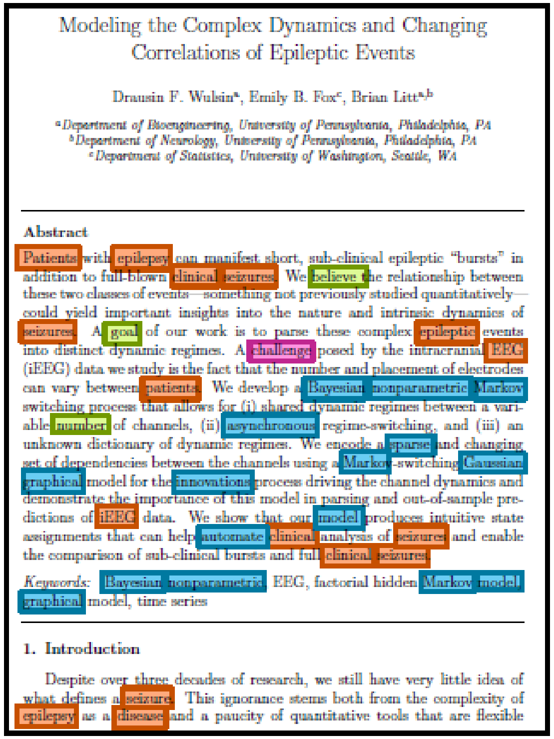
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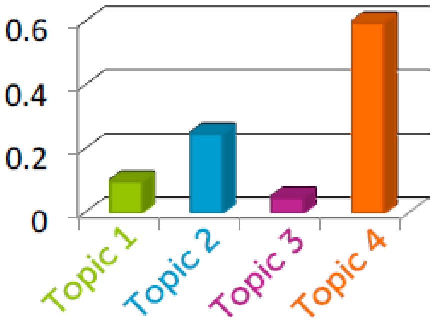
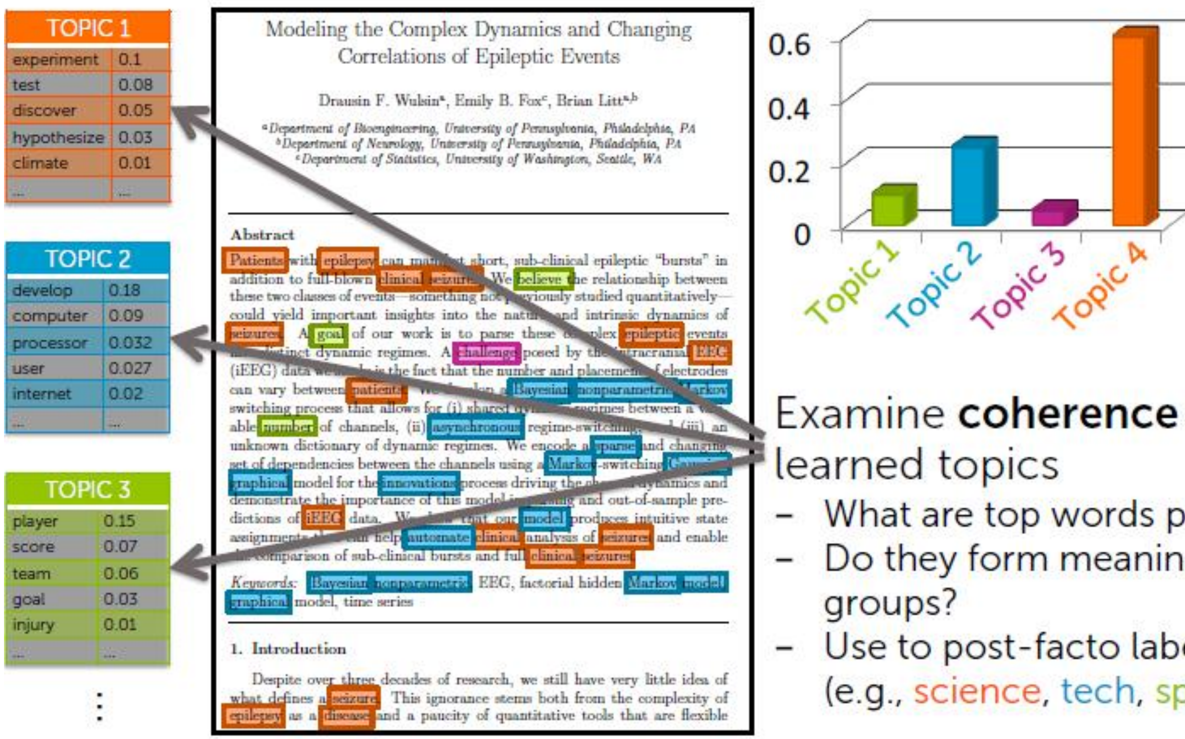


# Inference in LDA models



## Interpreting LDA outputs




Examine **coherence** of learned topics

- What are top words per topic?
- Do they form meaningful groups?
- Use to post-facto label topics (e.g., science, tech, sports,...)

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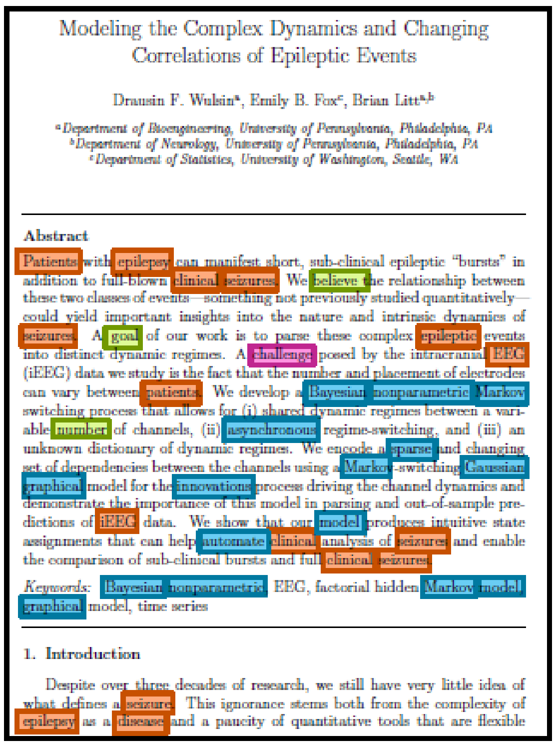

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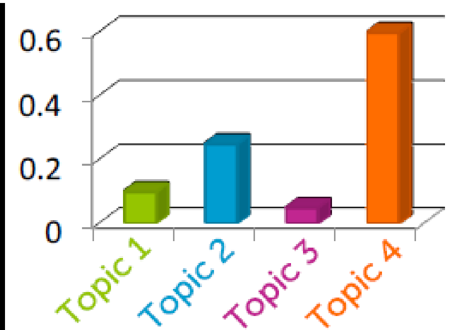


↑

Doc-specific topic proportions can be used to:

- Relate documents
- Study user topic preferences
- Assign docs to multiple categories

# Inference in LDA models



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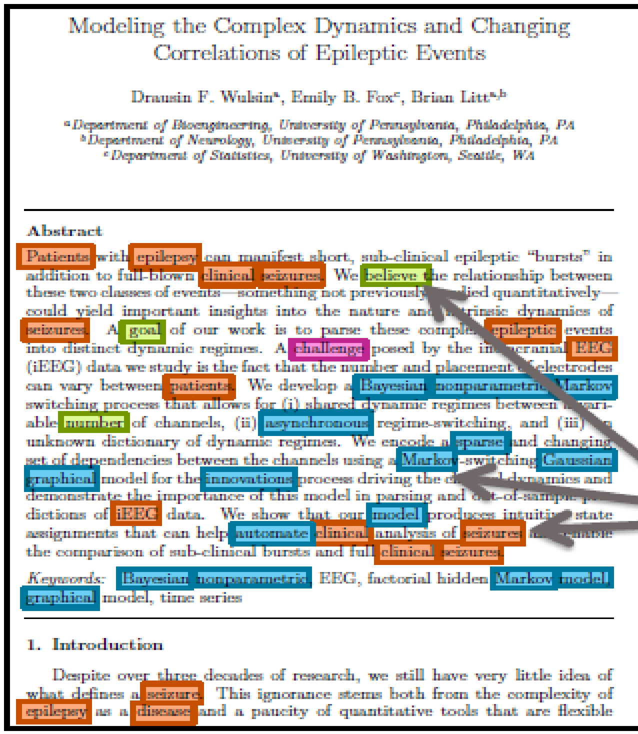

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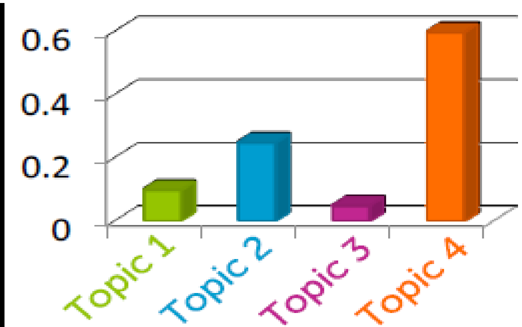


Typically **not** interested in word assignments

# An inference algorithm for LDA: Gibbs sampling

# Clustering so far



## k-means

Assign observations to closest cluster center

$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

Revise cluster centers

$$\mu_j \leftarrow \arg\min_\mu \sum_{i:z_i=j} ||\mu - \mathbf{x}_i||_2^2$$

**Iterative hard assignment to max objective**

## EM for MoG

**E-step:** estimate cluster responsibilities

$$\hat{r}_{ik} = \frac{\hat{\pi}_k N(x_i \mid \hat{\mu}_k, \hat{\Sigma}_k)}{\sum_{j=1}^K \hat{\pi}_j N(x_i \mid \hat{\mu}_j, \hat{\Sigma}_j)}$$

**M-step:** maximize likelihood over parameters

$$\hat{\pi}_k, \hat{\mu}_k, \hat{\Sigma}_k \mid \{\hat{r}_{ik}, x_i\}$$

**Iterative soft assignment to max objective**

What can we do for our bag-of-words models?



# Part 1: Clustering model

| SCIENCE | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
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| ... | ... |

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**Can derive EM algorithm:**

– Gaussian likelihood of tf-idf vector

↓

multinomial likelihood of word counts ($m_w$ successes of word w)

– **Result:** mixture of multinomial model

# What can we do for our bag-of-words models?



## Part 2: LDA model

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
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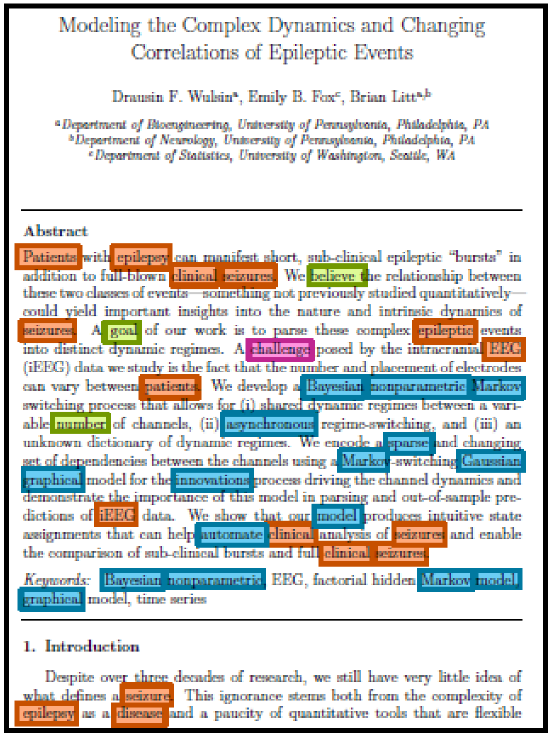

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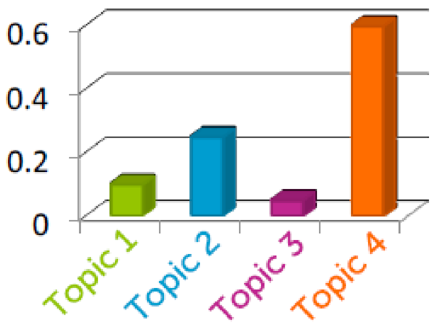



Can derive
EM algorithm,
but not common
(performs poorly)

# An inference algorithms



## Typical LDA implementations

Normally LDA is specified as a **Bayesian model**
(otherwise, “probabilistic latent semantic analysis/indexing”)

- Account for uncertainty in parameters when making predictions
- Naturally regularizes parameter estimates in contrast to MLE

EM-like algorithms (e.g., “variational EM”), or...

