

INTRODUCTION TO DATA SCIENCE

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

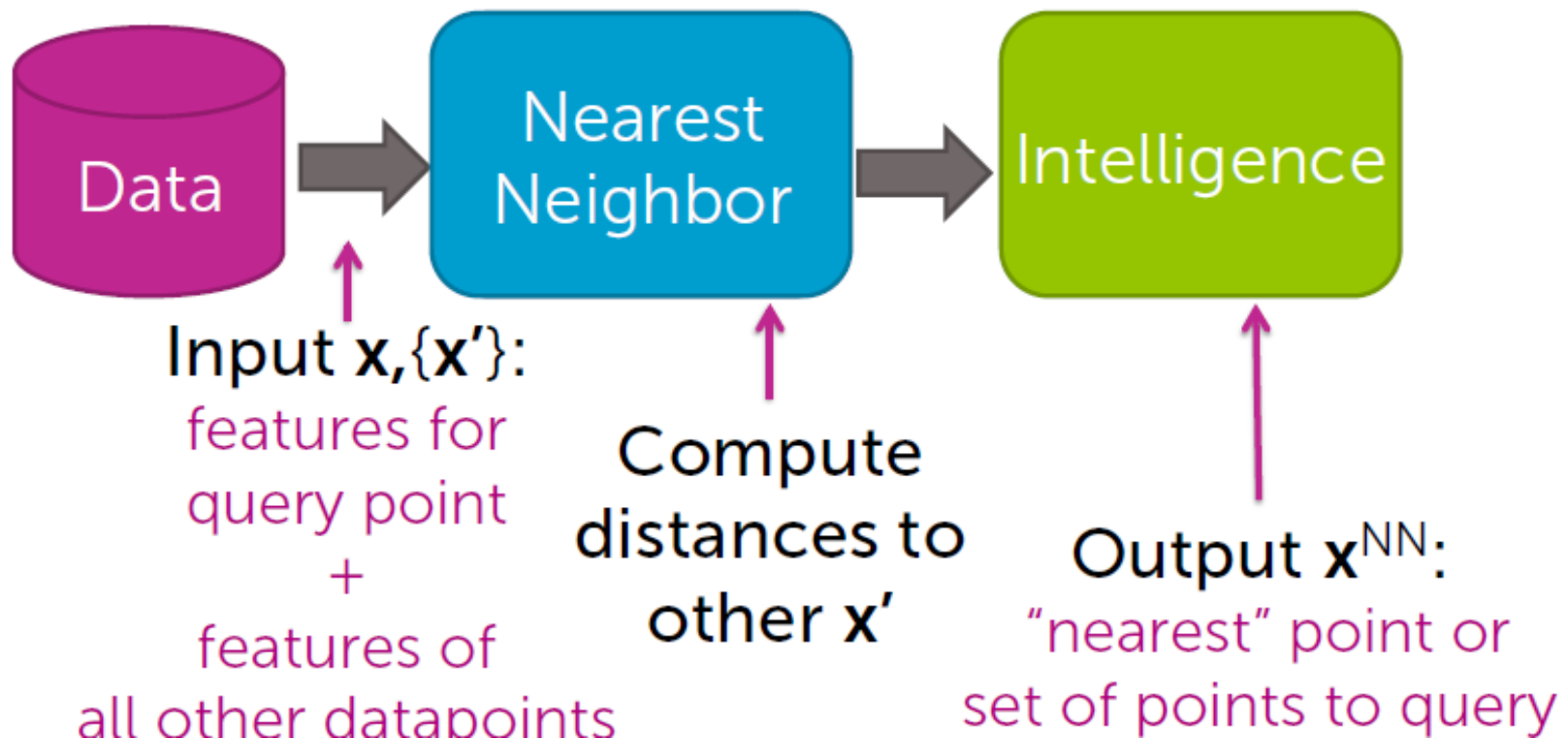
29/11, 6/12 2023

WFAiS UJ, Informatyka Stosowana
I stopień studiów

What is retrieval?

2

Search for related items



What is retrieval?

3

Retrieve “nearest neighbor” article

Space of all articles,
organized by similarity of text

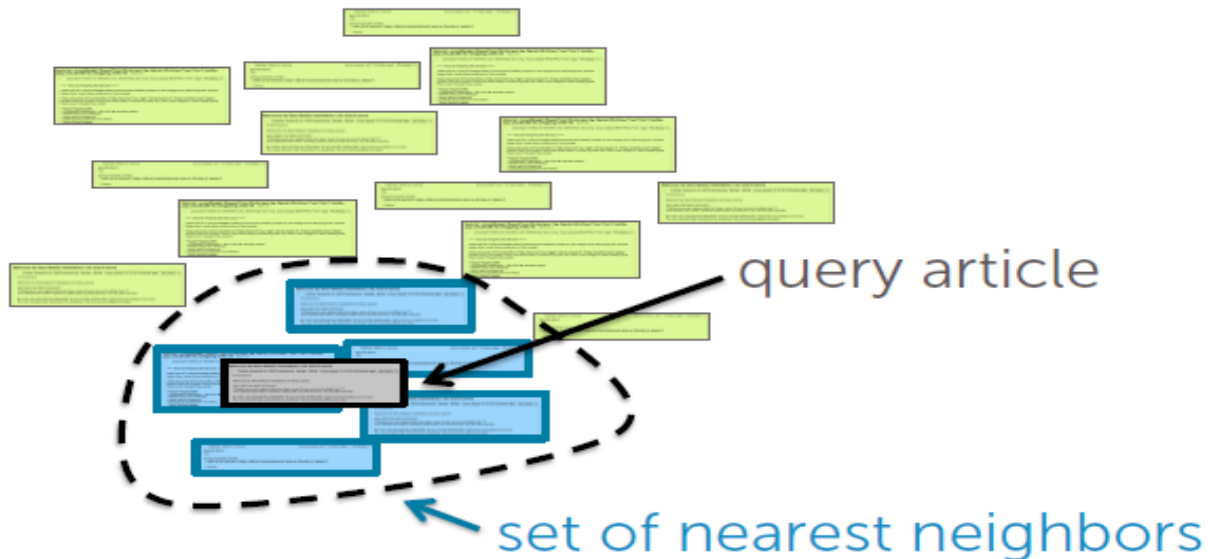


What is retrieval?

4

Or set of nearest neighbors

Space of all articles,
organized by similarity of text



Retrieval applications

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Just about everything...

Images



Products



Streaming content:

- Songs
- Movies
- TV shows
- ...

News articles



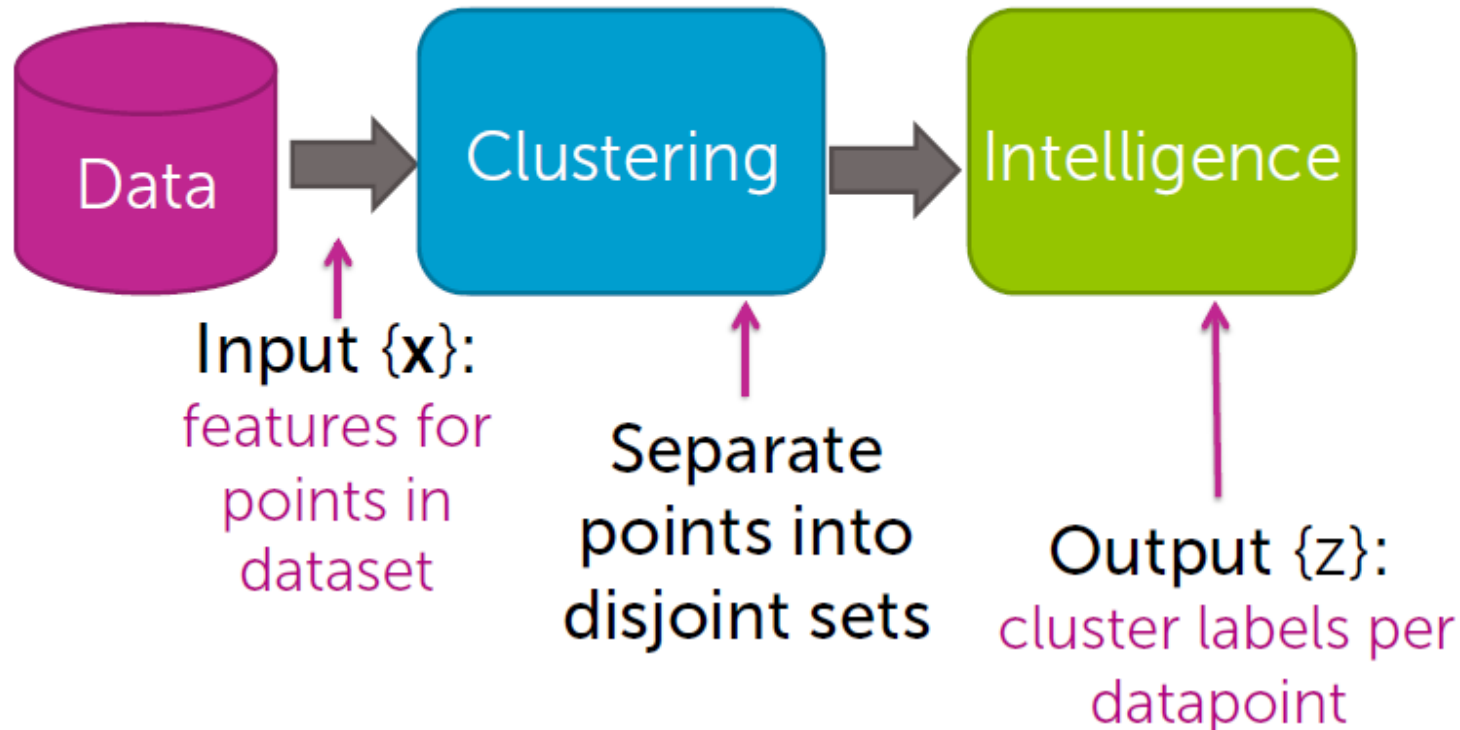
Social networks
(people you might want
to connect with)



What is clustering?

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Discover groups of similar inputs



Clustering applications

7

Clustering documents by "topic"



Clustering applications

8

Clustering images

For search, group as:

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



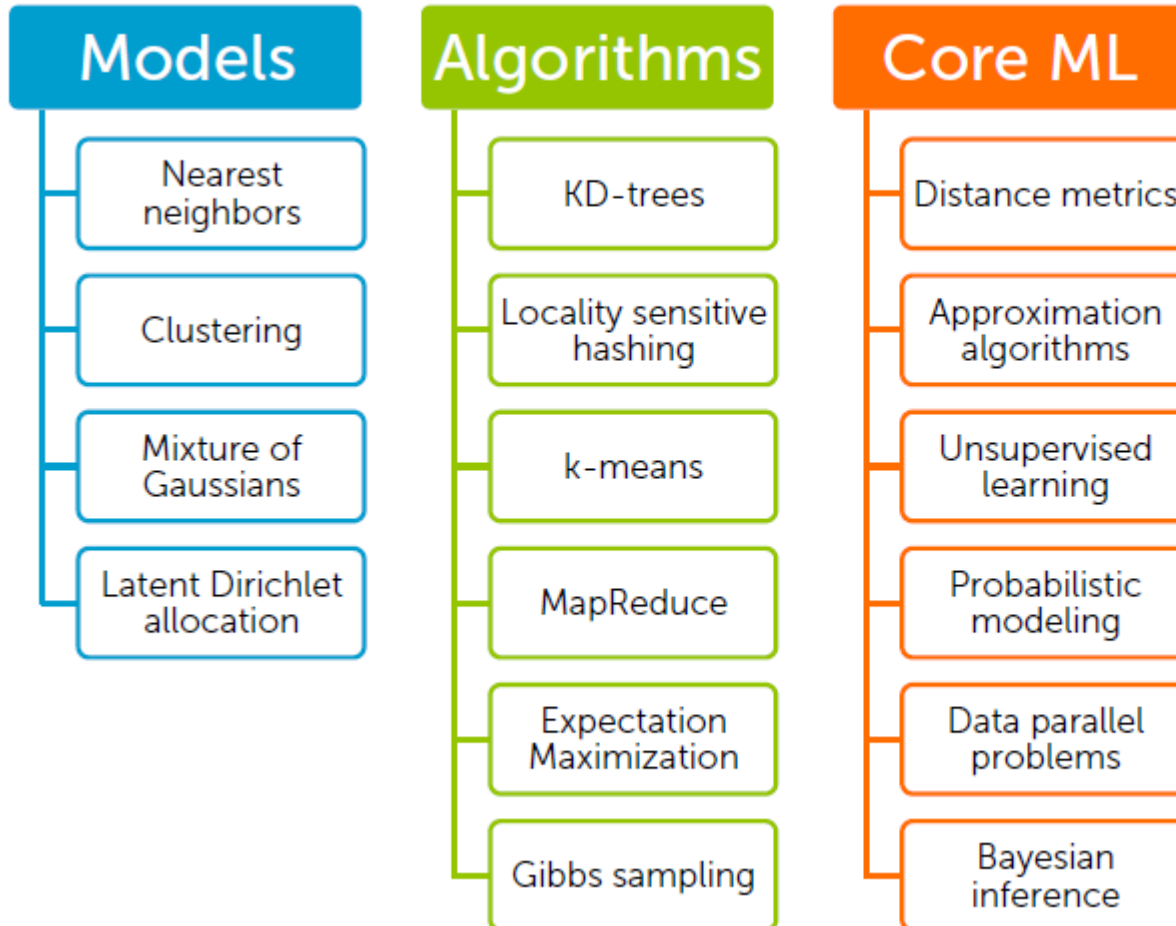
Impact of retrieval & clustering

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- 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)

Overview of content

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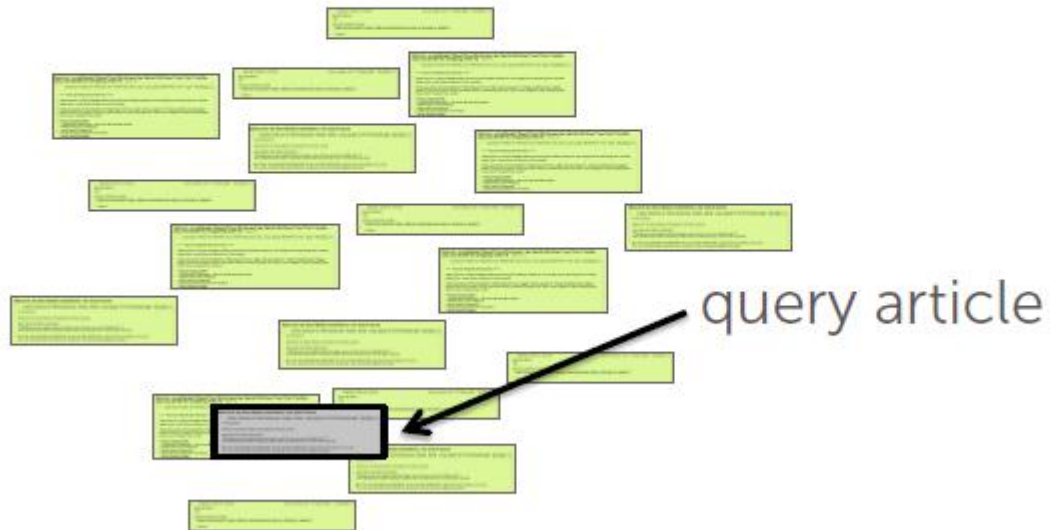


Retrieval as k-nearest neighbor search

1-NN search for retrieval

12

Space of all articles,
organized by similarity of text

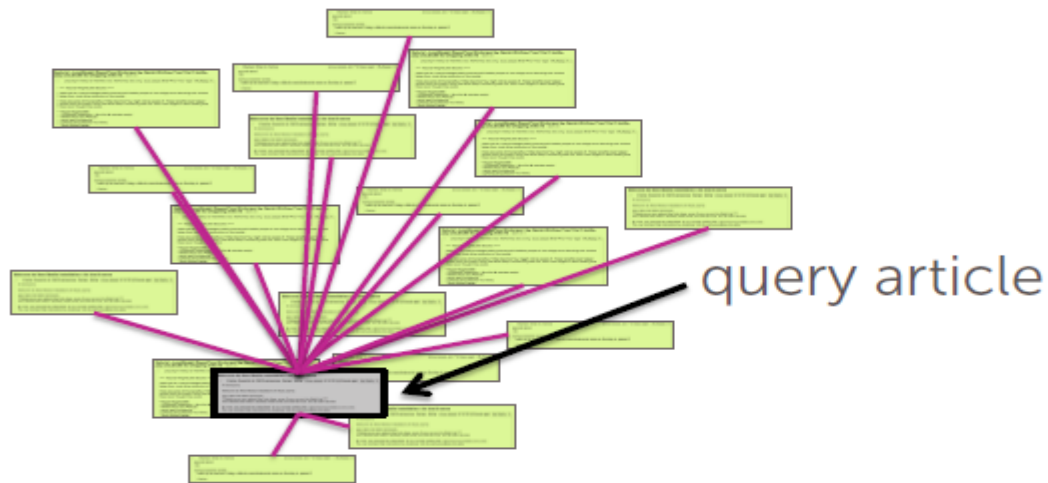


1-NN search for retrieval

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Compute distances to all docs