## Gibbs sampling

Iterative **random** hard assignment!

Benefits:

- Typically intuitive updates
- Very straightforward to implement

# Gibbs sampling for LDA

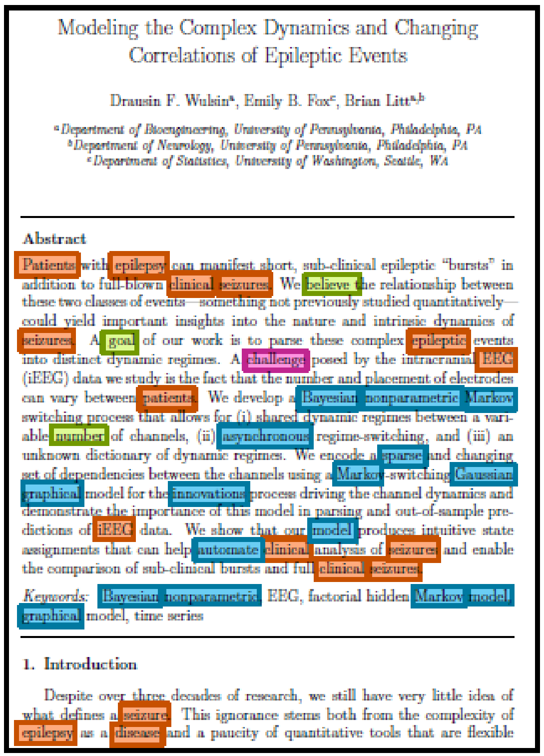


| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮



Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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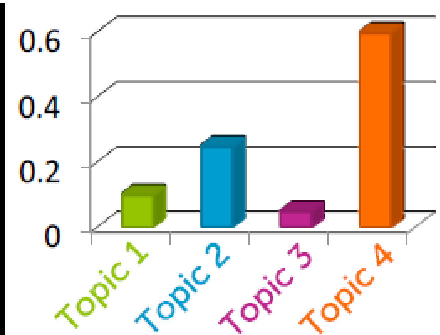


Current set of assignments

# Gibbs sampling for LDA



| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
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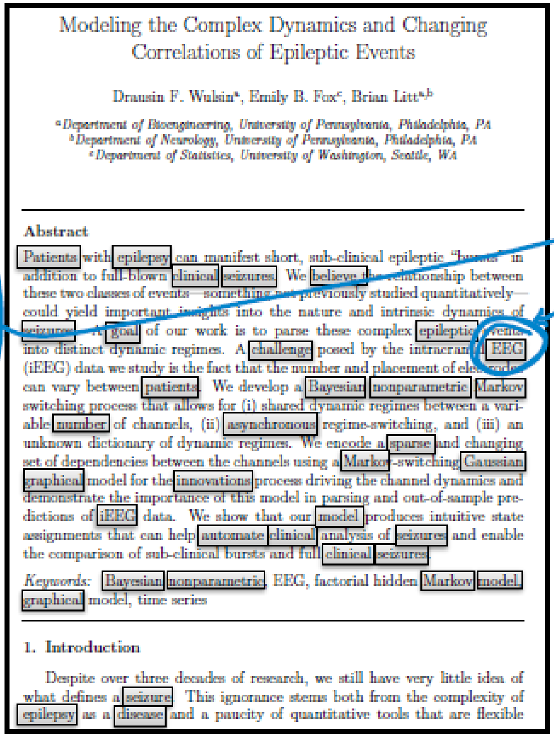
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮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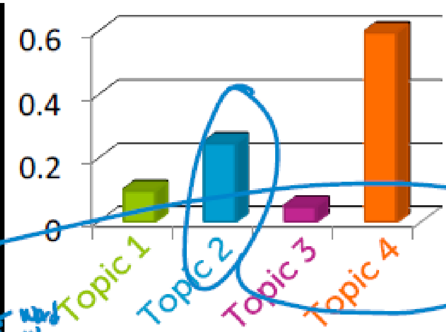


word w in doc i

**Step 1:** Randomly reassign all $z_{iw}$ based on
- doc topic proportions
- topic vocab distributions

Draw randomly from responsibility vector $[r_{iw1}\ r_{iw2}\ \ldots\ r_{iwK}]$

prior of

prob. $z_{iw}=2$

$$r_{iw2} = \frac{\pi_{i2} \cdot p(\text{"EEG"} \mid z_{iw}=2)}{\sum_{j=1}^{K} \pi_{ij}\, p(\text{"EEG"} \mid z_{iw}=j)}$$

prob. of assigning $z_{iw}=2$

# Gibbs sampling for LDA



| TOPIC 1 | |
|---|---|
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| test | 0.08 |
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| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

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| ... | ... |

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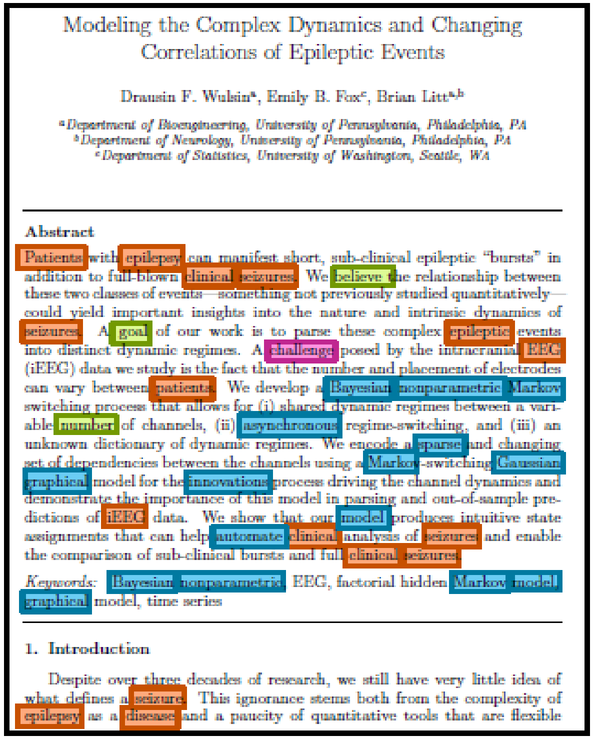

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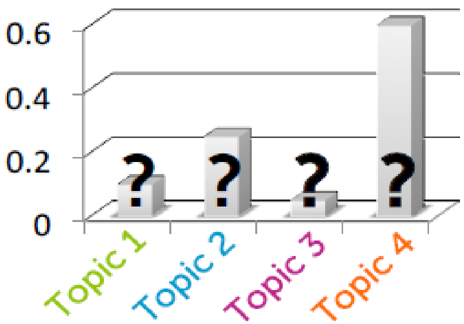


**Step 2:** Randomly reassign doc topic proportions based on assignments $z_{iw}$ in **current doc**

# Gibbs sampling for LDA



| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
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**Step 3:** Repeat for all docs

# Gibbs sampling for LDA

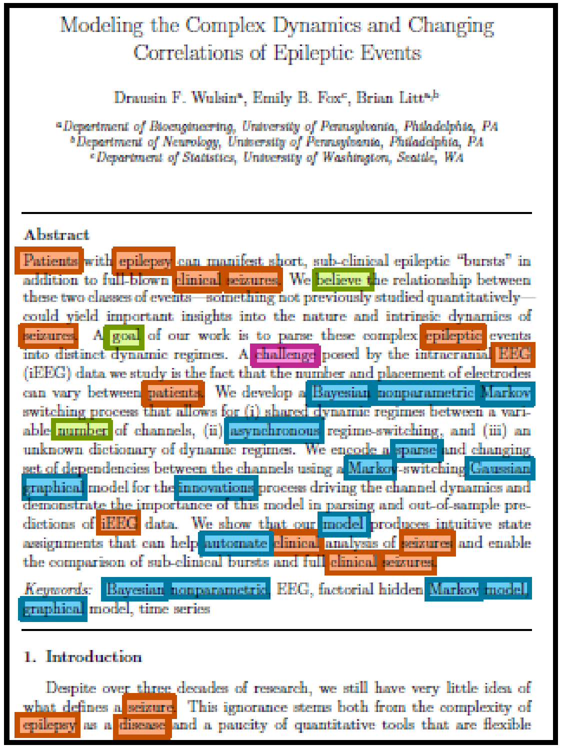


| TOPIC 1 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| ... | ... |

| TOPIC 2 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| ... | ... |

| TOPIC 3 | |
|---|---|
| Word 1 | ? |
| Word 2 | ? |
| Word 3 | ? |
| Word 4 | ? |
| Word 5 | ? |
| ... | ... |

⋮



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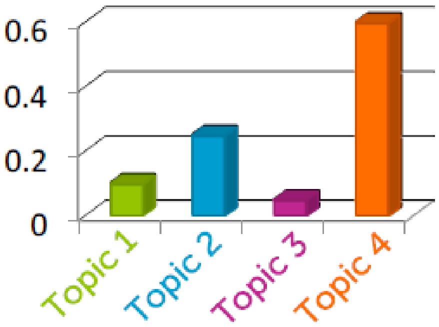



**Step 4:** Randomly reassign topic vocab distributions based on assignments $z_{iw}$ in **entire corpus**

# An inference algorithm: Gibbs sampling



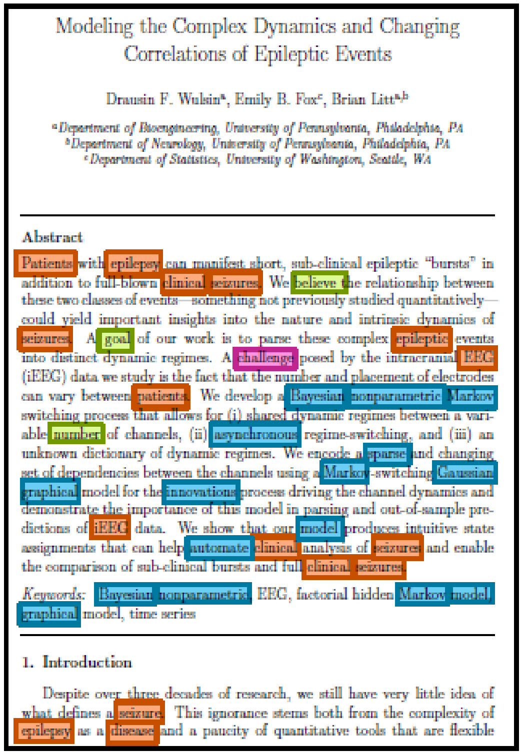
## Gibbs sampling for LDA

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮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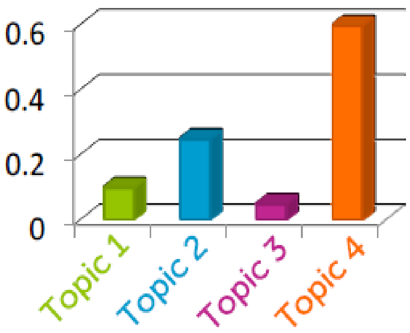