Space of all articles,
organized by similarity of text

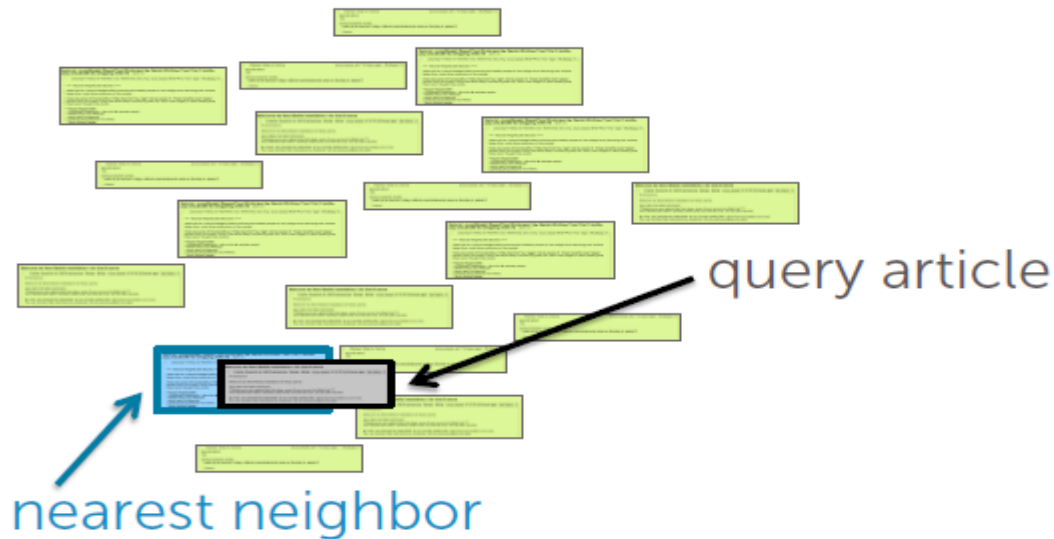


1-NN search for retrieval

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Retrieve “nearest neighbor”

Space of all articles,
organized by similarity of text

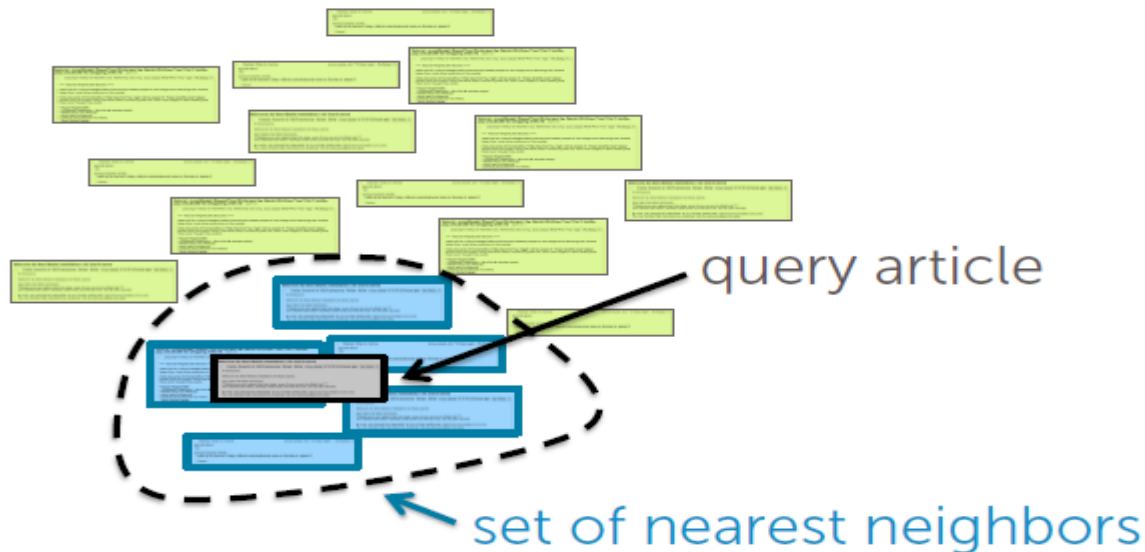


1-NN search for retrieval

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Or set of nearest neighbors

Space of all articles,
organized by similarity of text



1-NN algorithm

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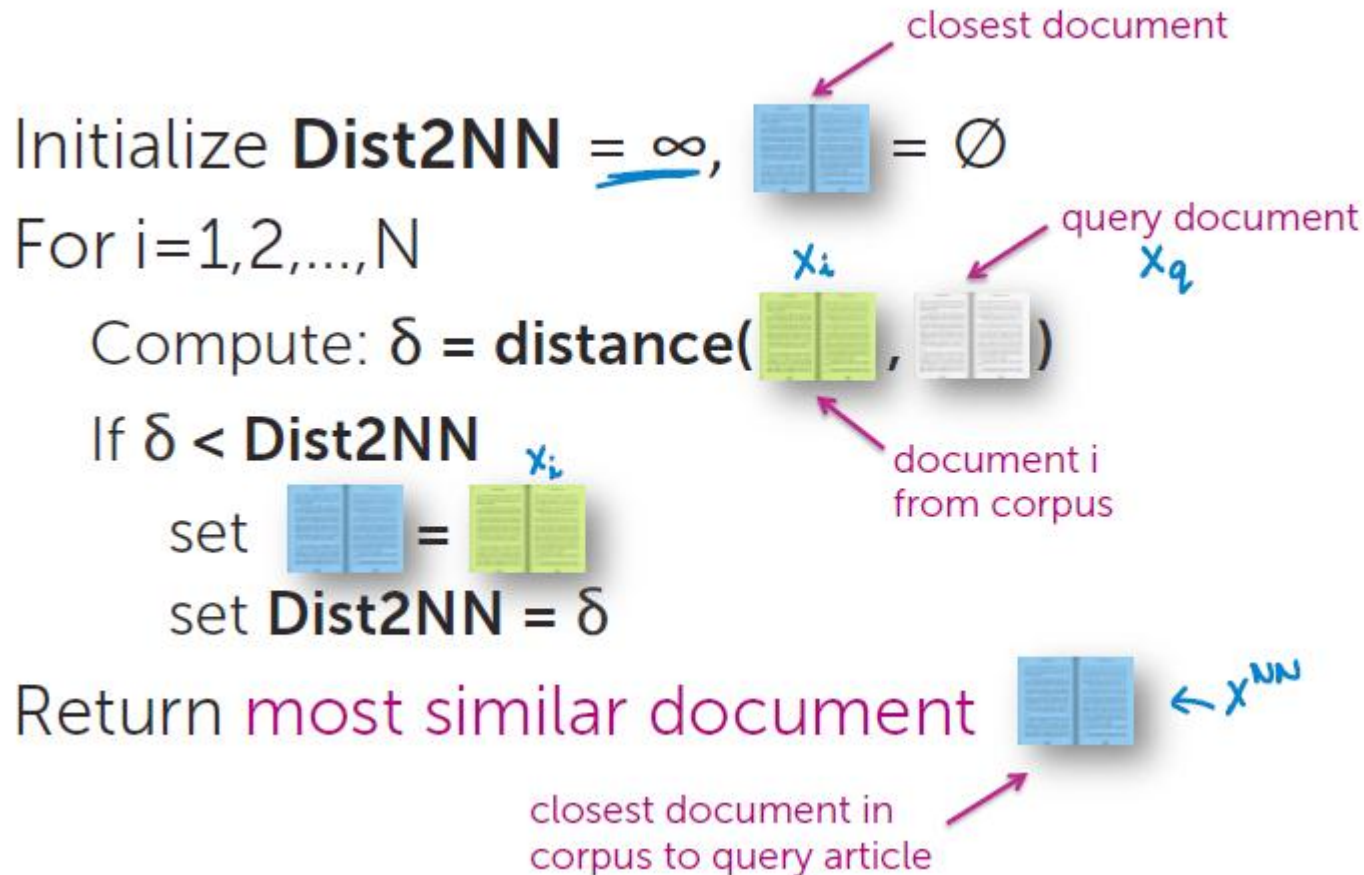
1 – Nearest neighbor

- **Input:** Query article  : \mathbf{x}_q
Corpus of documents (N docs)
 : $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$
- **Output:** *Most* similar article  $\leftarrow \mathbf{x}^{NN}$

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

1-NN algorithm

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k-NN algorithm

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- **Input:** Query article  : \mathbf{x}_q
Corpus of documents
 : $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$
- **Output:** *List of k* similar articles



Formally:

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

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

k-NN algorithm

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Initialize **Dist2kNN** = $\text{sort}(\delta_1, \dots, \delta_k)$ ← list of sorted distances
 = $\text{sort}(\dots, \text{dist}(\text{doc}_1, \text{query doc}), \dots, \text{dist}(\text{doc}_k, \text{query doc}))$ ← list of sorted docs

For $i=k+1, \dots, N$

Compute: $\delta = \text{distance}(\text{doc}_i, \text{query doc})$

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

find j such that $\delta > \text{Dist2kNN}[j-1]$ but $\delta < \text{Dist2kNN}[j]$

remove furthest house and shift queue:

$\text{Dist2kNN}[1:k] = \text{Dist2kNN}[1:j-1]$

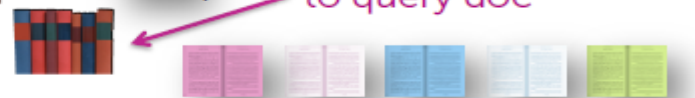
inserting new article

$\text{Dist2kNN}[j+1:k] = \text{Dist2kNN}[j:k-1]$

set $\text{Dist2kNN}[j] = \delta$ and $\text{docs}[j] = \text{doc}_i$

closest k docs to query doc

Return k most similar articles



Critical elements of NN search

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Item (e.g., doc) representation

$\mathbf{x}_q \leftarrow$



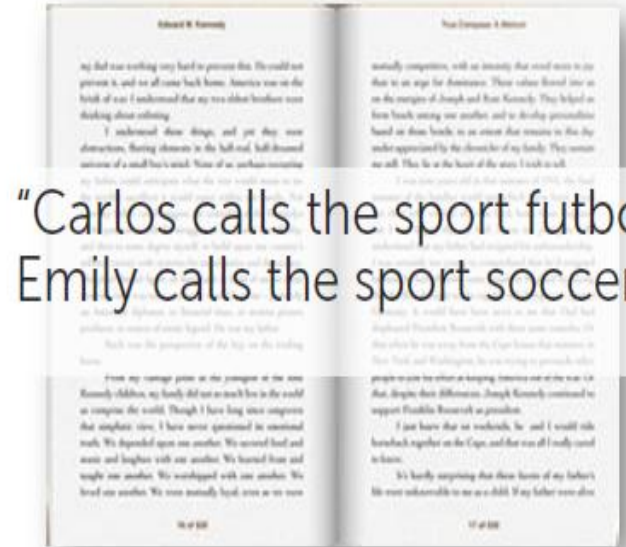
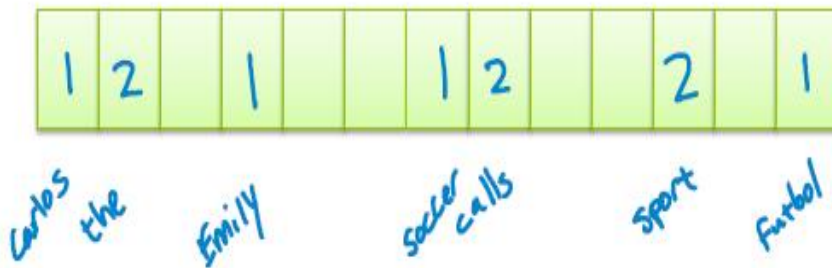
Measure of distance between items:

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

Document representation

Bag of words model

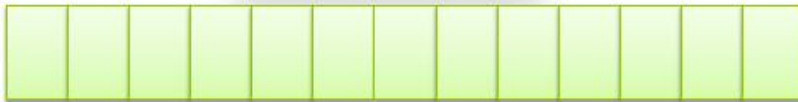
- Ignore order of words
- Count # of instances of each word in vocabulary



Document representation

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Issues with word counts – Rare words



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

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

Document representation

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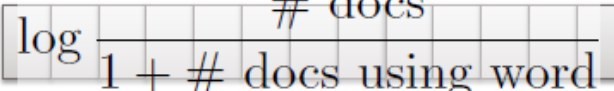
TF-IDF document representation

Emphasizes important words

- Appears frequently in document (common locally)

Term frequency = 

- Appears rarely in corpus (rare globally)

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

Trade off: local frequency vs. global rarity



tf * idf

Distance metrics:

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Distance metrics: Defining notion of “closest”

In 1D, just Euclidean distance:

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

In multiple dimensions:

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

Distance metrics:

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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



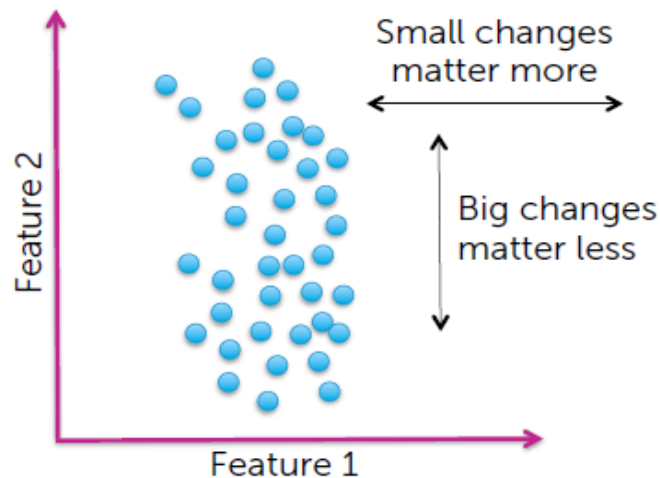
Distance metrics:

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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:

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Scaled Euclidean distance

Formally, this is achieved via

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

weight on each feature
(defining relative importance)

Distance metrics:

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Effect of binary weights

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

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

Setting weights as 0 or 1
is equivalent to
feature selection

Feature engineering/
selection is
important, but hard

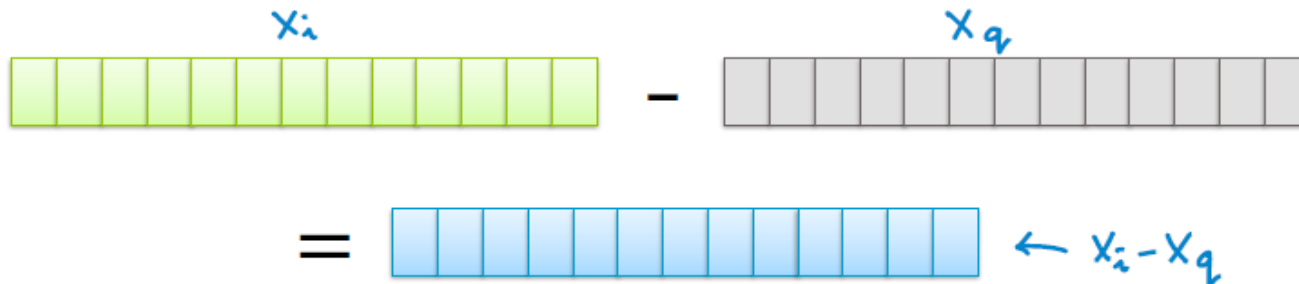
Distance metrics:

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(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:

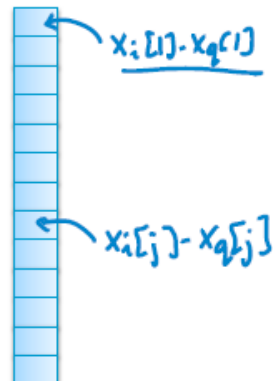
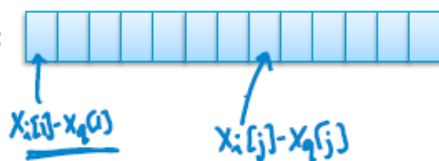
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(non-scaled) Euclidean distance

Defined in terms of inner product

$$\text{distance}(\mathbf{x}_i, \mathbf{x}_q) = \sqrt{(\mathbf{x}_i - \mathbf{x}_q)^T (\mathbf{x}_i - \mathbf{x}_q)} \leftarrow$$
$$\sqrt{(x_i[1] - x_q[1])^2 + \dots + (x_i[d] - x_q[d])^2}$$

distance² =



take
sq.r.t.