**Repeat Steps 1-4 until max iter reached**

# An inference algorithm: Gibbs sampling



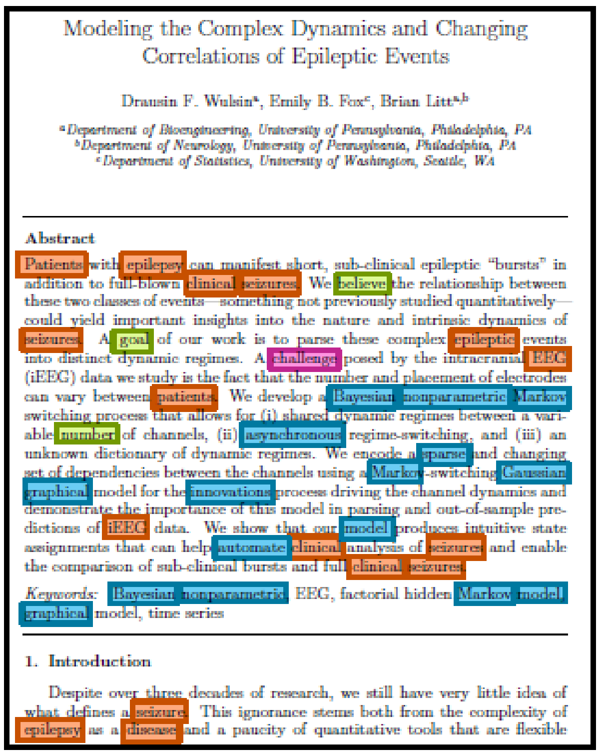
## Random sample #10000

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮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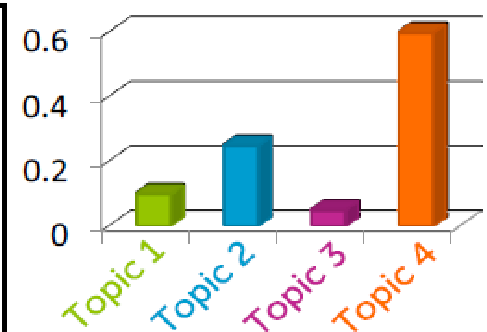



**Current set of assignments**

# An inference algorithm: Gibbs sampling



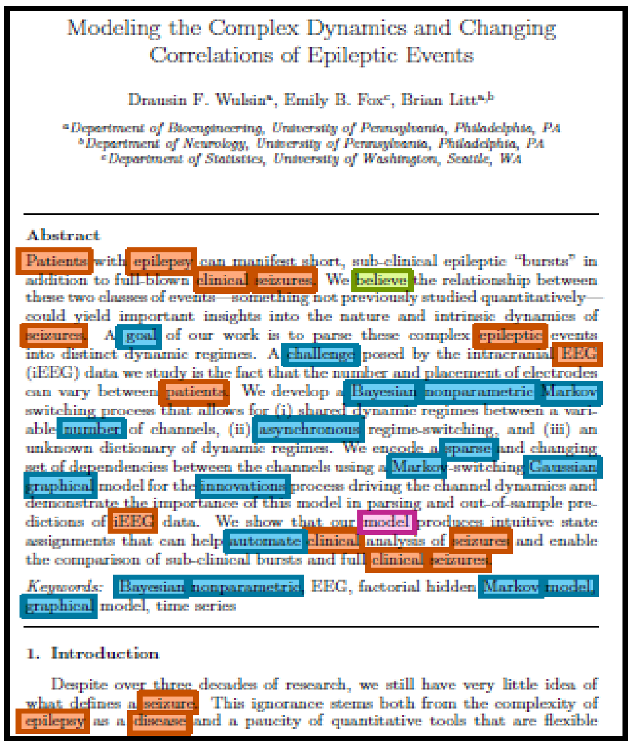
## Random sample #10001

| TOPIC 1 | |
|---|---|
| experiment | 0.12 |
| test | 0.06 |
| hypothesize | 0.042 |
| discover | 0.04 |
| climate | 0.011 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.16 |
| computer | 0.11 |
| user | 0.03 |
| processor | 0.029 |
| internet | 0.023 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| offense | 0.02 |
| defense | 0.018 |
| ... | ... |

⋮



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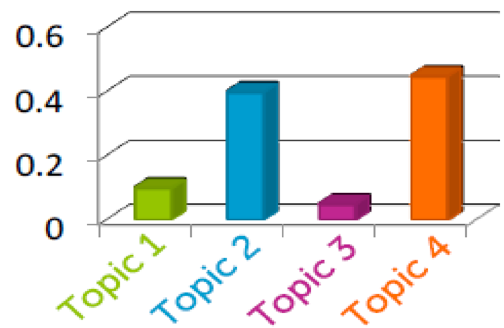



**Current set of assignments**

# An inference algorithm: Gibbs sampling



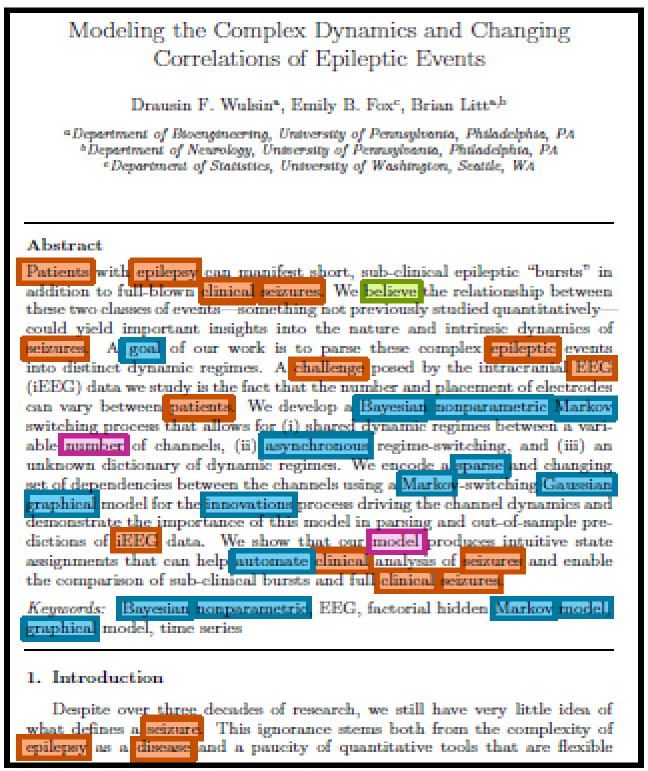
## Random sample #10002

| TOPIC 1 | |
|---|---|
| experiment | 0.10 |
| discover | 0.055 |
| hypothesize | 0.043 |
| test | 0.042 |
| examine | 0.015 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| computer | 0.12 |
| develop | 0.115 |
| user | 0.031 |
| device | 0.022 |
| cloud | 0.018 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.17 |
| score | 0.09 |
| game | 0.062 |
| team | 0.043 |
| win | 0.03 |
| ... | ... |

⋮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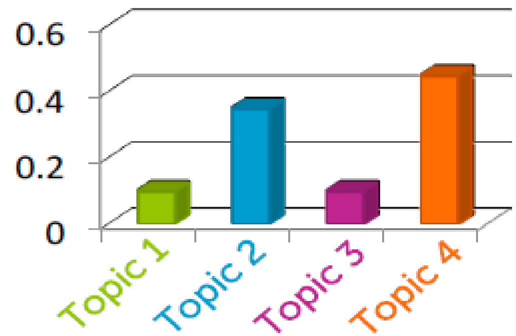


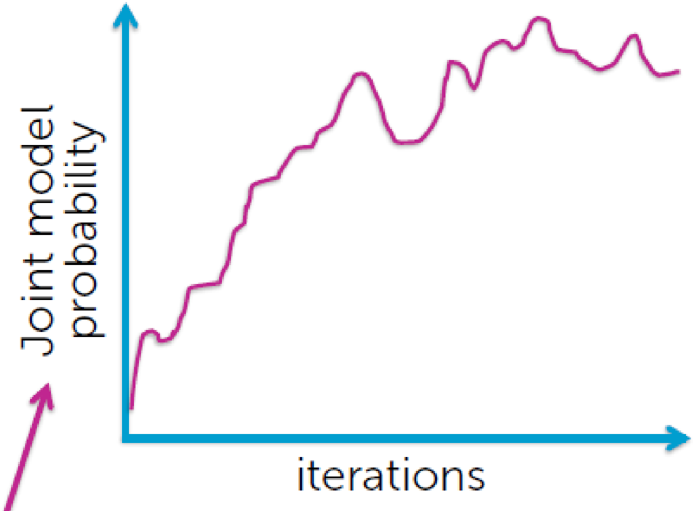

**Current set of assignments**

# An inference algorithm: Gibbs sampling



## What do we know about this process?

**Not an optimization algorithm**




probability of observations given variables/parameters
and probability of variables/parameters themselves

Eventually provides "correct" Bayesian estimates…

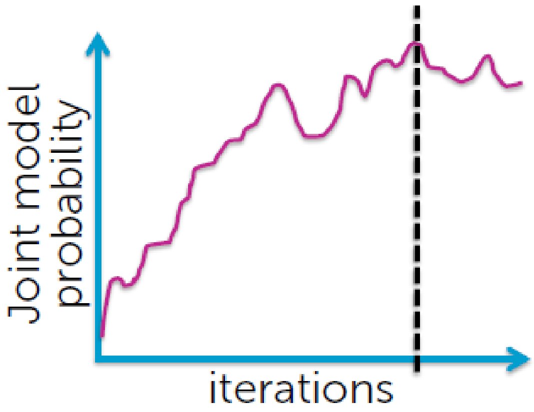
# What to do with sampling output?

**Predictions:**

1. Make prediction for each snapshot of randomly assigned variables/parameters (full iteration)
2. Average predictions for final result

**Parameter or assignment estimate:**

– Look at snapshot of randomly assigned variables/parameters that maximizes "joint model probability"



# Gibbs sampling algorithm



Iterative **random** hard assignment!