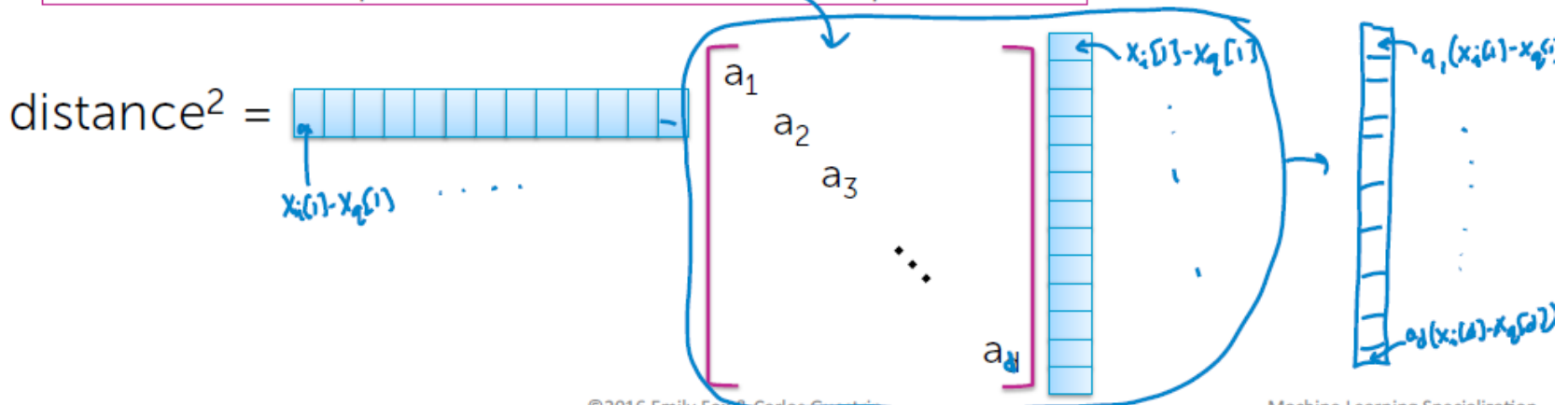
Distance metrics:

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Scaled Euclidean distance

Defined in terms of inner product

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





Distance metrics:

Another natural inner product measure



x_q

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



x_i

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

Similarity

$$\begin{aligned} &= \mathbf{x}_i^T \mathbf{x}_q \\ &= \sum_{j=1}^d \mathbf{x}_i[j] \mathbf{x}_q[j] \\ &= 13 \end{aligned}$$

Distance metrics:

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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

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Cosine similarity – normalize

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

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

$$\mathbf{a}^T \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos(\theta)$$

$$\mathbf{x}_i^T \mathbf{x}_q = \cos(\theta)$$

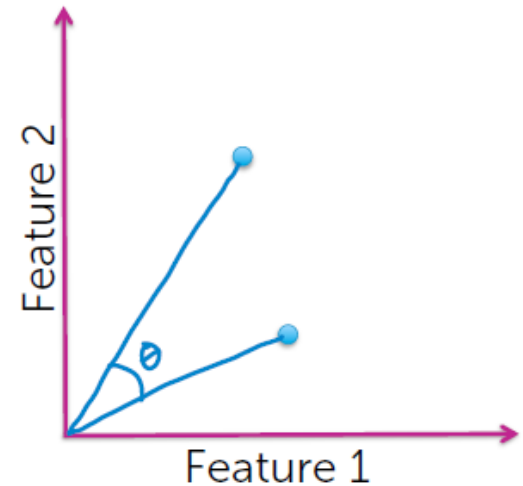
$$\frac{\mathbf{x}_i^T \mathbf{x}_q}{\|\mathbf{x}_i\| \|\mathbf{x}_q\|}$$

$$= \left(\frac{\mathbf{x}_i}{\|\mathbf{x}_i\|} \right)^T \left(\frac{\mathbf{x}_q}{\|\mathbf{x}_q\|} \right)$$

First normalize

- 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
---	---	---	---	---	---	---	---	---	---	---	---	---

← x_i

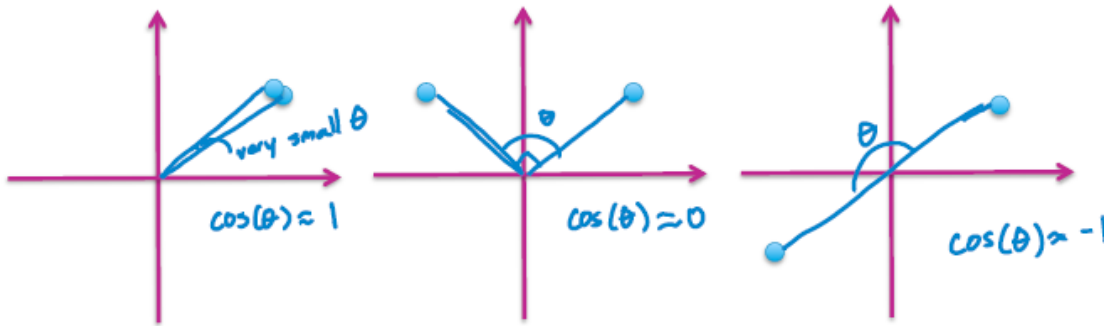
$$\sqrt{(1^2 + 5^2 + 3^2 + 1^2)} \leftarrow \|x_i\| = \sum_{j=1}^d x_i[j]^2$$

1				5	3			1				
/	0	0	0	/	/	0	0	/	0	0	0	0
6				6	6			6				

Distance metrics

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Cosine similarity



In general, $-1 < \text{similarity} < 1$

For positive features (like tf-idf)

$0 < \text{similarity} < 1$

} our focus



Define **distance = 1-similarity**

Distance metrics

To normalize or not?



1 0 0 0 5 3 0 0 1 0 0 0 0

3 1 0 0 2 0 0 1 0 1 0 0 0

Similarity = 13



2 0 0 0 10 6 0 0 2 0 0 0 0

6 2 0 0 4 0 0 2 0 2 0 0 0

Similarity = 52



Distance metrics

In the normalized case

Document 1

...the first part of the paper, the author ...

Document 2

...the second part of the paper, the author ...

Document 3

...the third part of the paper, the author ...

Document 4

...the fourth part of the paper, the author ...

1				5	3			1				
/	0	0	0	/	/	0	0	/	0	0	0	0
6				6	6			6				

3	1			1			1	1				
/	/	0	0	/	0	0	/	0	/	0	0	0
4	4			2			4	4				

Similarity = 13/24

Document 1

...the first part of the paper, the author ...

Document 2

...the second part of the paper, the author ...

Document 3

...the third part of the paper, the author ...

Document 4

...the fourth part of the paper, the author ...

1				5	3			1				
/	0	0	0	/	/	0	0	/	0	0	0	0
6				6	6			6				

3	1			1			1	1				
/	/	0	0	/	0	0	/	0	/	0	0	0
4	4			2			4	4				

Similarity = 13/24

Distance metrics

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But not always desired...



long document

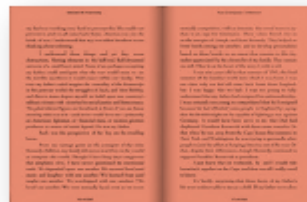


short tweet

Normalizing can
make dissimilar
objects appear
more similar



long document



long document

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

Distance metrics

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Other distance metrics

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

Combining distance metrics

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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

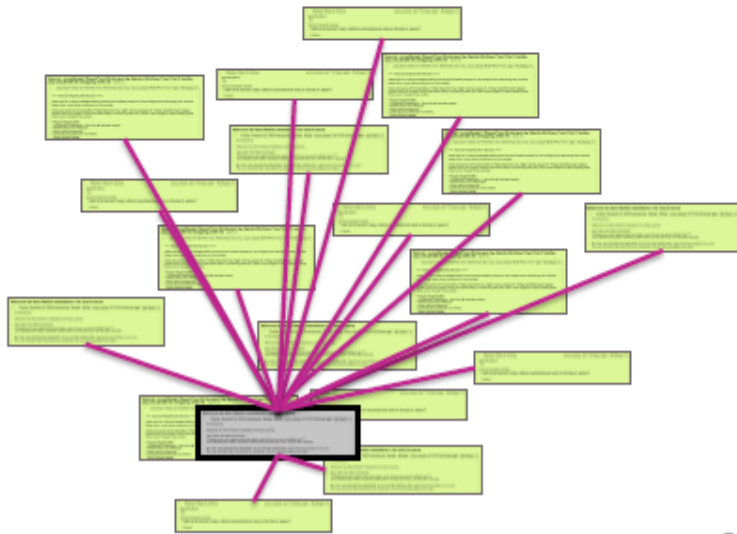
Scaling up k-NN search by storing data in a KD-tree

Complexity of brute-force search

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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)

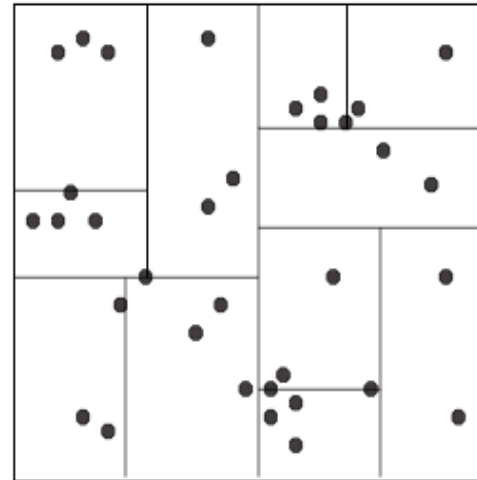
KD-trees

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Structured organization of documents

- Recursively partitions points into axis aligned boxes.

Enables more efficient pruning of search space



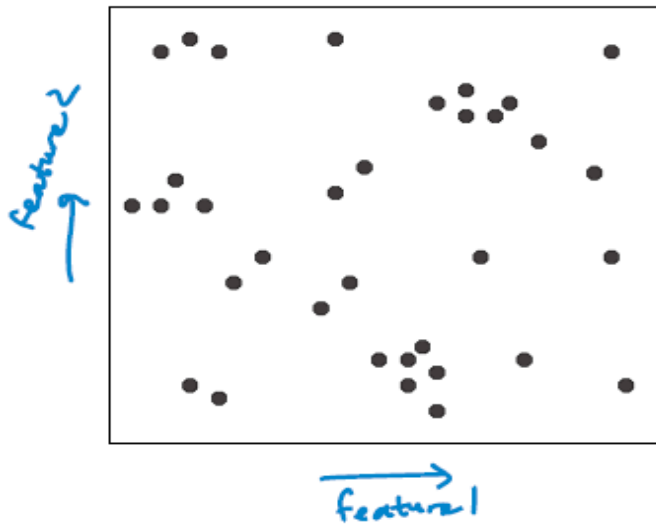
Works "well" in "low-medium" dimensions

- We'll get back to this...

KD-trees

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KD-tree construction



Start with a list of d-dimensional points.

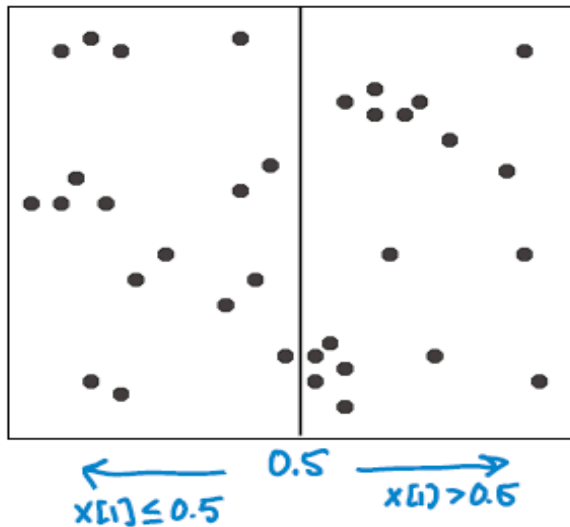
Pt	x[1]	x[2]
1	0.00	0.00
2	1.00	4.31
3	0.13	2.85
...

obs. indices
↑
Feat. 1 (word 1)
↑
Feat. 2 (word 2)
↑

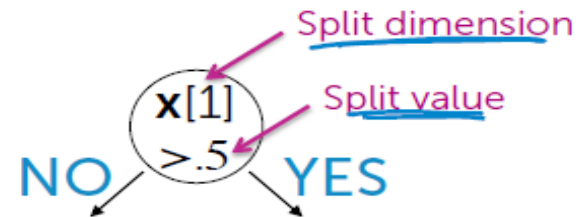
KD-trees

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KD-tree construction



Split points into 2 groups

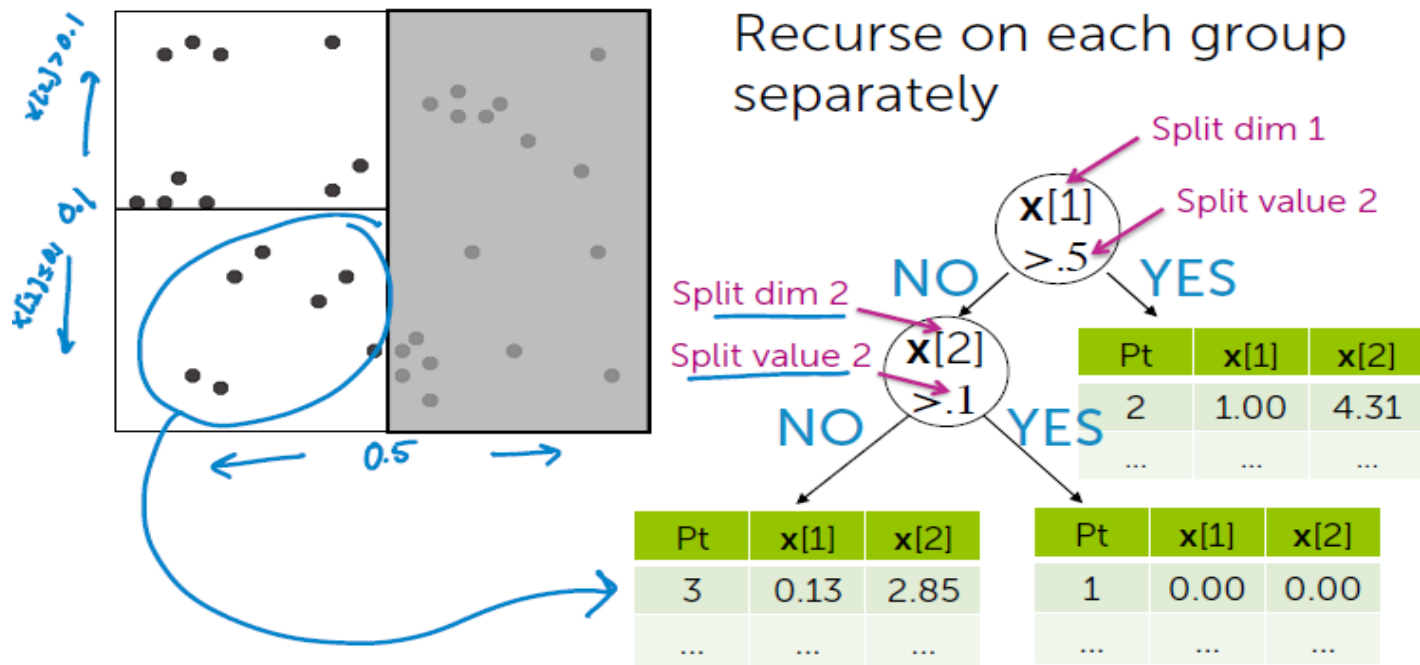


Pt	x[1]	x[2]	Pt	x[1]	x[2]
1	0.00	0.00	2	1.00	4.31
3	0.13	2.85
...