Assignment variables and model parameters treated similarly

Iteratively draw variable/parameter from conditional distribution having fixed:

- all other variables/parameters
  - values randomly selected in previous rounds
  - changes from iter to iter
- observations
  - always the same values

# „Collapsed" Gibbs sampling for LDA



Based on special structure of LDA model, can sample **just** indicator variables $z_{iw}$

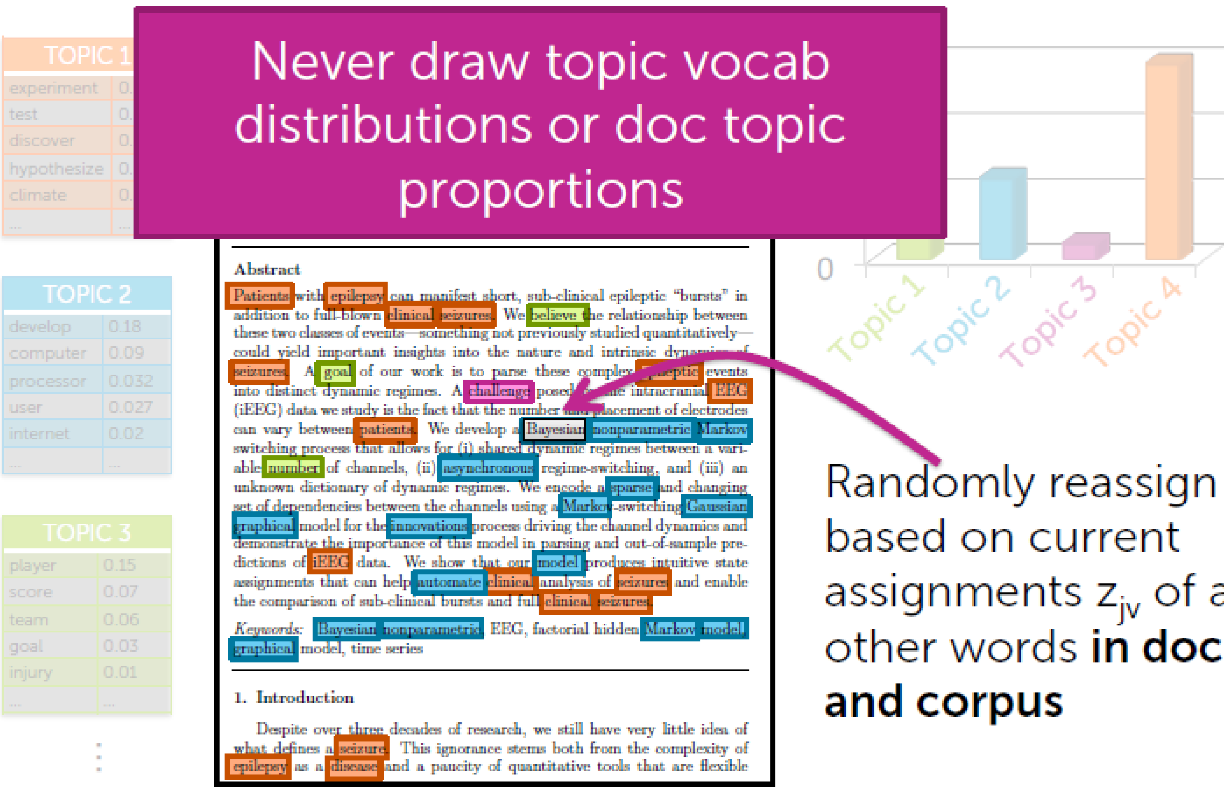
- No need to sample other parameters
  - corpus-wide topic vocab distributions
  - per-doc topic proportions

Often leads to much better performance because examining uncertainty in smaller space

# Collapsed Gibbs sampling for LDA



Never draw topic vocab distributions or doc topic proportions




Randomly reassign $z_{iw}$ based on current assignments $z_{jv}$ of all other words **in document and corpus**

# Collapsed Gibbs sampling for LDA



## Select a document

| | | | | |
|---|---|---|---|---|
| | | | | |
| epilepsy | dynamic | Bayesian | EEG | model |

5 word document

# Collapsed Gibbs sampling for LDA



## Randomly assign topics

| | | | | |
|---|---|---|---|---|
| 3 | 2 | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |

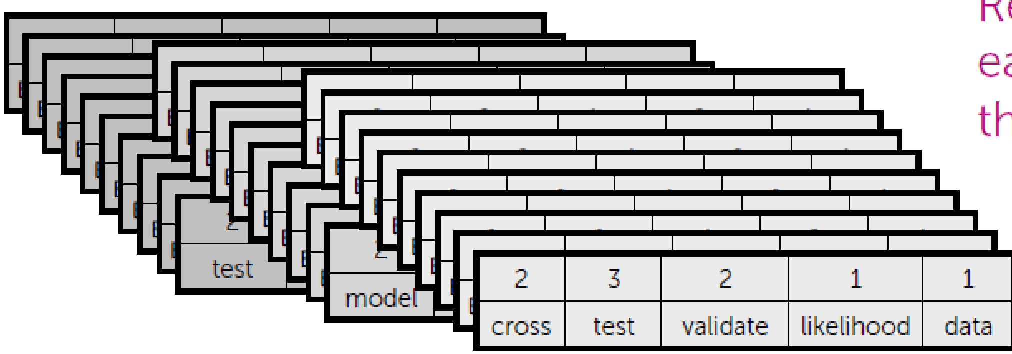
(one possible approach)

# Collapsed Gibbs sampling for LDA



## Randomly assign topics

| 3 | 2 | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |




Repeat for each doc in the corpus

# Collapsed Gibbs sampling for LDA



## Maintain local statistics

| | | | | |
|---|---|---|---|---|
| 3 | 2 | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 2 | 1 | 2 |

# Collapsed Gibbs sampling for LDA



## Maintain global statistics

| 3 | 2 | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 2 | 1 | 2 |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| epilepsy | 1 | 0 | 35 |
| Bayesian | 50 | 0 | 1 |
| model | 42 | 1 | 0 |
| EEG | 0 | 0 | 20 |
| dynamic | 10 | 8 | 1 |
| … | | | |

Total counts from **all** docs

# Collapsed Gibbs sampling for LDA



## Randomly reassign topics

| 3 | ~~2~~ | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |

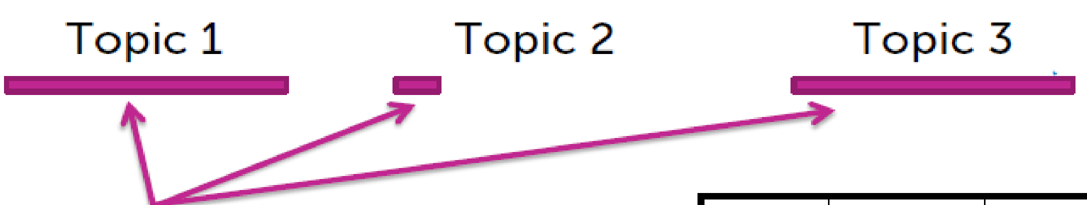
| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 2 | 0 ~~1~~ | 2 |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| epilepsy | 1 | 0 | 35 |
| Bayesian | 50 | 0 | 1 |
| model | 42 | 1 | 0 |
| EEG | 0 | 0 | 20 |
| dynamic | 10 | 7 ~~8~~ | 1 |
| … | | | |

decrementing counts after removing current assignment $z_{iw} = 2$

## Probability of new assignment

| 3 | ? | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |




How much doc "likes" each topic based on other assignments in doc

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 2 | 0 | 2 |

# current assignments to topic k in doc i → $\dfrac{n_{ik} + \alpha}{N_i - 1 + K\alpha}$ ← smoothing param from Bayes prior

# words in doc i → $N_i$

ignore current word

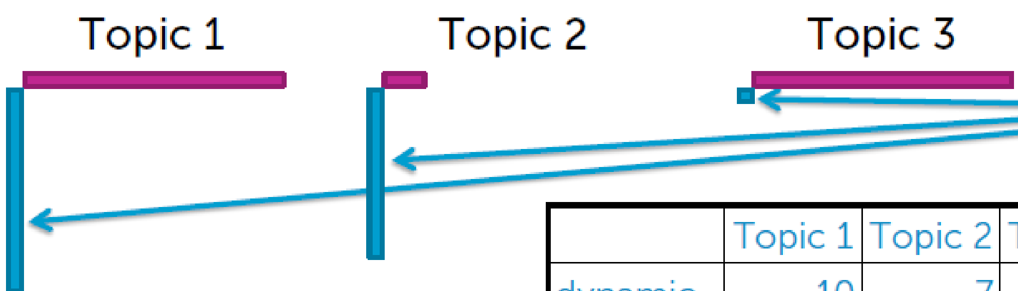
63

# Collapsed Gibbs sampling for LDA



## Probability of new assignment

| 3 | ? | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |




How much each topic likes the word "dynamic" based on assignments in other docs in corpus

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| dynamic | 10 | 7 | 1 |

# assignments **corpus-wide** of word "dynamic" to topic k

$$\frac{m_{\text{dynamic},k} + \gamma}{\sum_{w \in V} m_{w,k} + V\gamma}$$

smoothing param from Bayes prior

size of vocab

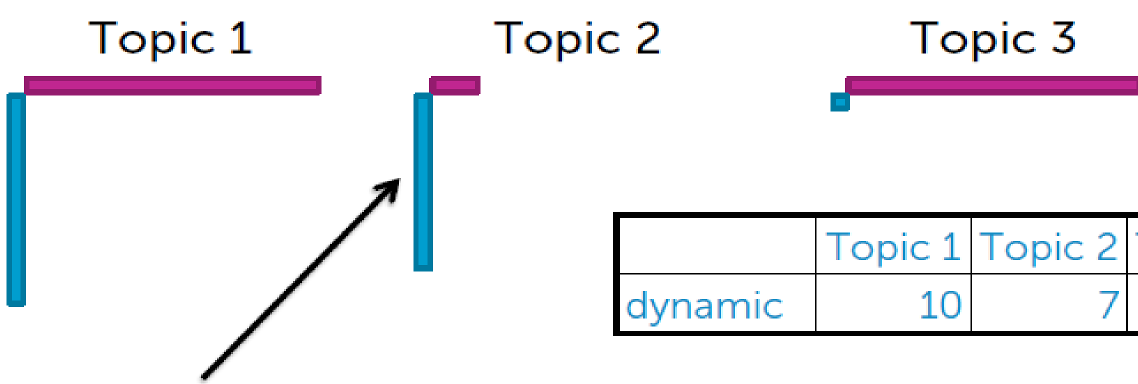
64

# Collapsed Gibbs sampling for LDA



## Probability of new assignment

| | | | | |
|---|---|---|---|---|
| 3 | ? | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |




| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| dynamic | 10 | 7 | 1 |

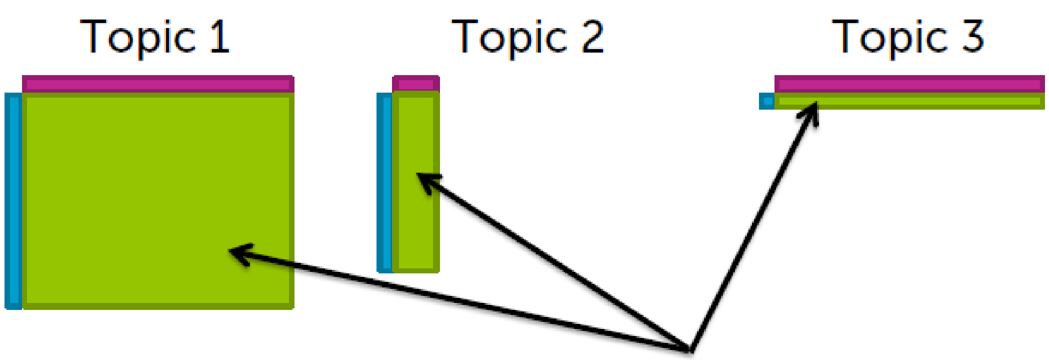
Topic 2 also really likes "dynamic",
but in a different context...
e.g., a topic on fluid dynamics

# Collapsed Gibbs sampling for LDA



## Probability of new assignment

| | | | | |
|---|---|---|---|---|
| 3 | ? | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |



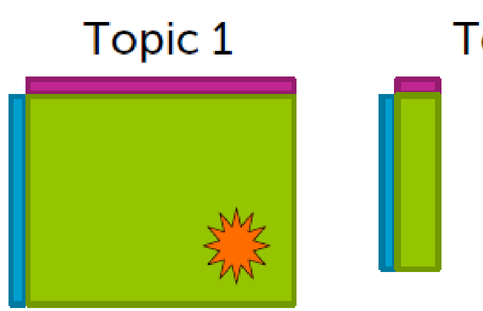

How much doc likes topic $\frac{n_{ik} + \alpha}{N_i - 1 + K\alpha} \frac{m_{\text{dynamic},k} + \gamma}{\sum_{w \in V} m_{w,k} + V\gamma}$ How much topic likes word

# Collapsed Gibbs sampling for LDA



## Randomly draw a new topic indicator

| 3 | ? | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |





**To draw new topic assignment** (equivalently):

- roll K-sided die with these probabilities
- throw dart at these regions

Normalize this product of terms over K possible topics!

How much doc likes topic

$$\boxed{\frac{n_{ik}+\alpha}{N_i-1+K\alpha}\;\frac{m_{\text{dynamic},k}+\gamma}{\sum_{w\in V} m_{w,k}+V\gamma}}$$

How much topic likes word

# Collapsed Gibbs sampling for LDA



## Update counts

| 3 | 1 | 1 | 3 | 1 |
|---|---|---|---|---|
| epilepsy | dynamic | Bayesian | EEG | model |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 3 ~~2~~ | 0 | 2 |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| epilepsy | 1 | 0 | 35 |
| Bayesian | 50 | 0 | 1 |
| model | 42 | 1 | 0 |
| EEG | 0 | 0 | 20 |
| dynamic | 11 ~~10~~ | 7 | 1 |
| … | | | |

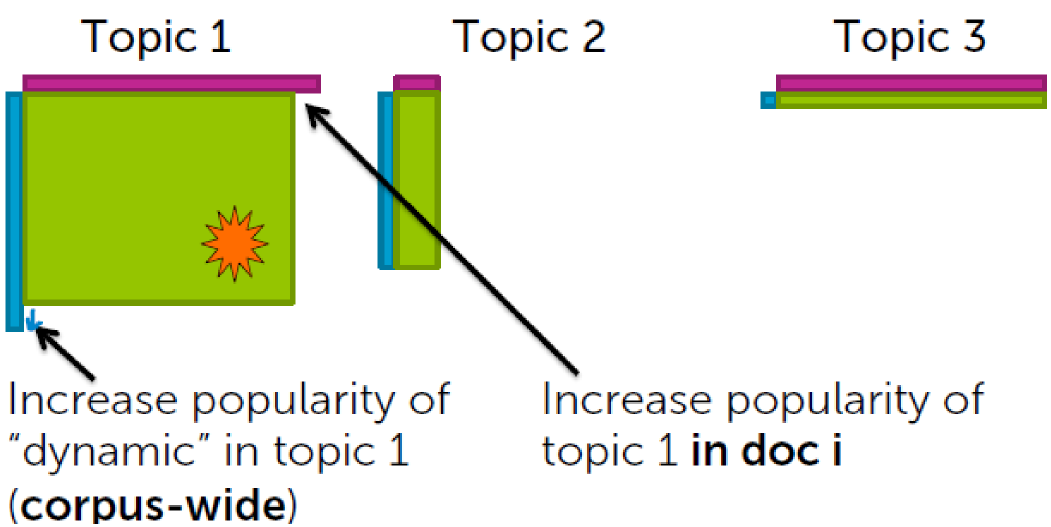
increment counts based on new assignment of $z_{iw}=1$

# Collapsed Gibbs sampling for LDA



## Geometrically…

| | | | | |
|---|---|---|---|---|
| 3 | 1 | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |



# Collapsed Gibbs sampling for LDA



## Iterate through all words/docs

| | | | | |
|---|---|---|---|---|
| 3 | 1 | 1 | 3 | 1 |
| epilepsy | dynamic | Bayesian | EEG | model |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| epilepsy | 1 | 0 | 35 |
| Bayesian | 50 | 0 | 1 |
| model | 42 | 1 | 0 |
| EEG | 0 | 0 | 20 |
| dynamic | 10 | 7 | 1 |
| ... | | | |

| | Topic 1 | Topic 2 | Topic 3 |
|---|---|---|---|
| Doc i | 2 | 0 | 2 |

# Collapsed Gibbs sampling for LDA



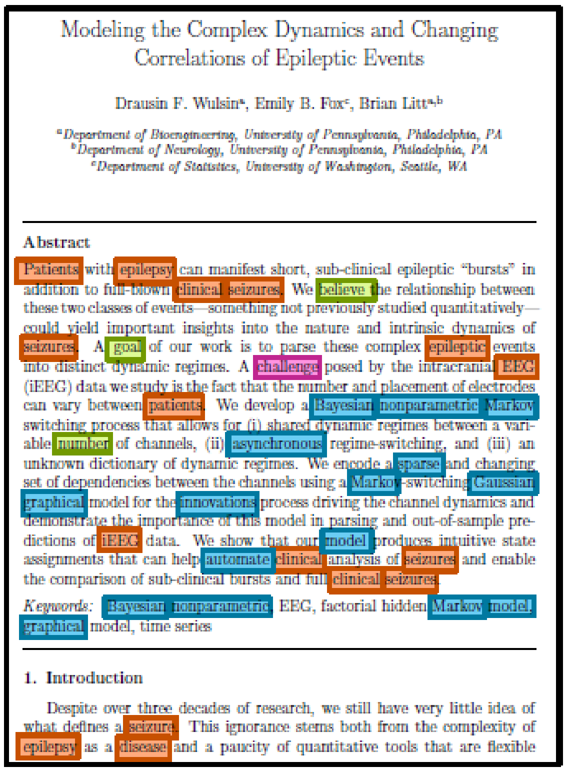
## What to do with the collapsed samples?

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
| player | 0.15 |
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮



Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

Drausin F. Wulsin[a], Emily B. Fox[c], Brian Litt[a,b]

[a]Department of Bioengineering, University of Pennsylvania, Philadelphia, PA
[b]Department of Neurology, University of Pennsylvania, Philadelphia, PA
[c]Department of Statistics, University of Washington, Seattle, WA

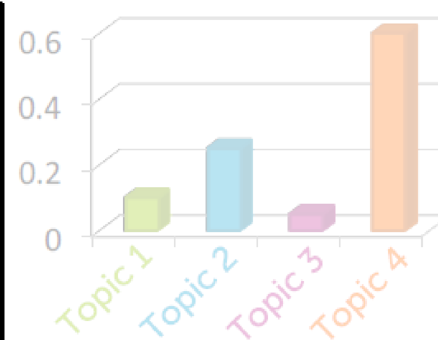
Abstract

Patients with epilepsy can manifest short, sub-clinical epileptic "bursts" in addition to full-blown clinical seizures. We believe the relationship between these two classes of events—something not previously studied quantitatively—could yield important insights into the nature and intrinsic dynamics of seizures. A goal of our work is to parse these complex epileptic events into distinct dynamic regimes. A challenge posed by the intracranial EEG (iEEG) data we study is the fact that the number and placement of electrodes can vary between patients. We develop a Bayesian nonparametric Markov switching process that allows for (i) shared dynamic regimes between a variable number of channels, (ii) asynchronous regime-switching, and (iii) an unknown dictionary of dynamic regimes. We encode a sparse and changing set of dependencies between the channels using a Markov-switching Gaussian graphical model for the innovations process driving the channel dynamics and demonstrate the importance of this model in parsing and out-of-sample predictions of iEEG data. We show that our model produces intuitive state assignments that can help automate clinical analysis of seizures and enable the comparison of sub-clinical bursts and full clinical seizures.

*Keywords:* Bayesian nonparametric, EEG, factorial hidden Markov model, graphical model, time series

1. Introduction

Despite over three decades of research, we still have very little idea of what defines a seizure. This ignorance stems both from the complexity of epilepsy as a disease and a paucity of quantitative tools that are flexible




From "best" sample of $\{z_{iw}\}$, can infer:

1. Topics from conditional distribution…
   need corpus-wide info

# Collapsed Gibbs sampling for LDA



## What to do with the collapsed samples?

| TOPIC 1 | |
|---|---|
| experiment | 0.1 |
| test | 0.08 |
| discover | 0.05 |
| hypothesize | 0.03 |
| climate | 0.01 |
| ... | ... |

| TOPIC 2 | |
|---|---|
| develop | 0.18 |
| computer | 0.09 |
| processor | 0.032 |
| user | 0.027 |
| internet | 0.02 |
| ... | ... |

| TOPIC 3 | |
|---|---|
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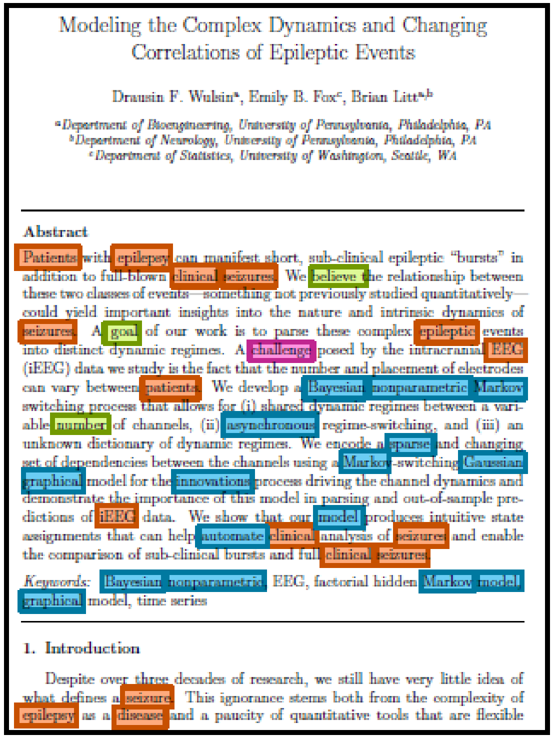
| score | 0.07 |
| team | 0.06 |
| goal | 0.03 |
| injury | 0.01 |
| ... | ... |

⋮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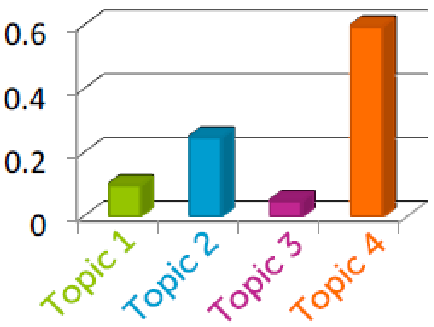


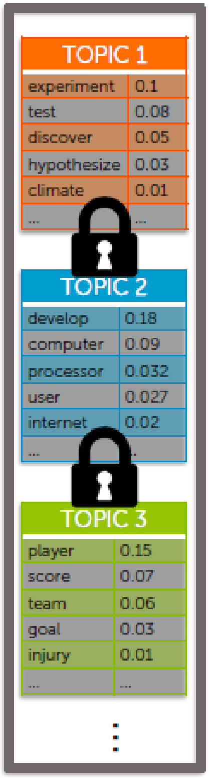

From "best" sample of $\{z_{iw}\}$, can infer:

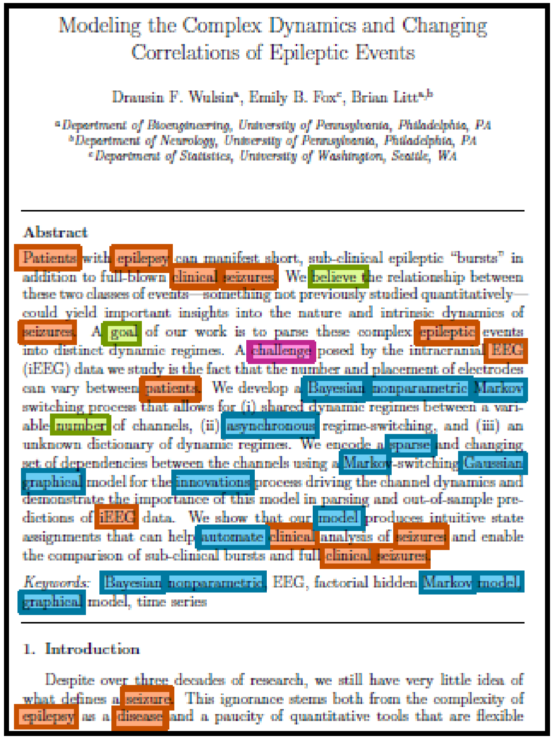
1. Topics from conditional distribution…
   need corpus-wide info
2. Document "embedding"…
   need doc info only

# Collapsed Gibbs sampling for LDA



## Embedding new documents



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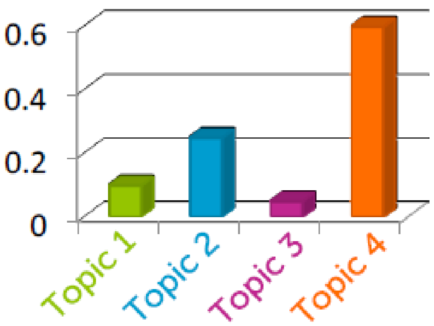



**Simple approach:**

1. Fix topics based on training set collapsed sampling
2. Run uncollapsed sampler on new doc(s) only

# What you can do now



- Compare and contrast clustering and mixed membership models
- Describe a document clustering model for the bag-of-words doc representation
- Interpret the components of the LDA mixed membership model
- Analyze a learned LDA model
  - Topics in the corpus
  - Topics per document
- Describe Gibbs sampling steps at a high level
- Utilize Gibbs sampling output to form predictions or estimate model parameters
- Implement collapsed Gibbs sampling for LDA

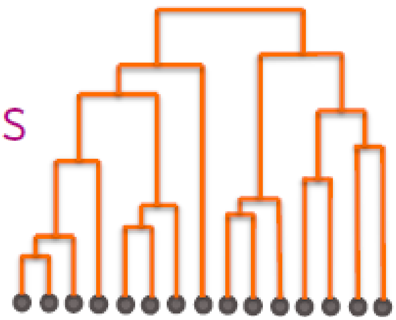
# Hierarchical clustering

# Why hierarchical clustering



- Avoid choosing # clusters beforehand

- Dendrograms help visualize different clustering granularities
  - No need to rerun algorithm

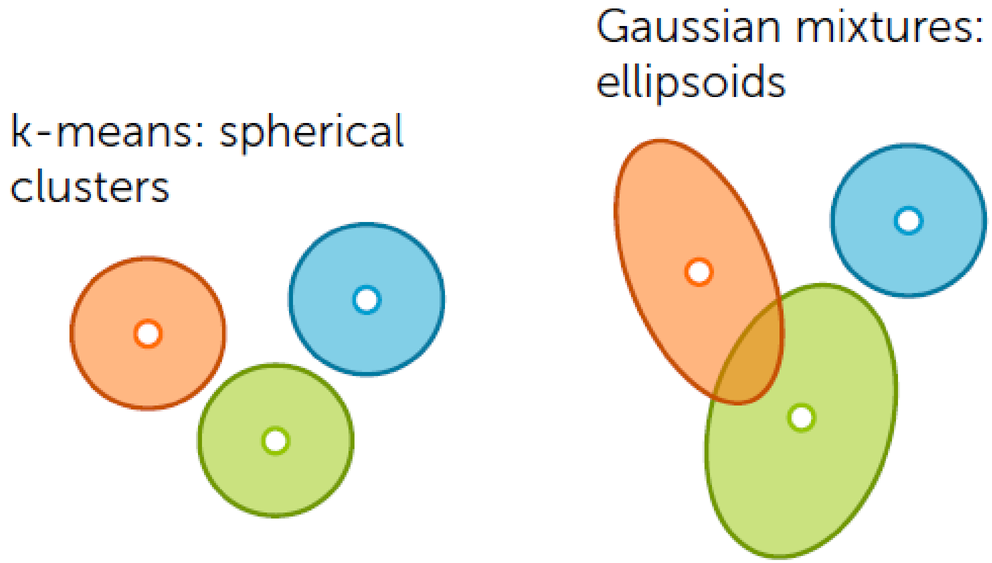


- Most algorithms allow user to choose any distance metric
  - k-means restricted us to Euclidean distance

# Why hierarchical clustering



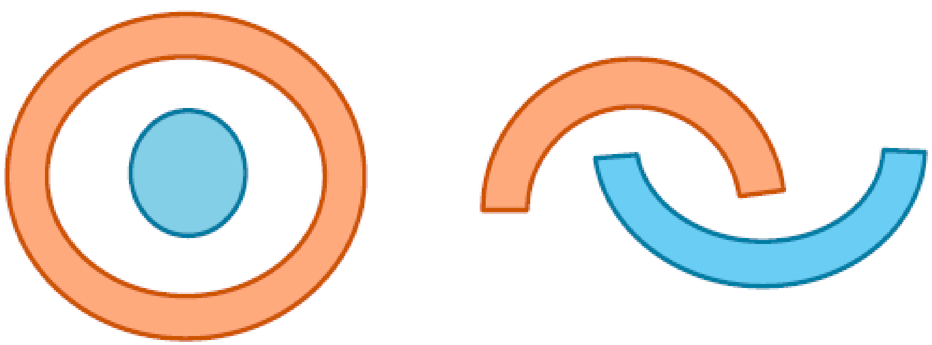
Can often find more complex shapes than k-means or Gaussian mixture models



# Why hierarchical clustering

Can often find more complex shapes than k-means or Gaussian mixture models

**What about these?**



# Two main types of algorithms



Divisive, *a.k.a top-down:* Start with all data in one big cluster and recursively split.

- Example: recursive k-means

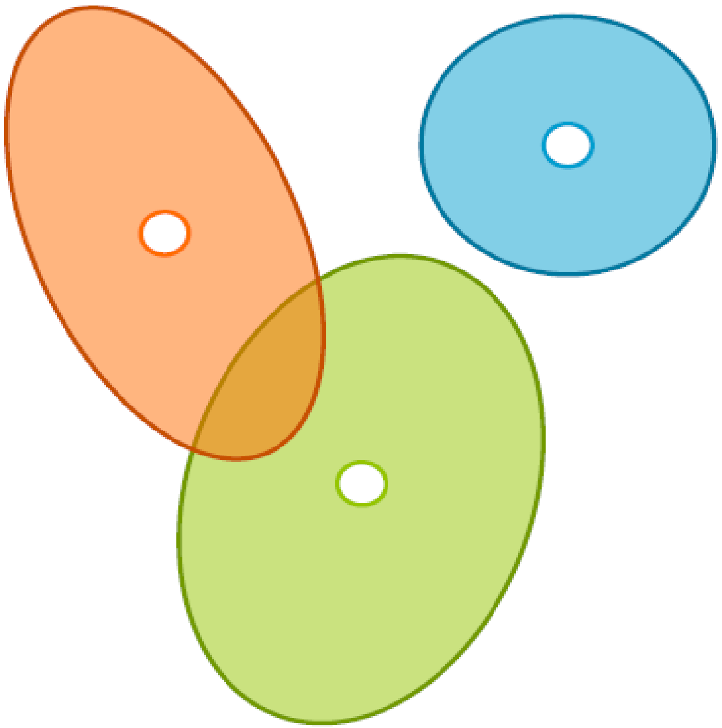
Agglomerative *a.k.a. bottom-up*: Start with each data point as its own cluster. Merge clusters until all points are in one big cluster.