KD-trees

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KD-tree construction

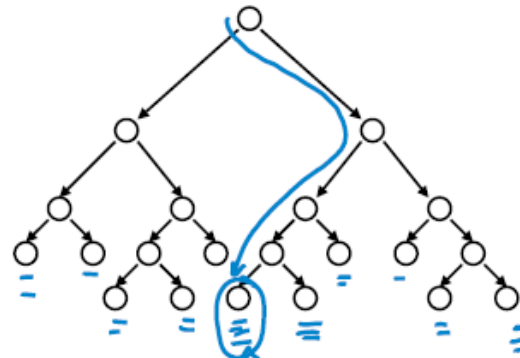
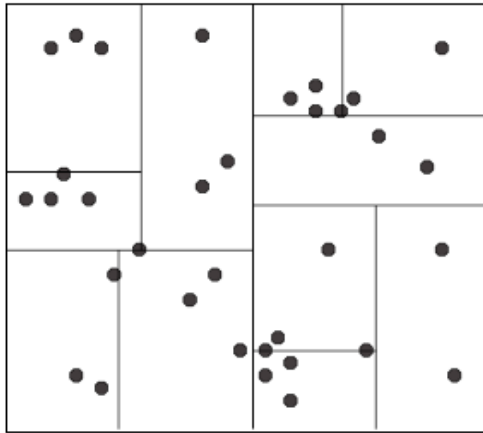


--

KD-trees

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KD-tree construction



points here
satisfy all
conditions down
the tree to
this leaf

Continue splitting points at each set

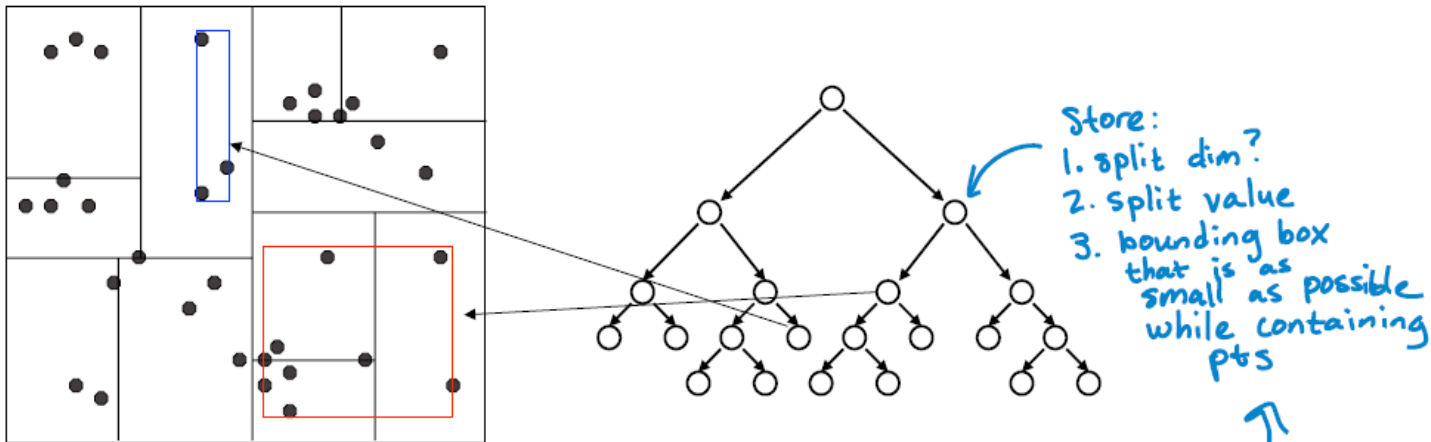
- Creates a binary tree structure

Each leaf node contains a list of points

KD-trees

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KD-tree construction



Keep one additional piece of info at each node:

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

KD-trees

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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

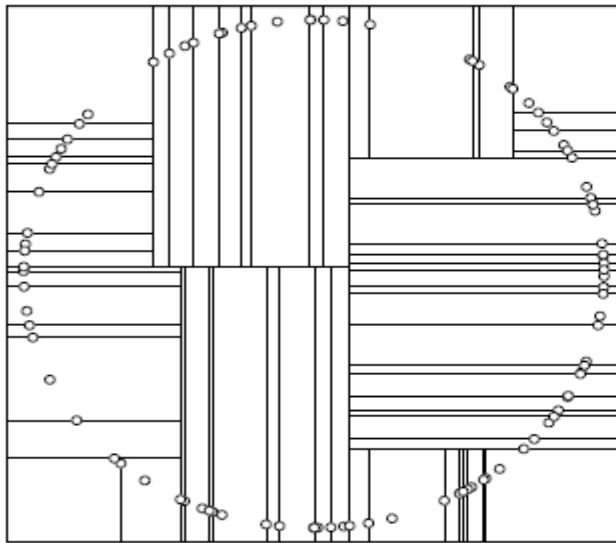
or

box hits minimum width

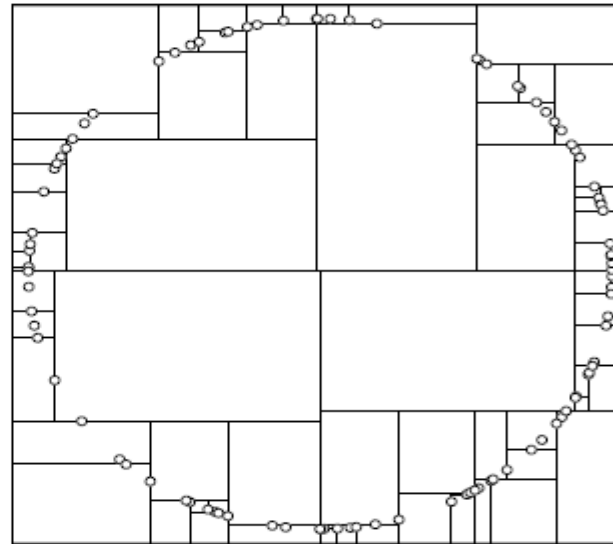
KD-trees

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Many heuristics...



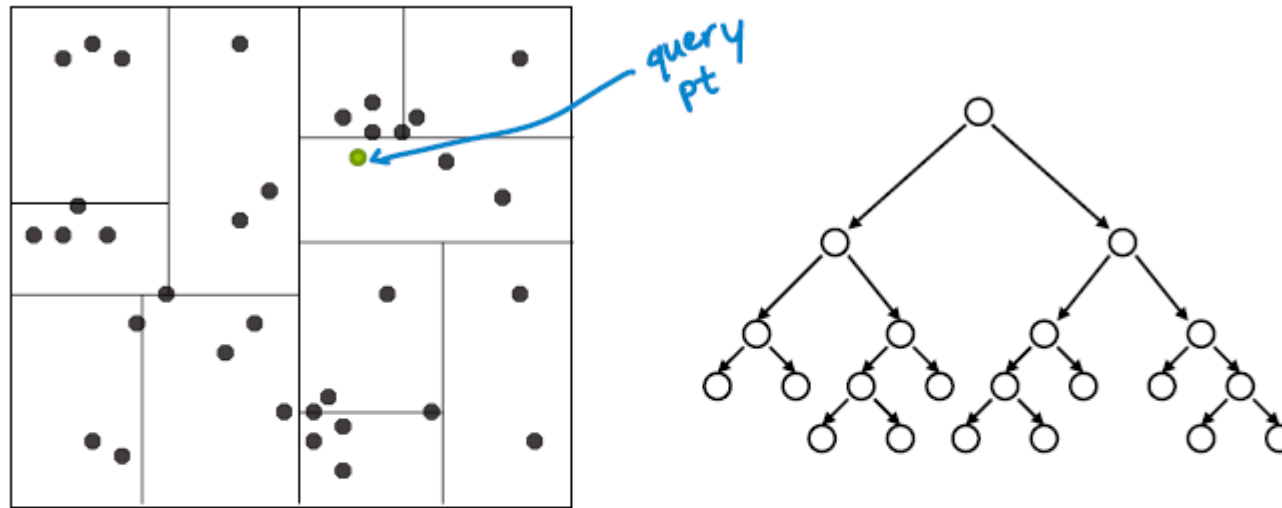
median heuristic



center-of-range
heuristic

Nearest neighbor with KD-trees

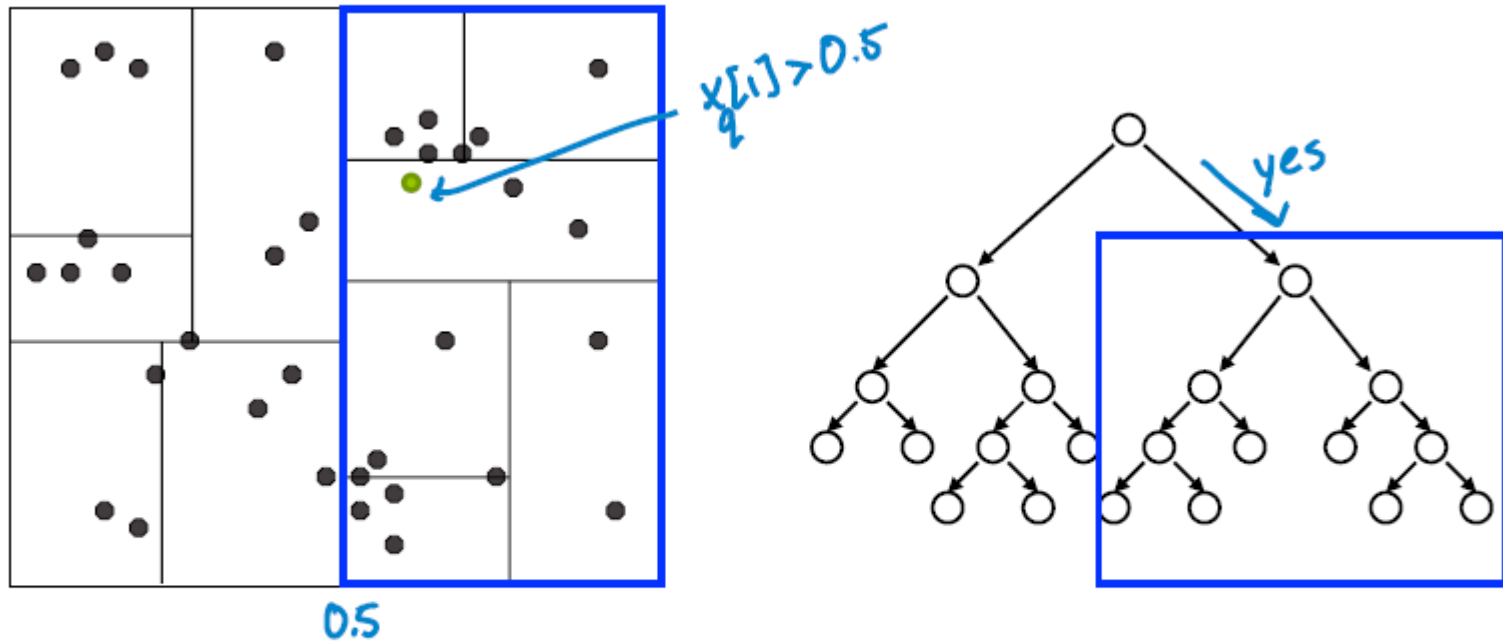
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Traverse tree looking for nearest neighbor to query point

Nearest neighbor with KD-trees

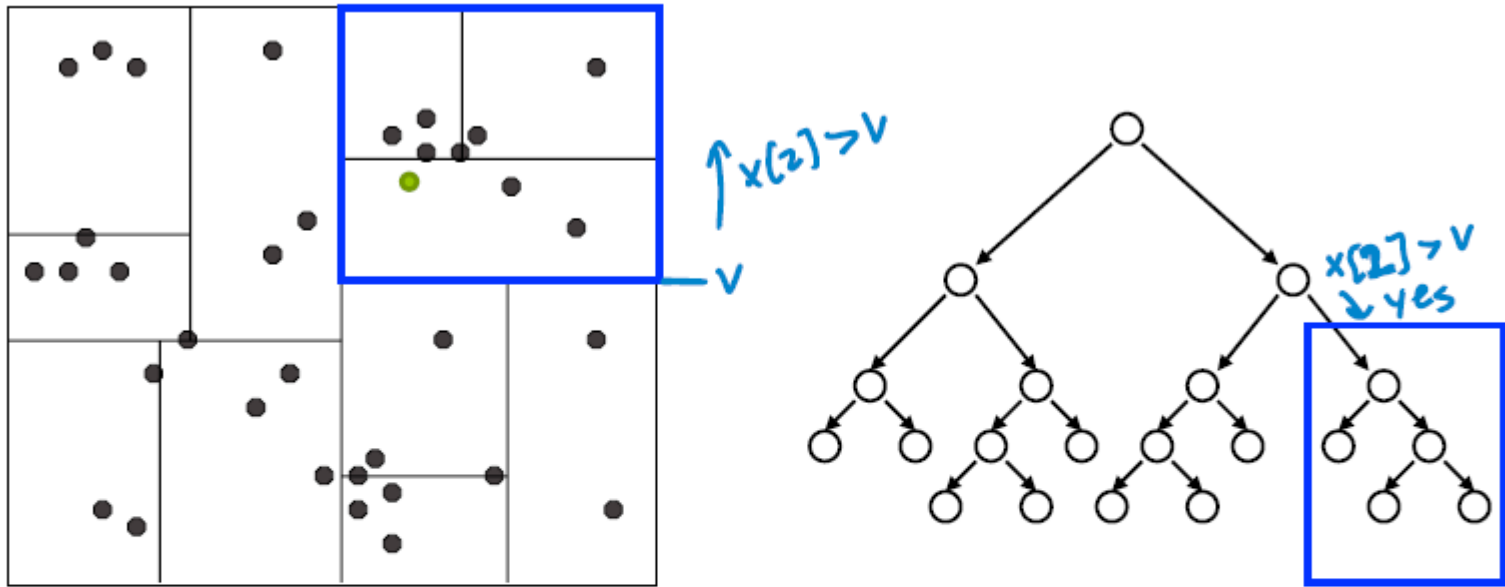
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1. Start by exploring leaf node containing query point

Nearest neighbor with KD-trees

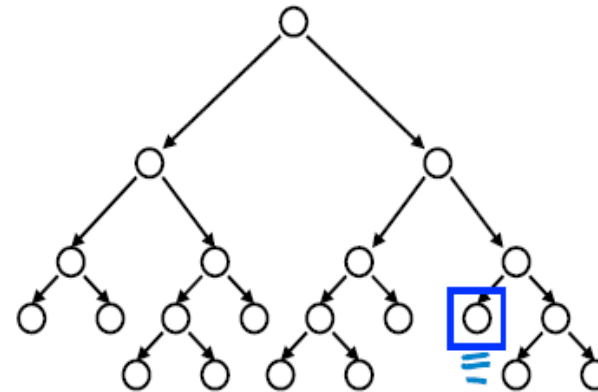
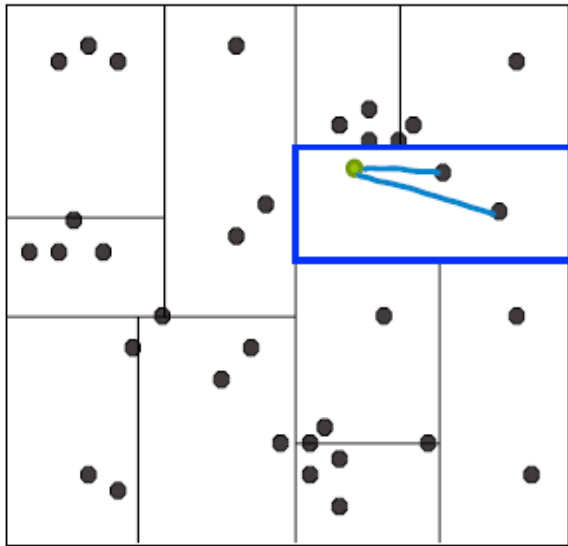
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1. Start by exploring leaf node containing query point

Nearest neighbor with KD-trees

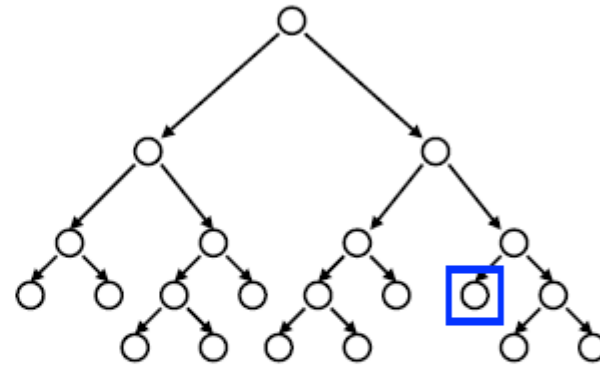
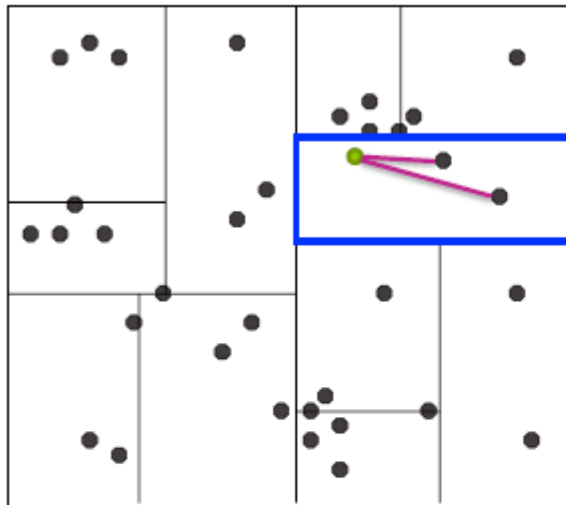
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1. Start by exploring leaf node containing query point