- Example: single linkage

# Divisive clustering



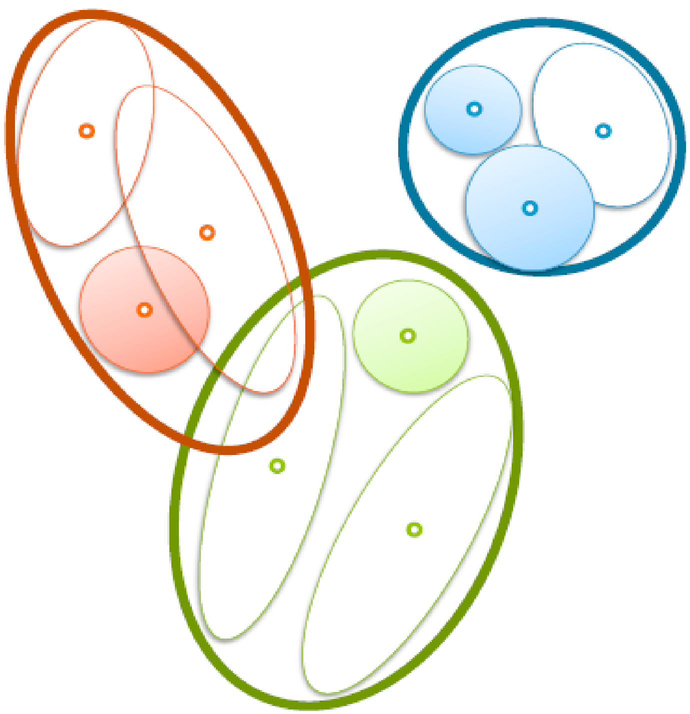
## Divisive in pictures – level 1



# Divisive clustering

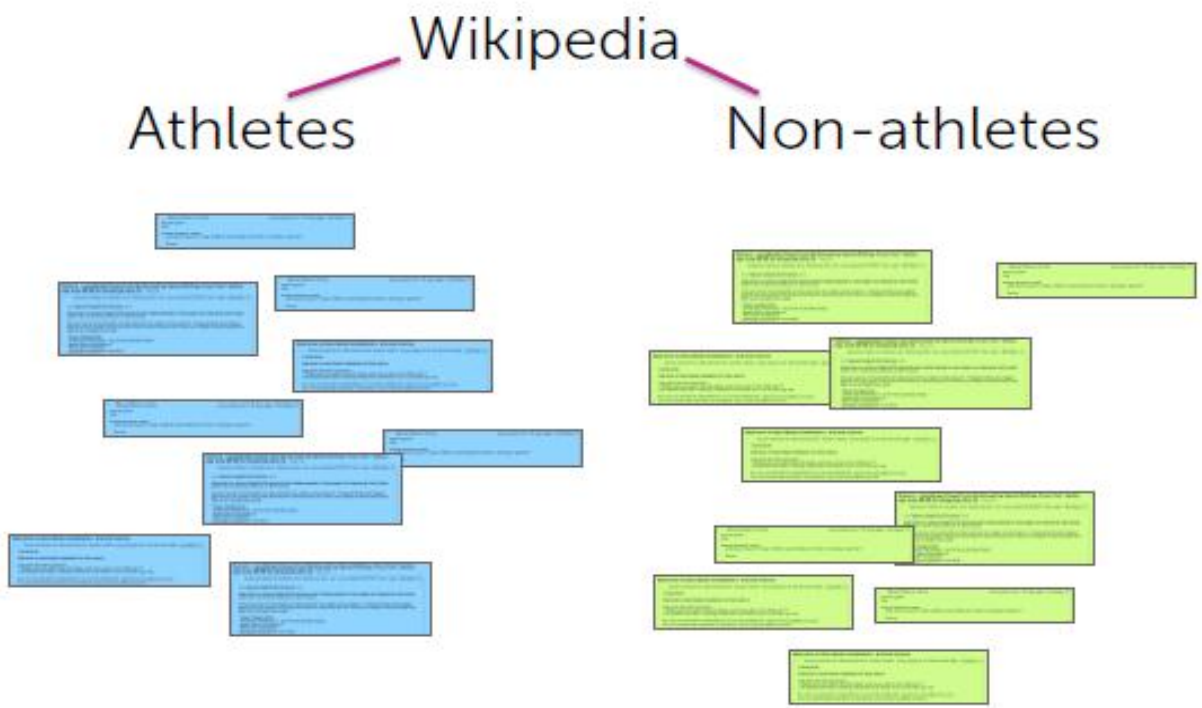


## Divisive in pictures – level 2



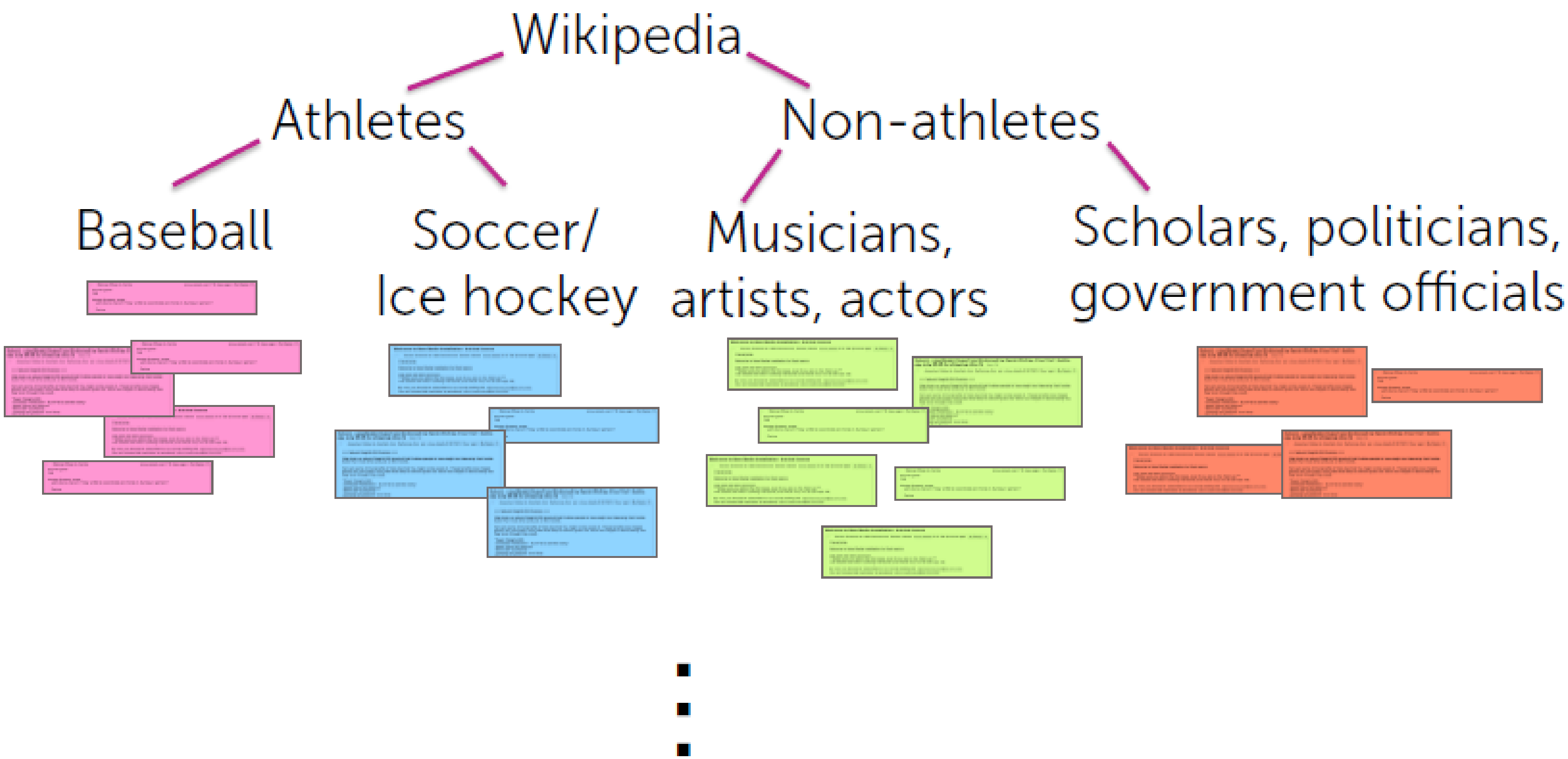
# Divisive: Recursive k-means





# Divisive: Recursive k-means





# Divisive: choices to be made

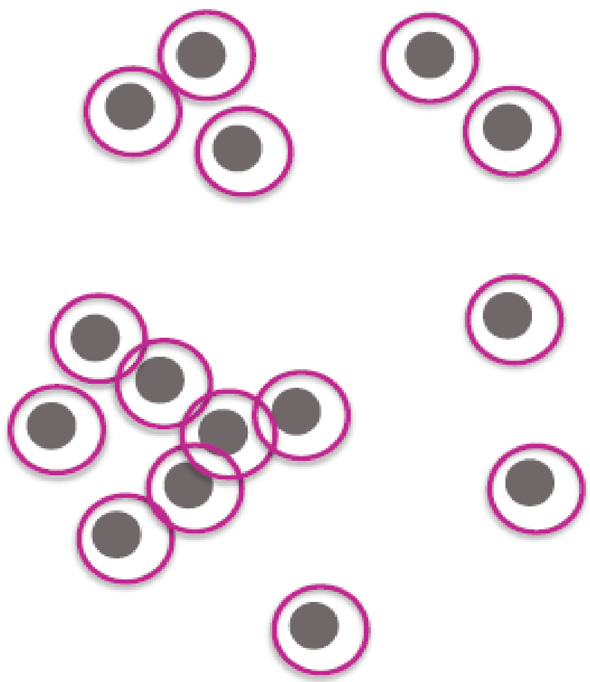


- Which algorithm to recurse
- How many clusters per split
- When to split vs. stop
  - Max cluster size:
    number of points in cluster falls below threshold
  - Max cluster radius:
    distance to furthest point falls below threshold
  - Specified # clusters:
    split until pre-specified # clusters is reached

# Aglomerative: Single linkage



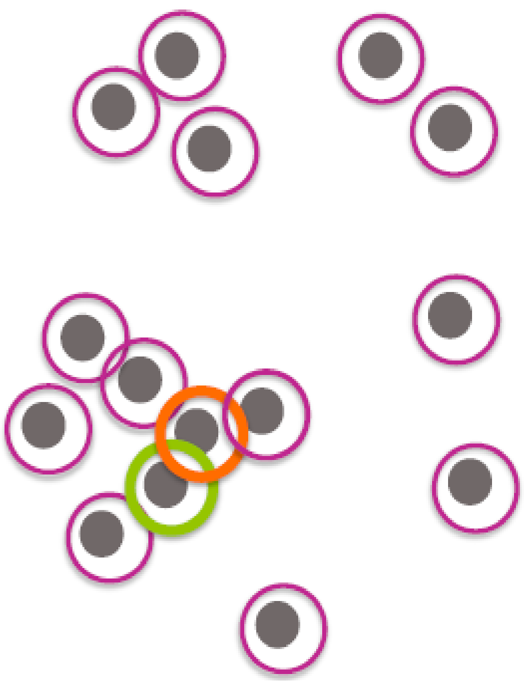
1. Initialize each point to be its own cluster



# Aglomerative: Single linkage



2. Define distance between clusters to be:



$$\text{distance}(C_1, C_2) = \boxed{\min_{\substack{x_i \text{ in } C_1,\\ x_j \text{ in } C_2}} d(\mathbf{x}_i, \mathbf{x}_j)}$$

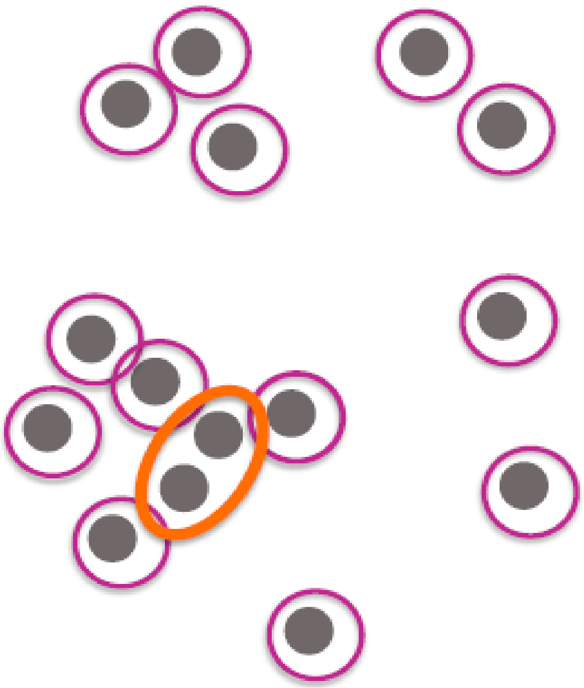
specified pairwise distance function

Linkage criteria

# Aglomerative: Single linkage



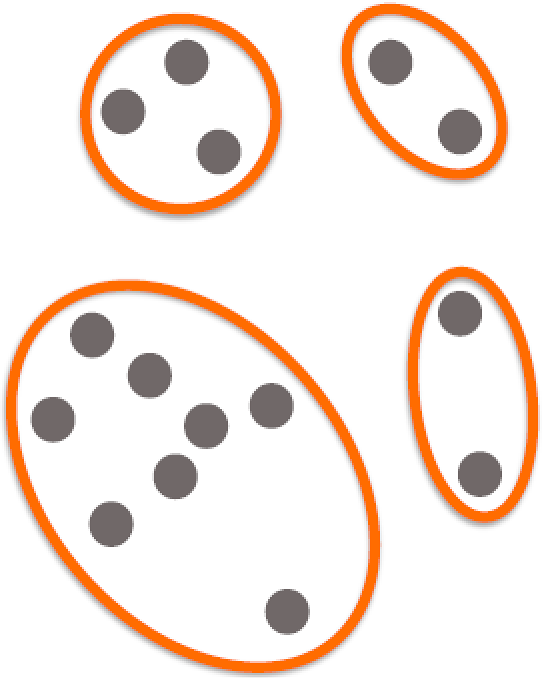
3. Merge the two closest clusters



# Aglomerative: Single linkage



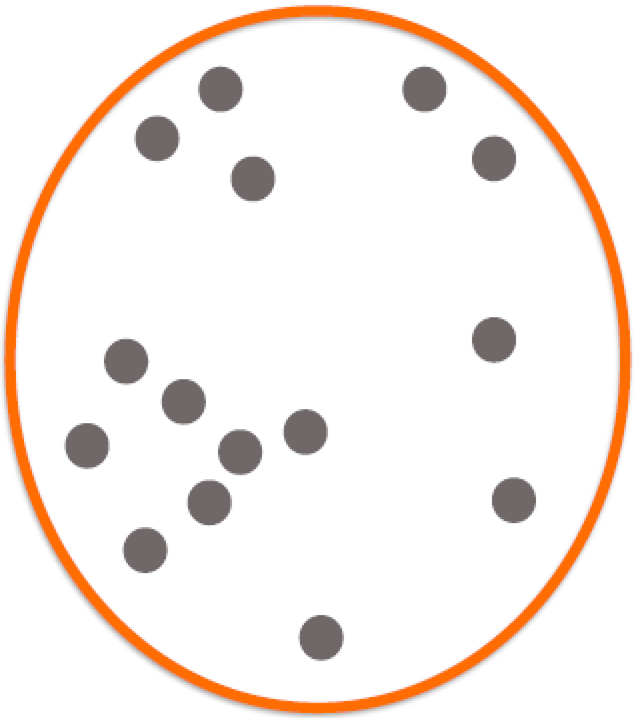
4. Repeat step 3 until all points are in one cluster