Nearest neighbor with KD-trees

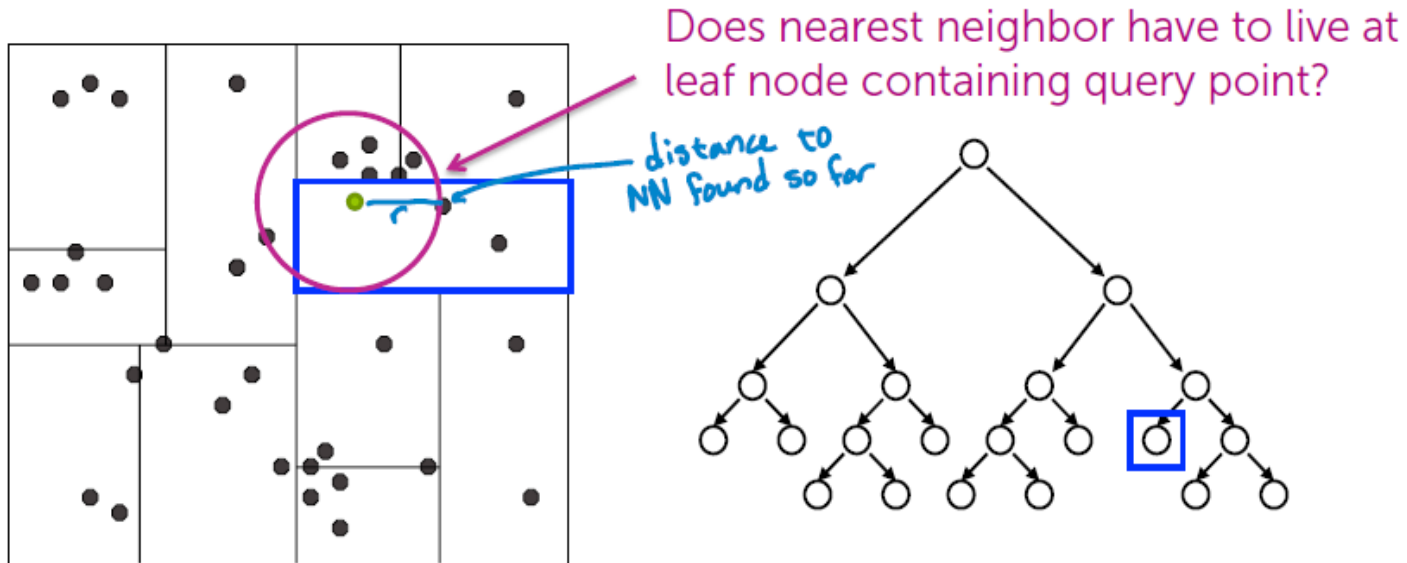
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1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node

Nearest neighbor with KD-trees

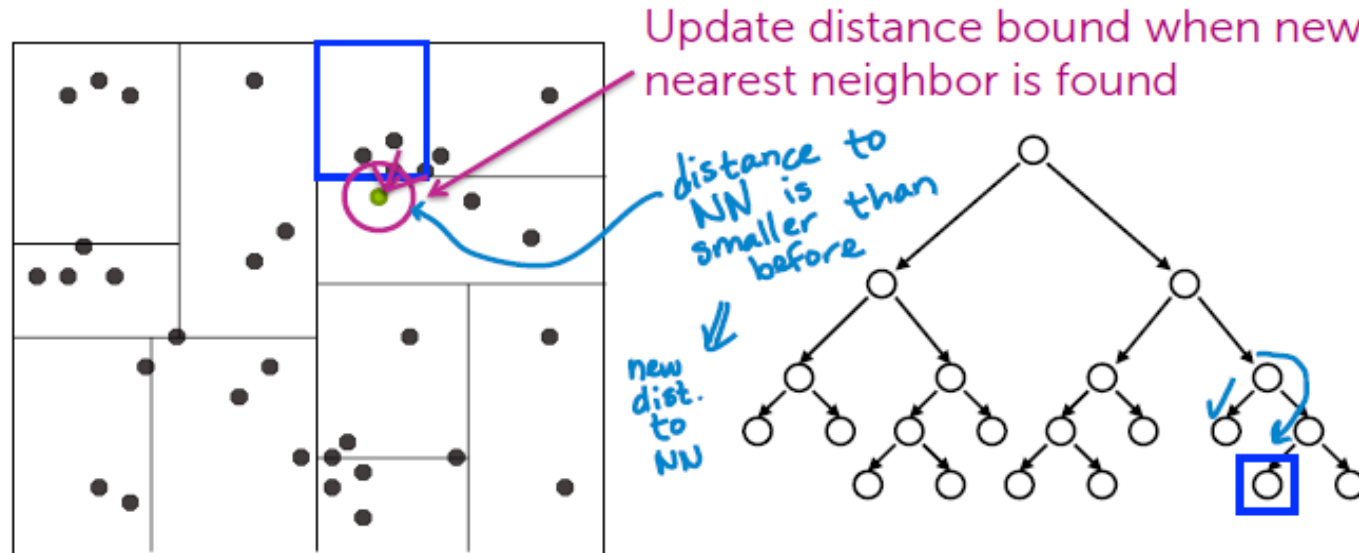
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1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node

Nearest neighbor with KD-trees

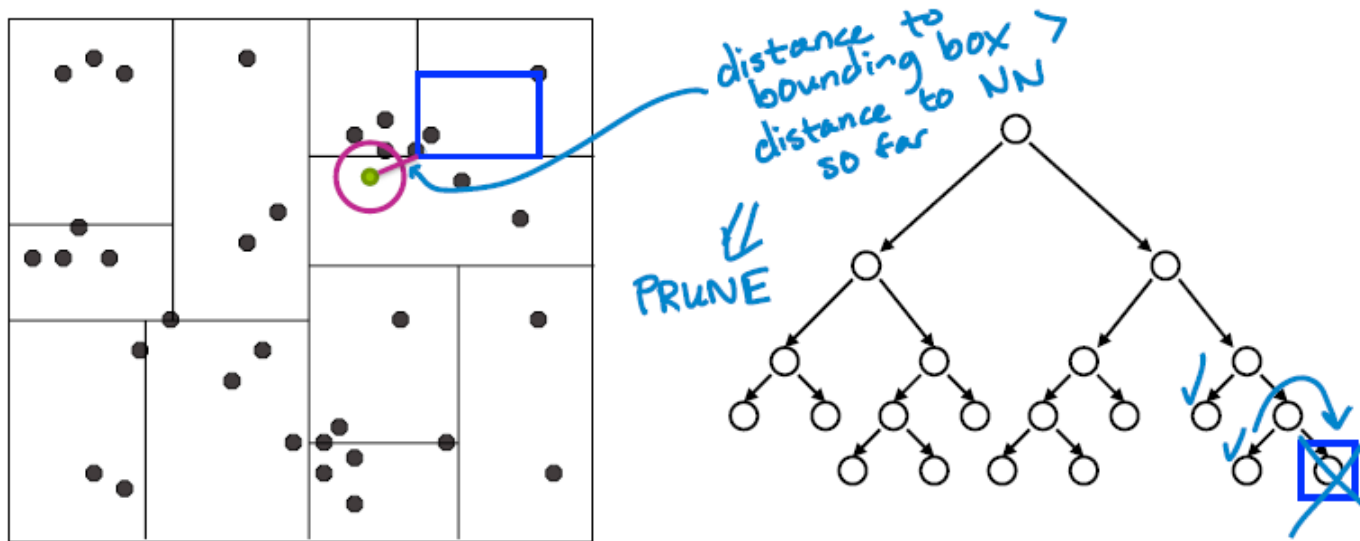
60



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

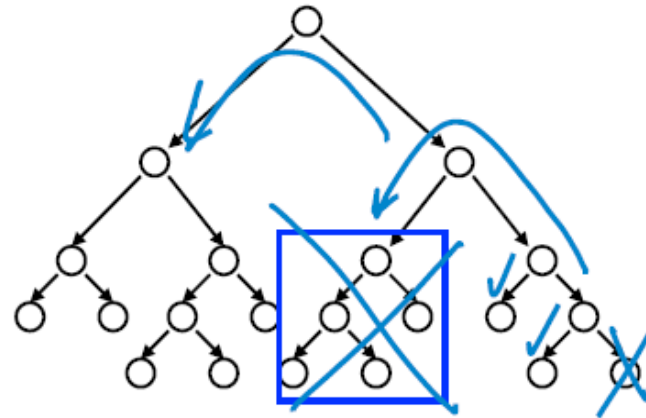
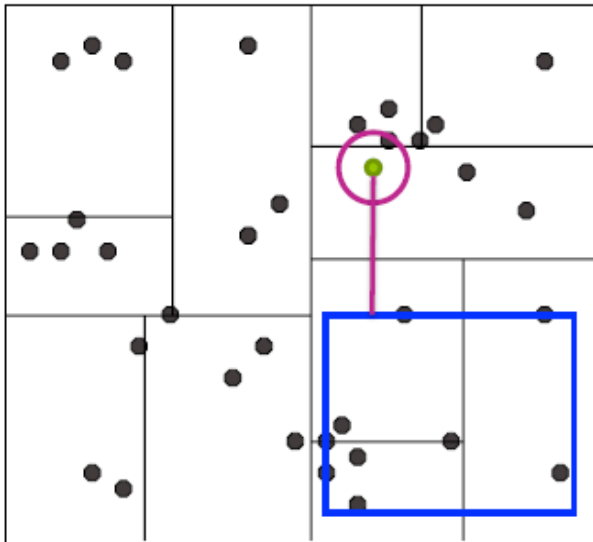
61



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

Nearest neighbor with KD-trees

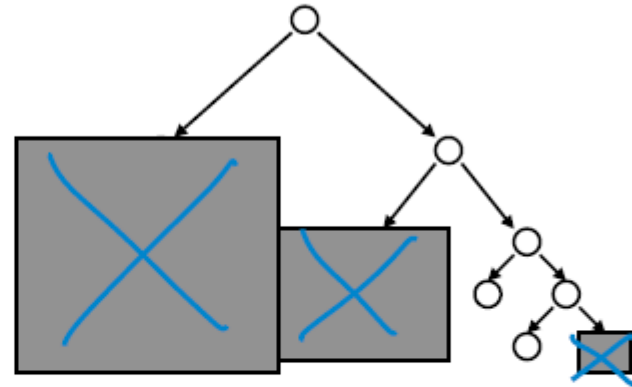
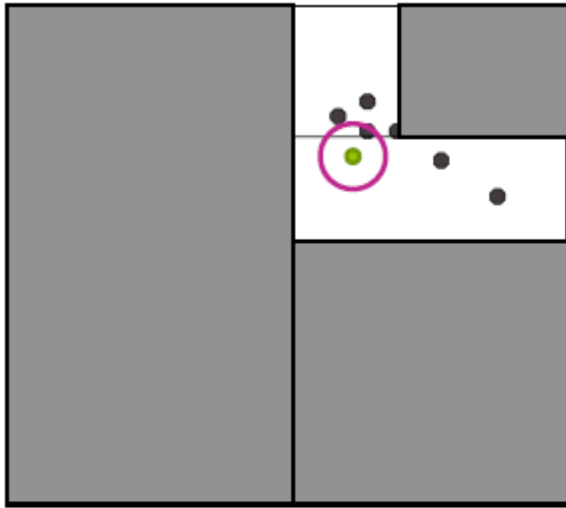
62



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

Nearest neighbor with KD-trees

63



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

Nearest neighbor with KD-trees

64

Complexity



For (nearly) balanced, binary trees...

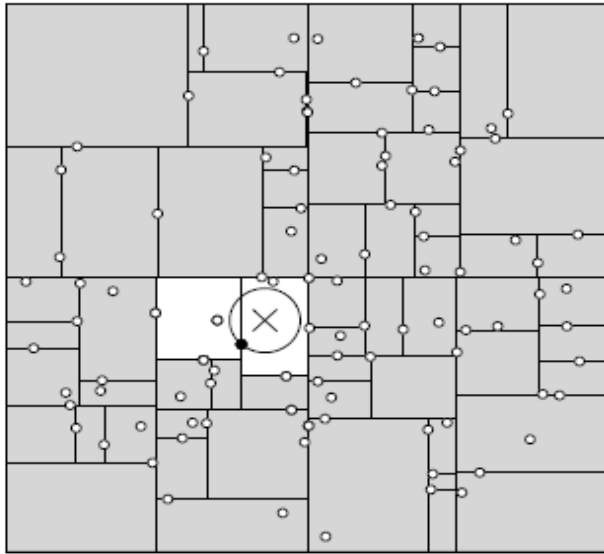
- Construction
 - Size: $2N-1$ nodes if 1 datapoint at each leaf $\rightarrow \underline{O(N)}$
 - Depth: $O(\log N)$
 - Median + send points left right: $O(N)$ at every level of the tree
 - Construction time: $O(N \log N)$
- 1-NN query
 - Traverse down tree to starting point: $O(\log N)$
 - Maximum 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 $O(\log N)$ but exponential in d

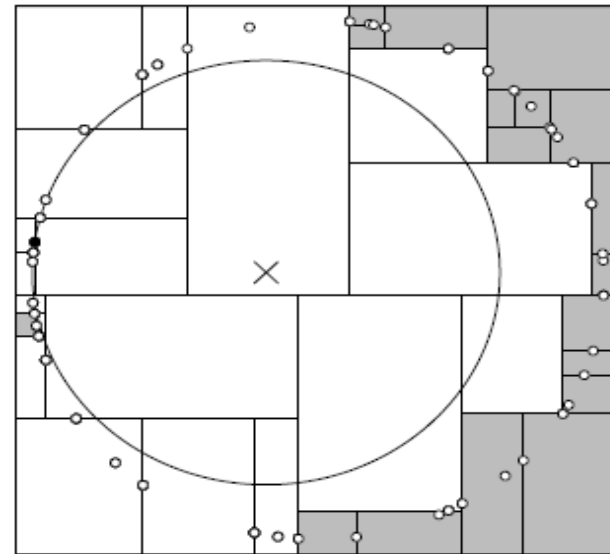
Nearest neighbor with KD-trees

65

Complexity



pruned many
(closer to $O(\log N)$)



pruned few
(closer to $O(N)$)

Complexity for N queries

66

- Ask for nearest neighbor to each doc

N queries

- Brute force 1-NN:

$O(N^2)$

- kd-trees:

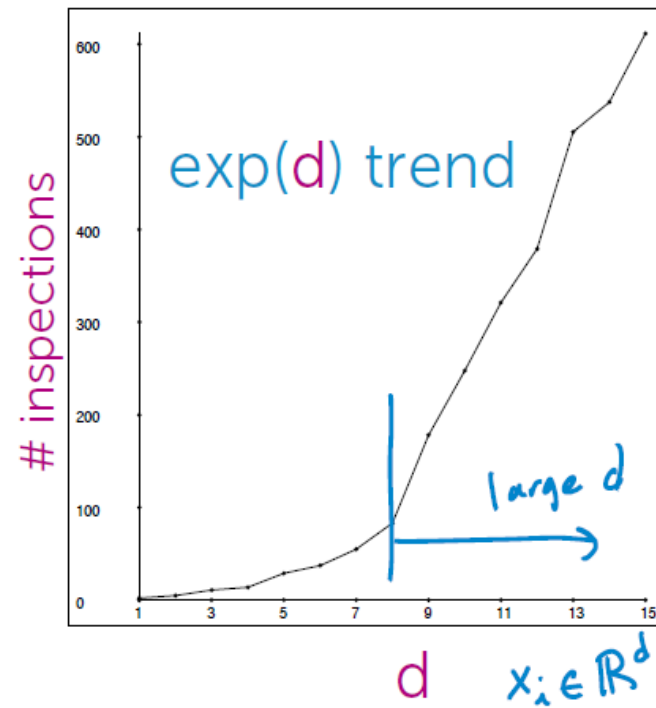
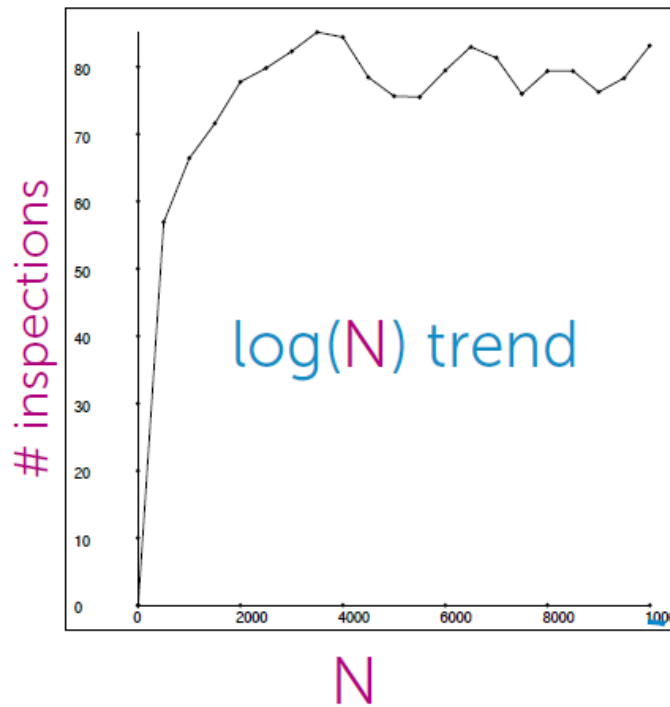
$O(N \log N) \rightarrow O(N^2)$