# Aglomerative: Single linkage



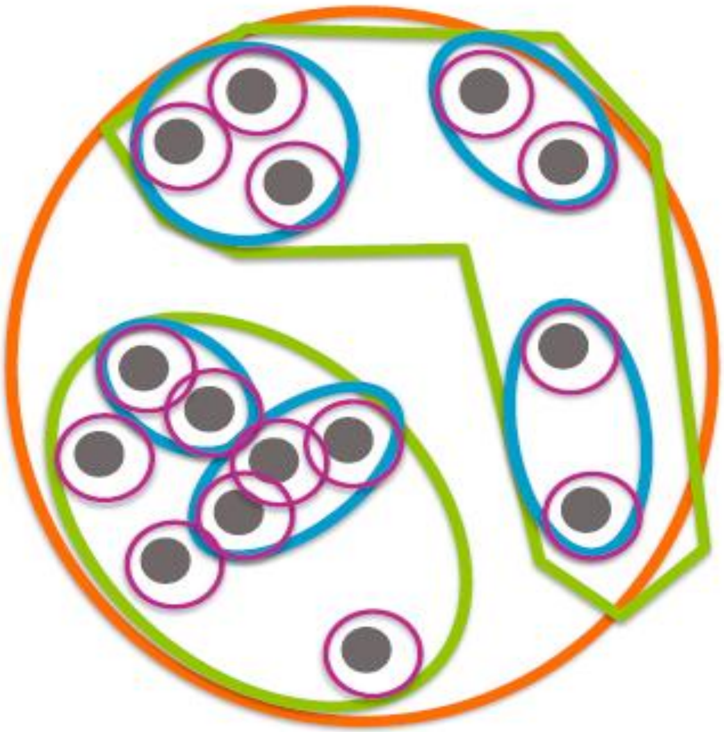
4. Repeat step 3 until all points are in one cluster



# Cluster of clusters



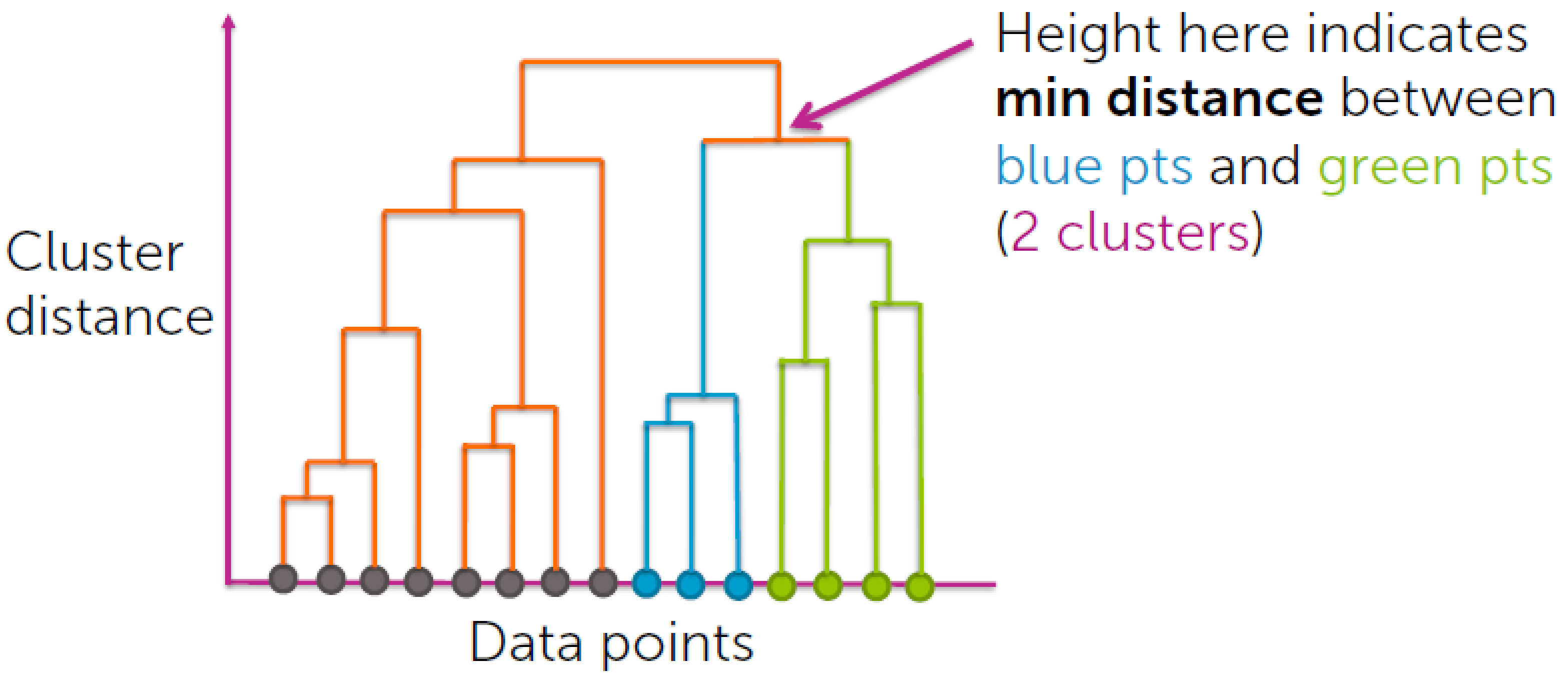
Just like our picture for divisive clustering...



# The dendrogram



- x axis shows data points (carefully ordered)
- y-axis shows distance between pair of clusters

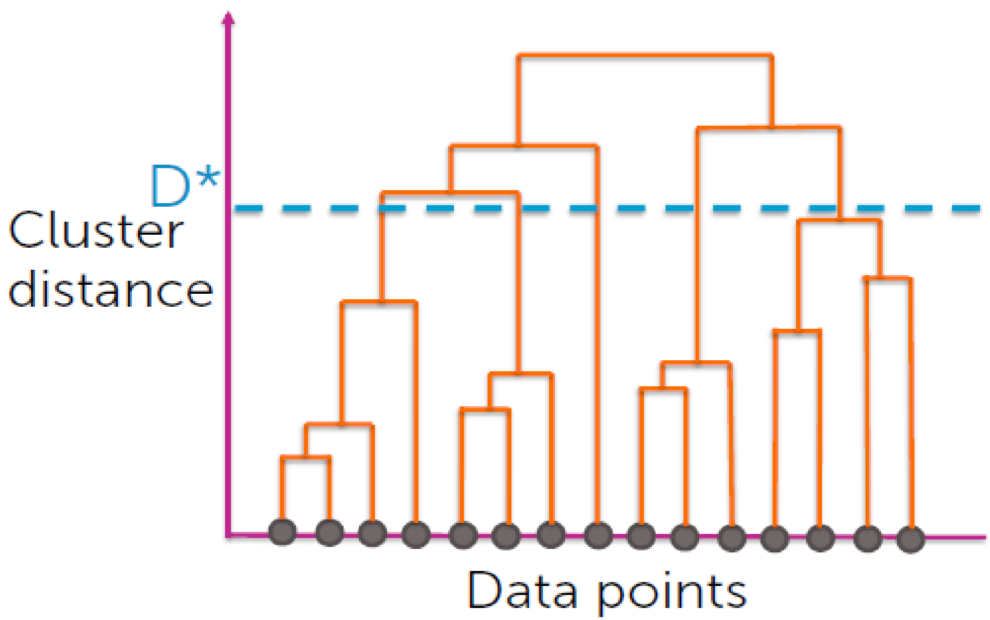


# Extracting a partition



Choose a distance D* at which to cut dendogram

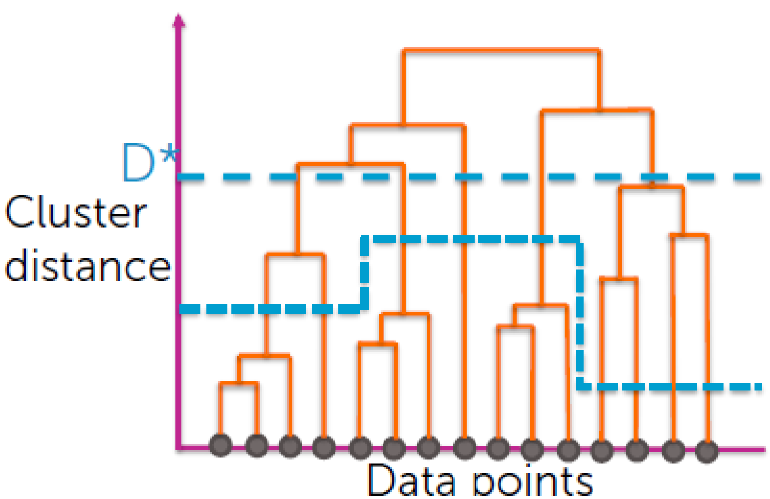
Every branch that crosses D* becomes a separate cluster



# Agglomerative: choices to be made



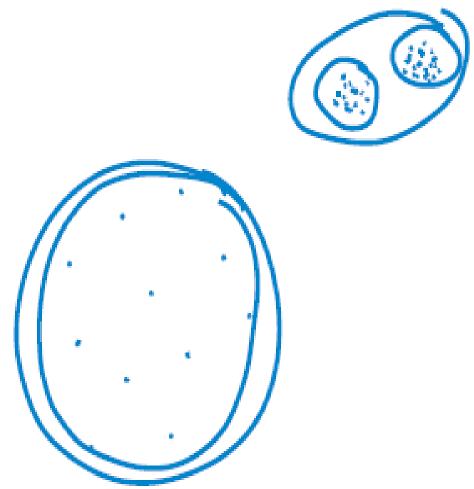
- Distance metric: $d(\mathbf{x}_i, \mathbf{x}_j)$
- Linkage function: e.g., $\min_{\mathbf{x}_i \text{ in } C_1, \mathbf{x}_j \text{ in } C_2} d(\mathbf{x}_i, \mathbf{x}_j)$
- Where and how to cut dendrogram



# More on cutting dendrogram



- For visualization, smaller # clusters is preferable
- For tasks like outlier detection, cut based on:
  - Distance threshold
  - Inconsistency coefficient
    - Compare height of merge to average merge heights below
    - If top merge is substantially higher, then it is joining two subsets that are relatively far apart compared to the members of each subset internally
    - Still have to choose a threshold to cut at, but now in terms of "inconsistency" rather than distance
- No cutting method is "incorrect", some are just more useful than others



# Computational considerations



- Computing all pairs of distances is expensive
  - Brute force algorithm is $O(N^2 \log(N))$

    # datapoints

- Smart implementations use triangle inequality to rule out candidate pairs

- Best known algorithm is $O(N^2)$