*↑
potentially
very large
savings for
large N!*

Complexity for N queries

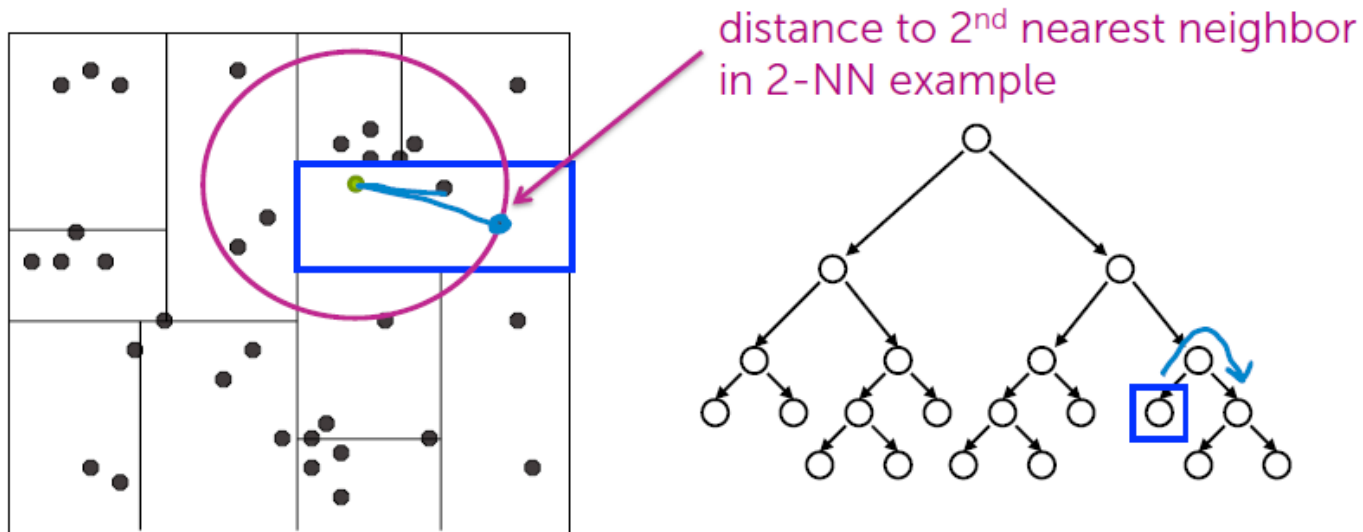
67

Inspections vs. N and d



k-NN with KD-trees

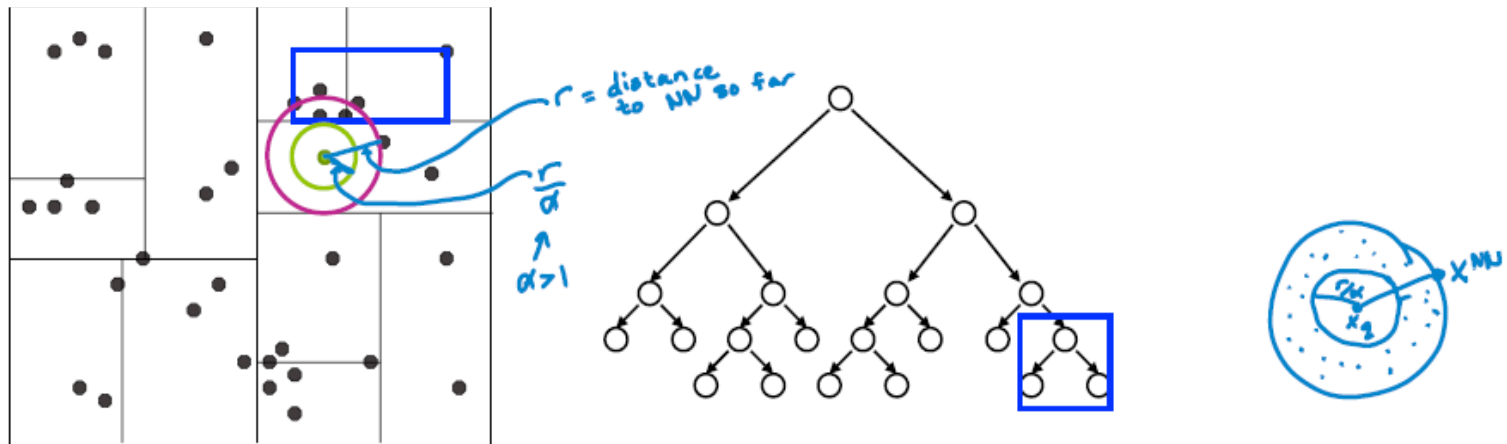
68



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

Approximate k-NN with KD-trees

69



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/α

← 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

70

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

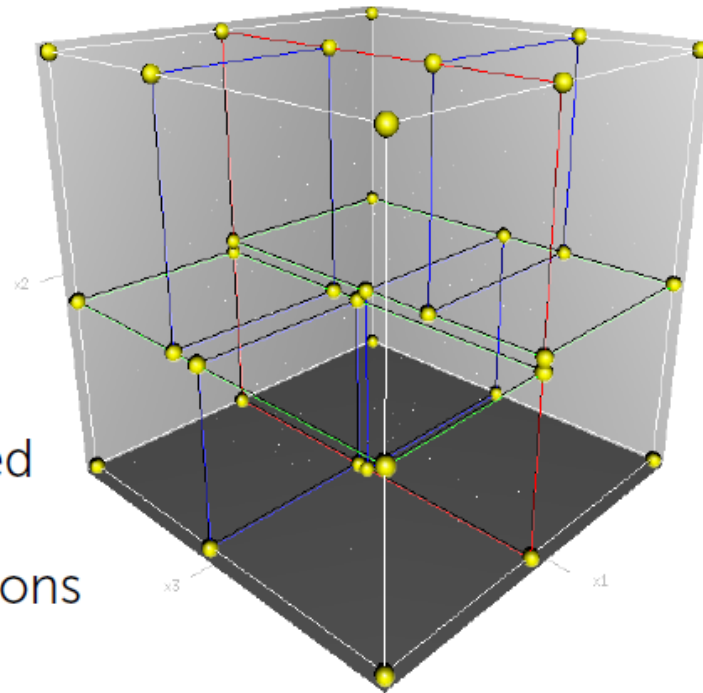
For both, high-dim spaces are hard!

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

KD-tree in high dimensions

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- 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

72

- 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

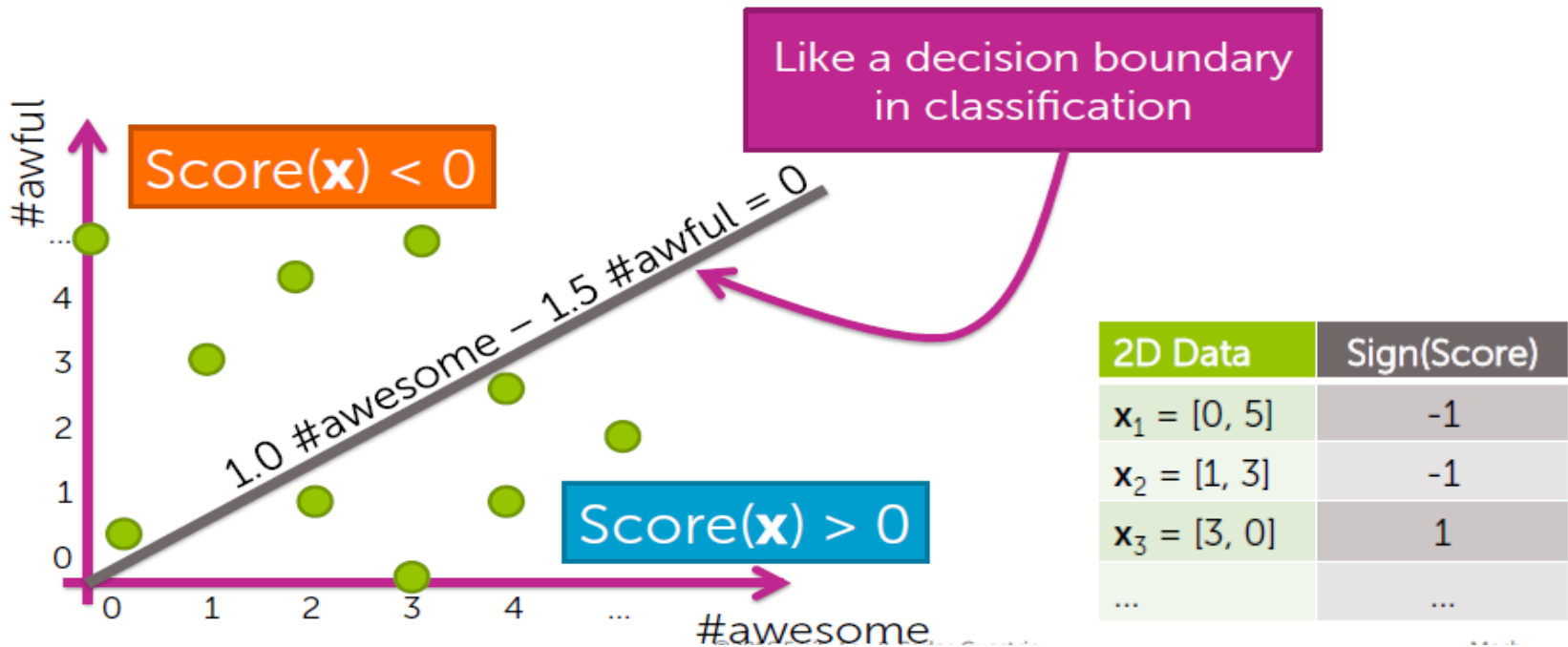
Locality Sensitive Hashing (LHS) as alternative to KD-trees

Locality sensitive hashing

74

Simple "binning" of data into 2 bins

$$\text{Score}(\mathbf{x}) = 1.0 \text{ \#awesome} - 1.5 \text{ \#awful}$$



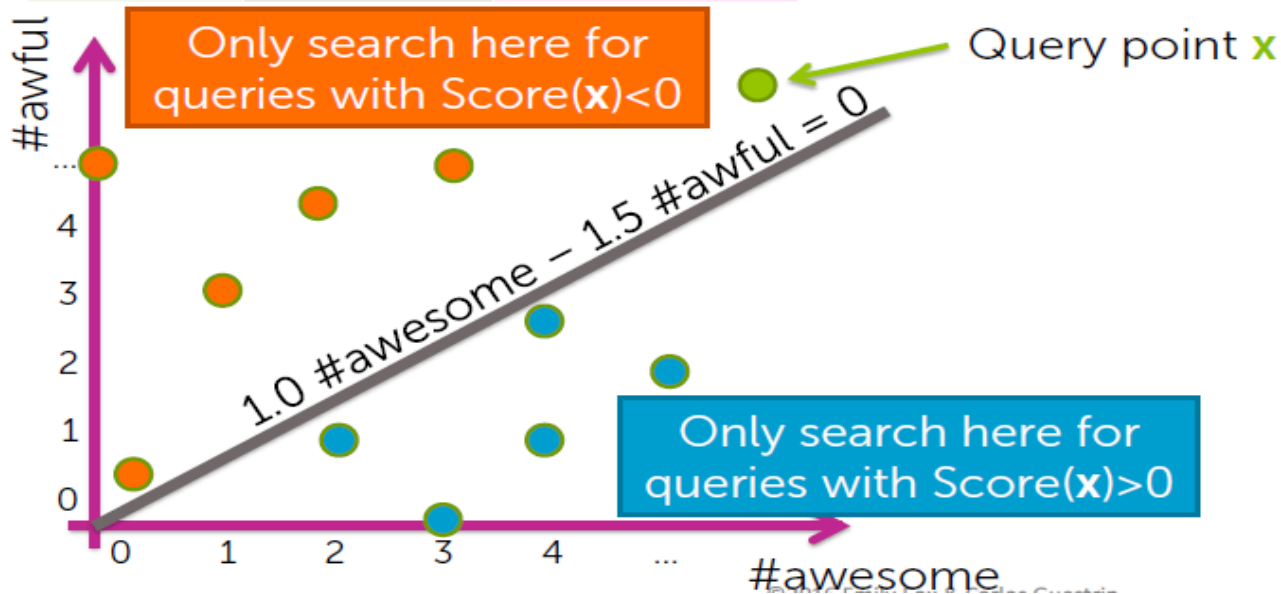
Locality sensitive hashing

75

Using bins for NN search

2D Data	Sign(Score)	Bin index
$x_1 = [0, 5]$	-1	0
$x_2 = [1, 3]$	-1	0
$x_3 = [3, 0]$	1	1
...

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



Locality sensitive hashing

76

Using score for NN search

2D Data	Sign(Score)	Bin index
$x_1 = [0, 5]$	-1	0
$x_2 = [1, 3]$	-1	0
$x_3 = [3, 0]$	1	1
...

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



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

HASH TABLE

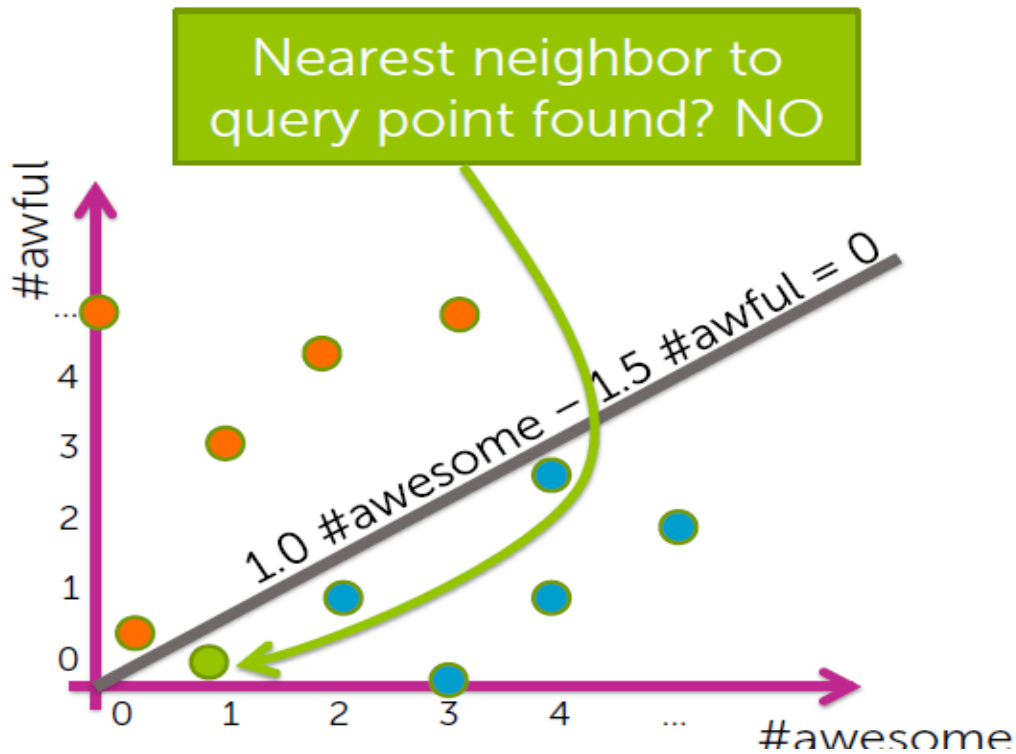
search for NN amongst this set



Locality sensitive hashing

77

Provides approximate NN



Locality sensitive hashing

78

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

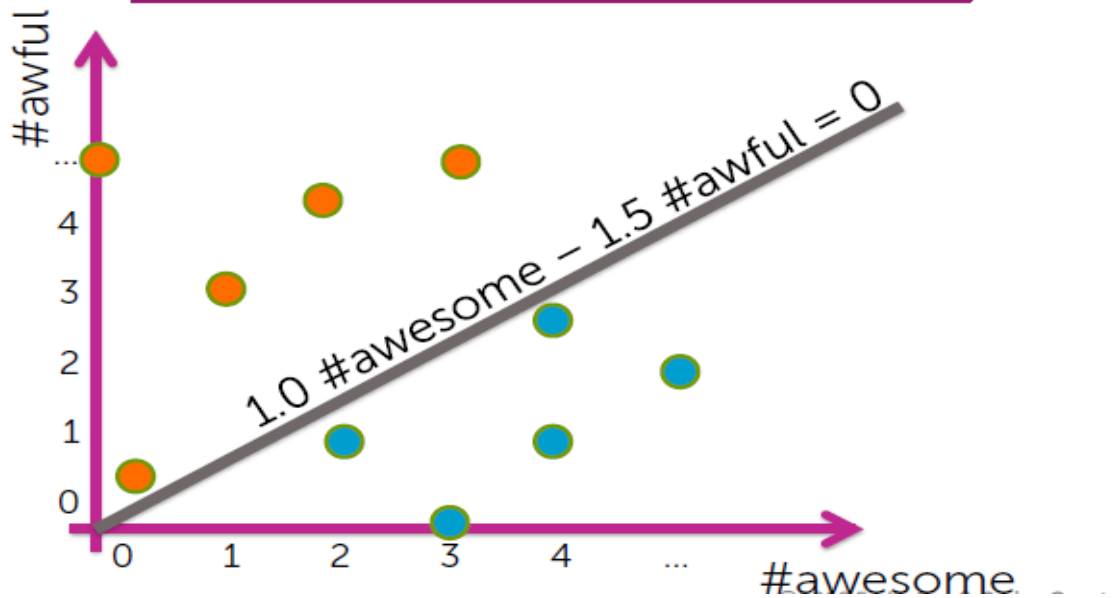
Bin	0	1
List containing indices of datapoints:	{1,2,4,7,...}	{3,5,6,8,...}

Locality sensitive hashing

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How to define the line?

Crazy idea:
Define line randomly!

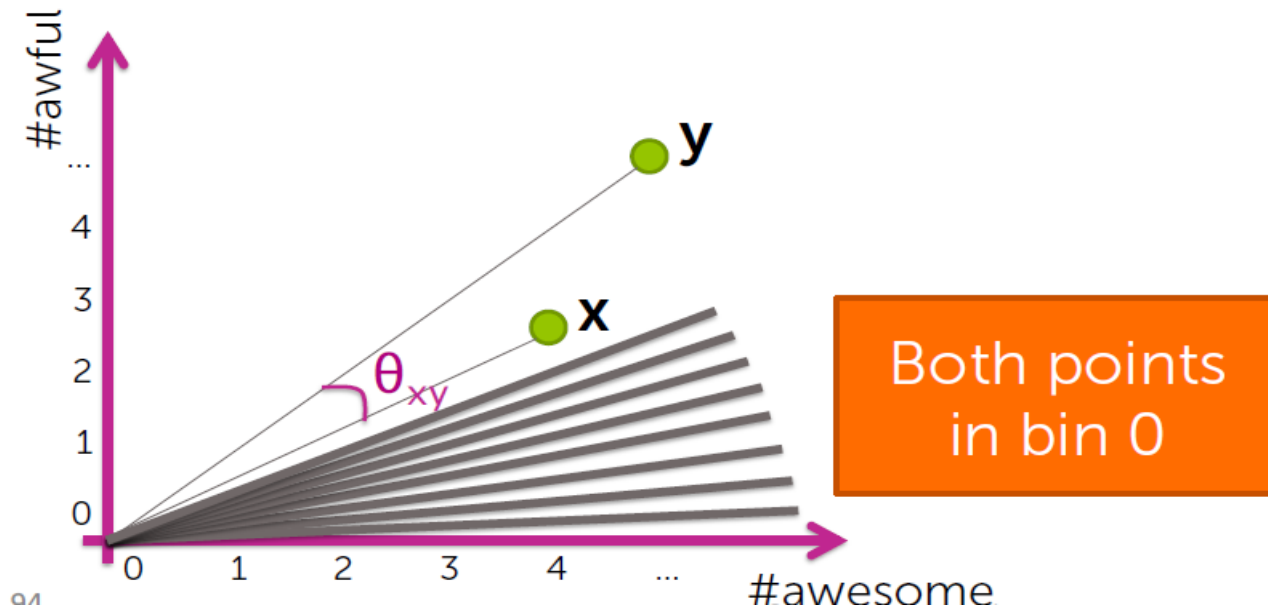


Locality sensitive hashing

80

How bad can a random line be?

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

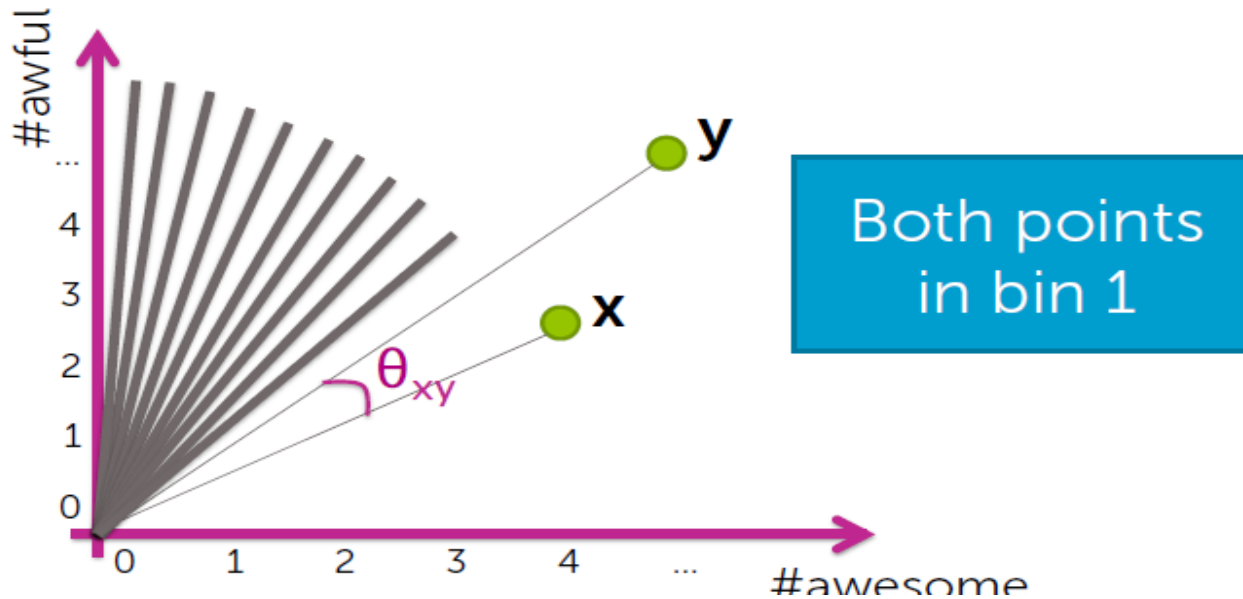


Locality sensitive hashing

81

How bad can a random line be?

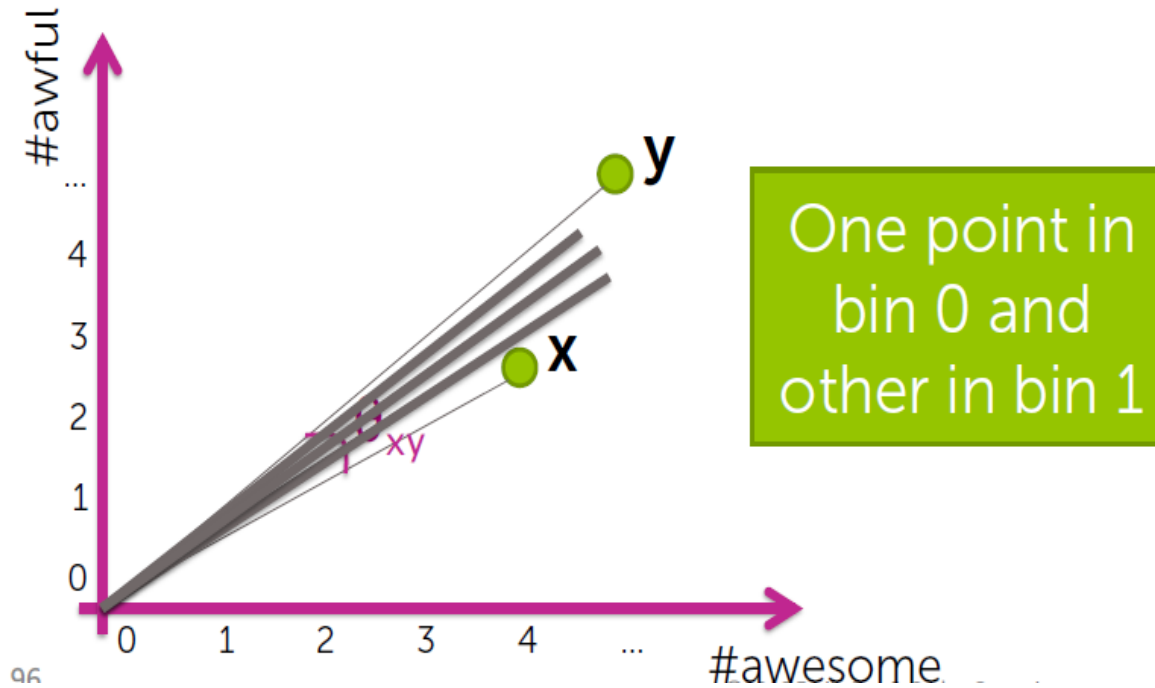
Goal: If x, y are close (according to cosine similarity), want binned values to be the same.



Locality sensitive hashing

82

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

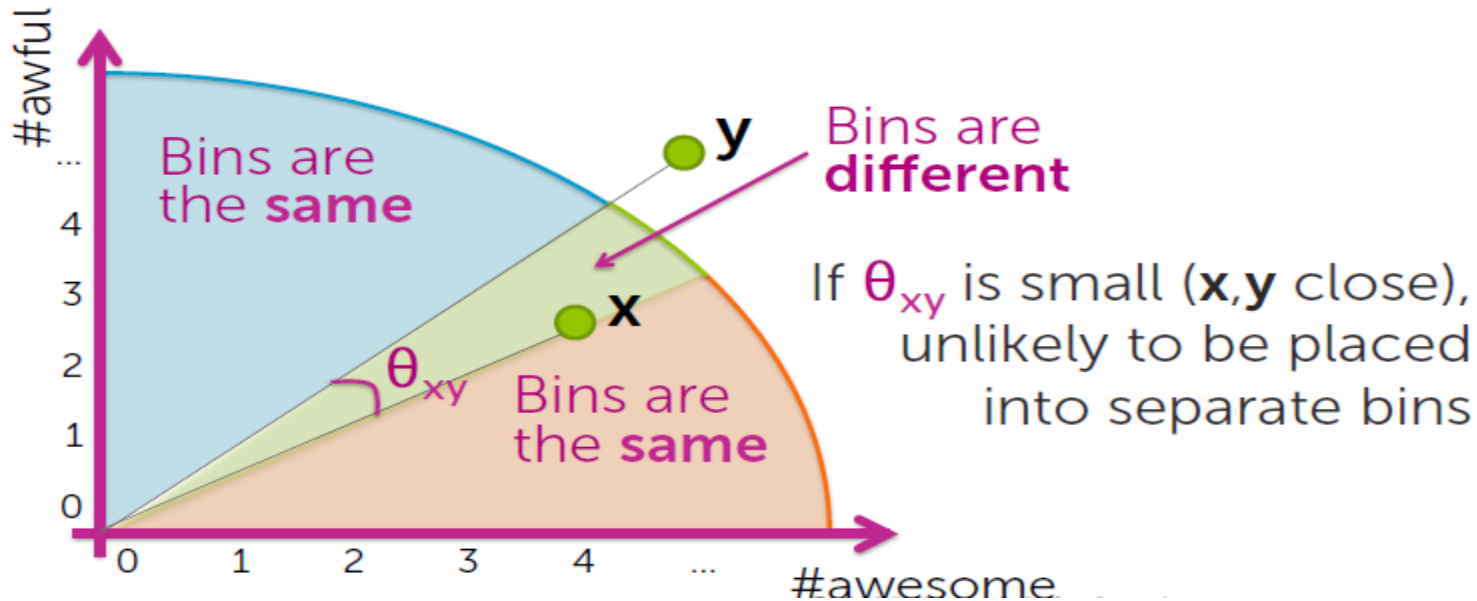


Locality sensitive hashing

83

How bad can a random line be?

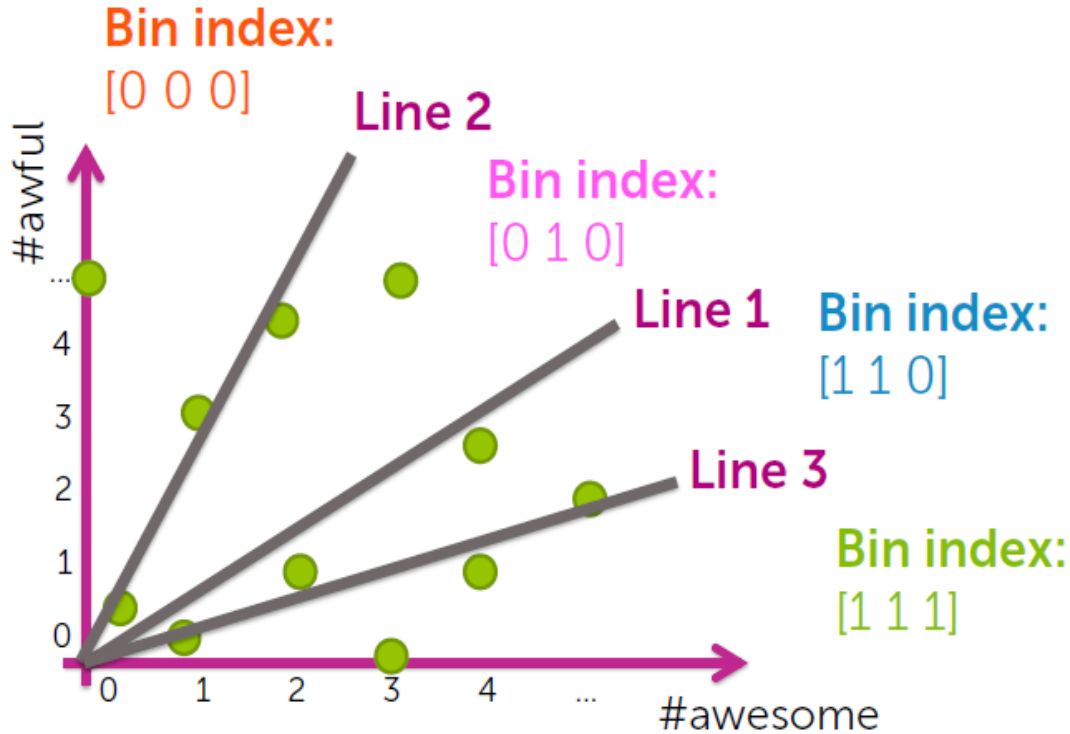
Goal: If \mathbf{x}, \mathbf{y} are close (according to cosine similarity), want binned values to be the same.



LSH: improving efficiency

84

Reducing search cost through **more bins**



LSH: improving efficiency

85

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
$x_1 = [0, 5]$	-1	0	-1	0	-1	0
$x_2 = [1, 3]$	-1	0	-1	0	-1	0
$x_3 = [3, 0]$	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

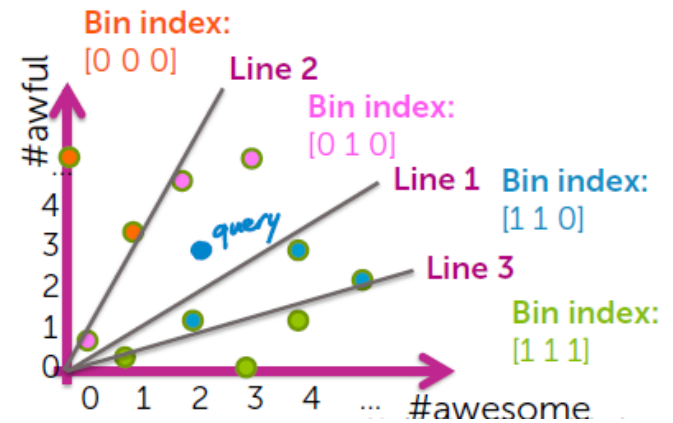
Improving search quality by searching neighboring bins

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



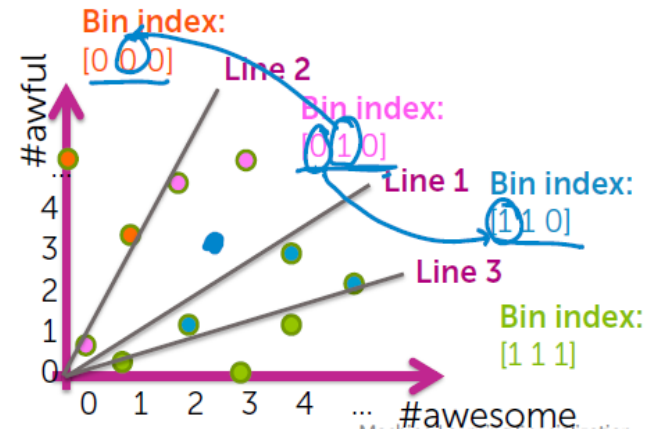
LSH: improving efficiency

87

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:	<u>{1,2}</u>	--	<u>{4,8,11}</u>	--	--	--	<u>{7,9,10}</u>	{3,5,6}

Next closest bins
(flip 1 bit)

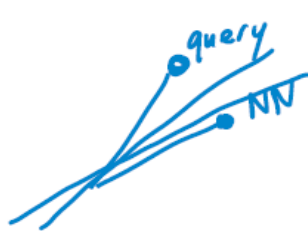


LSH: improving efficiency

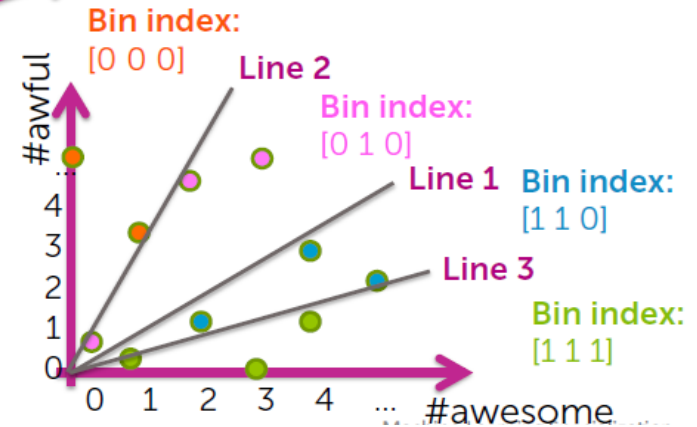
88

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

89

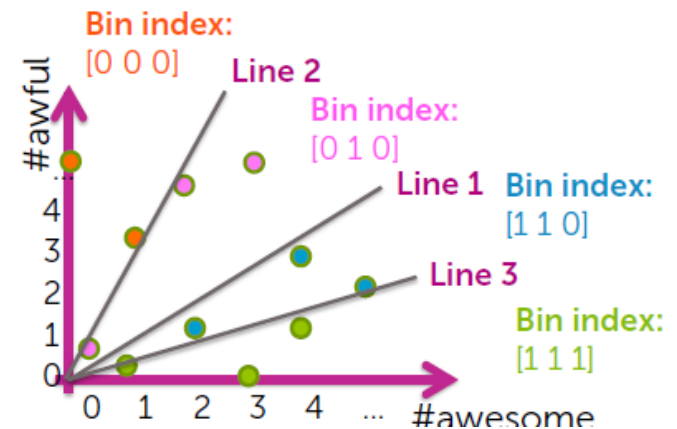
Improving search quality by searching neighboring bins

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



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LSH recap

90

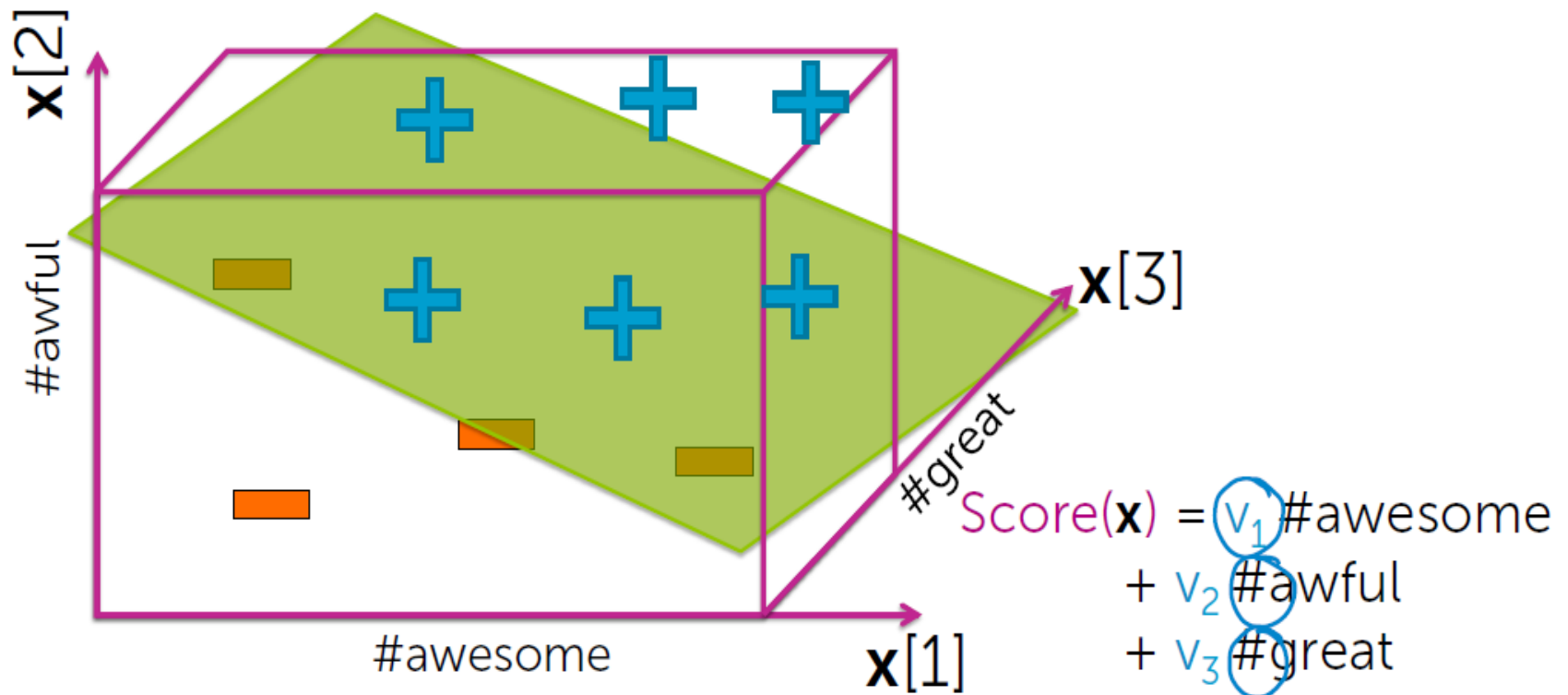
kd-tree competitor
data structure

- 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 \mathbf{x} , search $\text{bin}(\mathbf{x})$, then neighboring bins until time limit

LSH: moving to higher dimensions d

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Draw random *planes*



LSH: moving to higher dimensions d

92

Cost of binning points in d -dim

$$\text{Score}(\mathbf{x}) = v_1^{(i)} \# \text{awesome} \\ + v_2^{(i)} \# \text{awful} \\ + v_3^{(i)} \# \text{great}$$

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 ...

93

- 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

95

Goal: Structure documents by topic

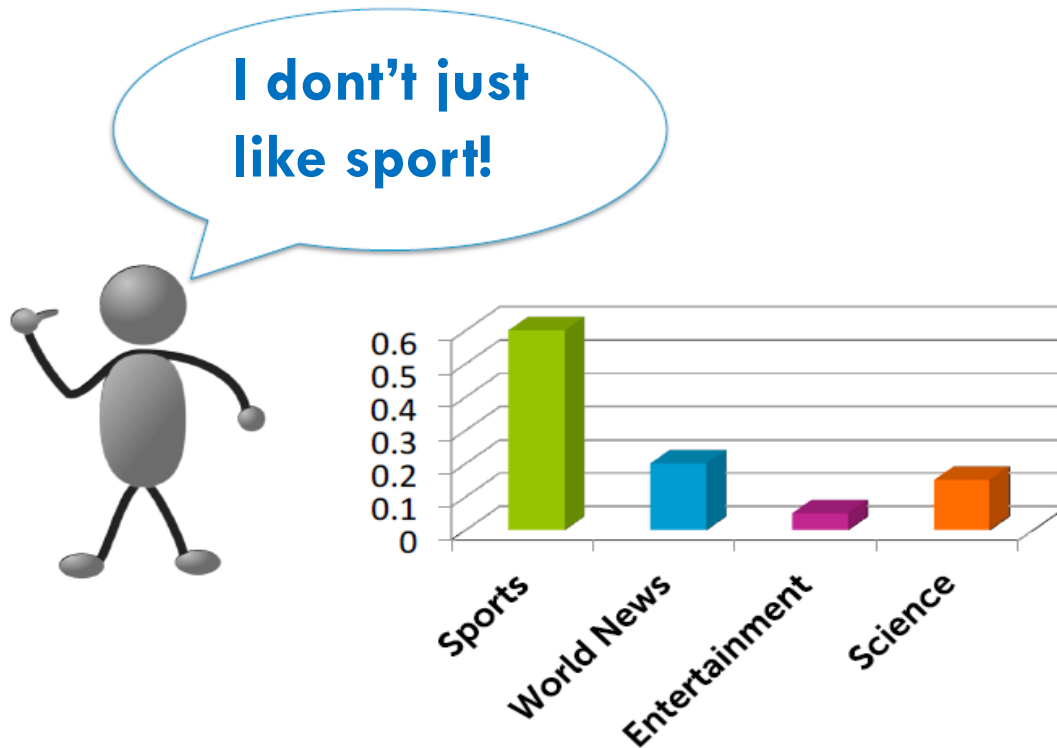
Discover groups (*clusters*) of related articles



Motivation

96

Why might clustering be useful?

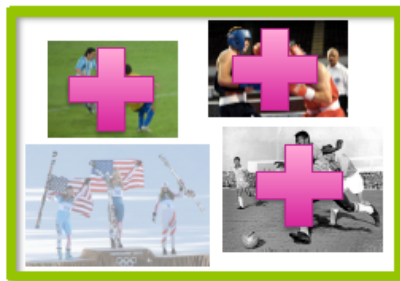


Motivation

97

Learn user preferences

Set of clustered documents read by user



Cluster 1



Cluster 2



Cluster 3



Cluster 4



Use feedback
to learn user
preferences
over topics

Clustering: a supervised learning

98

What if some of the labels are known?

Training set of labeled docs



SPORTS



WORLD NEWS



ENTERTAINMENT

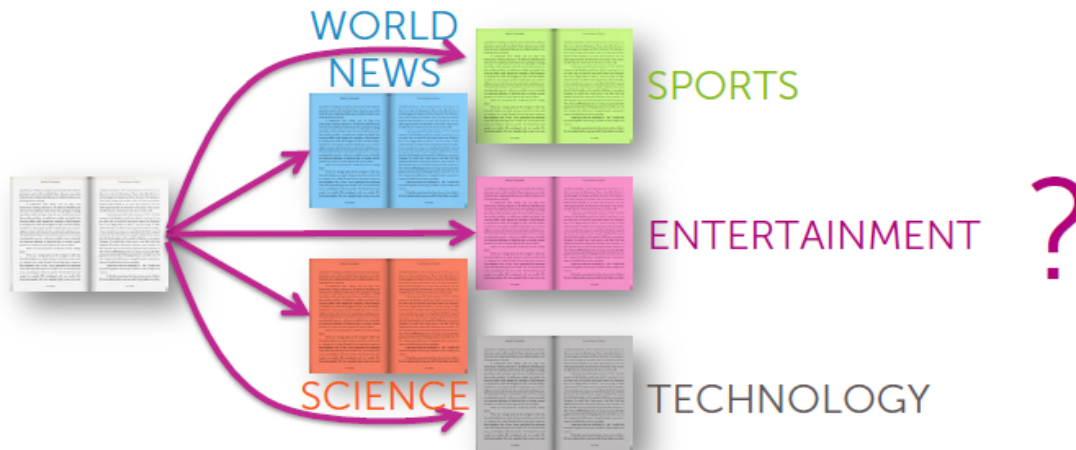


SCIENCE

Clustering: a supervised learning

99

Multiclass classification problem



Example of supervised learning

Clustering: an unsupervised learning

100

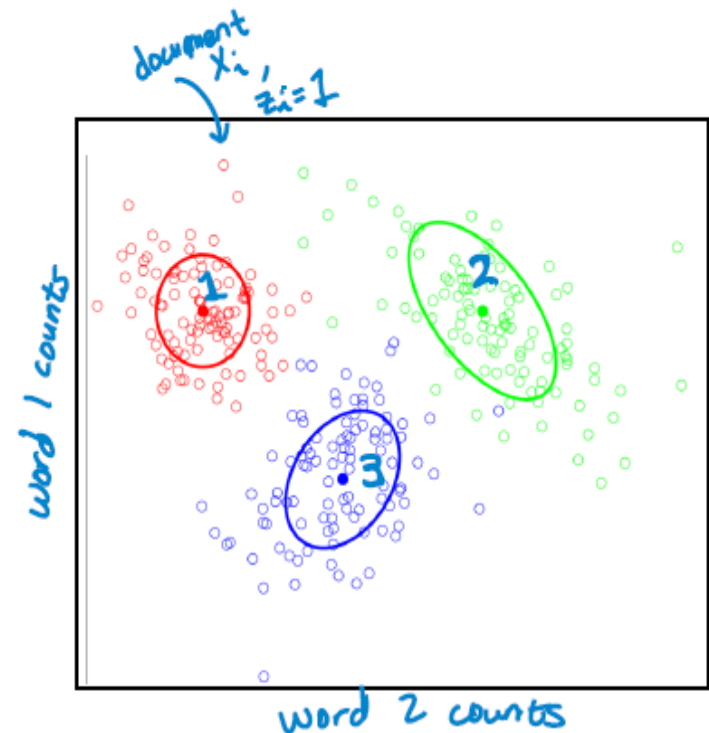
No labels provided

...uncover cluster structure
from input alone

Input: docs as vectors \mathbf{x}_i

Output: cluster labels z_i

An unsupervised
learning task



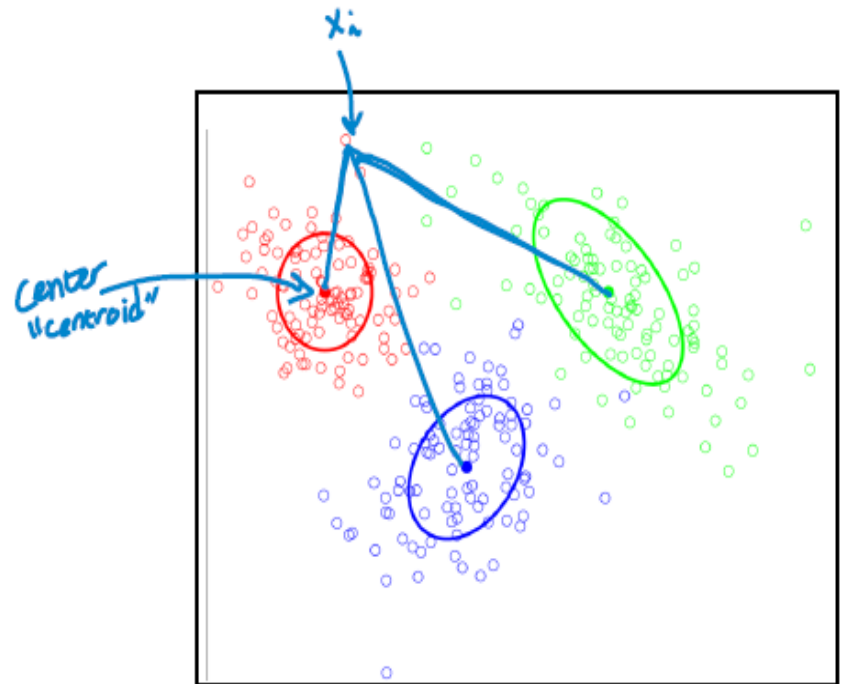
What defines a cluster ?

101

Cluster defined by
center & shape/spread

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

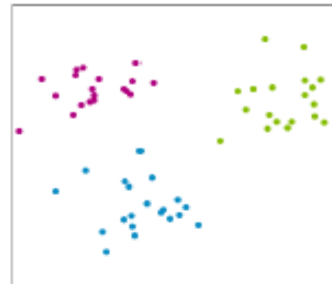
- Score under cluster k is higher than under others
- For simplicity, often define score as distance to cluster center (ignoring shape)



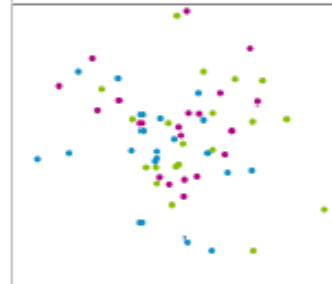
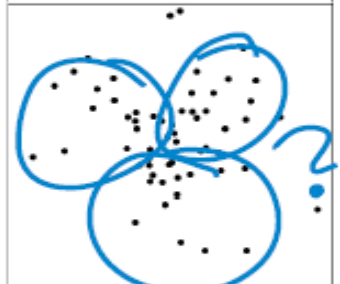
Hope for unsupervised learning

102

Easy



Impossible



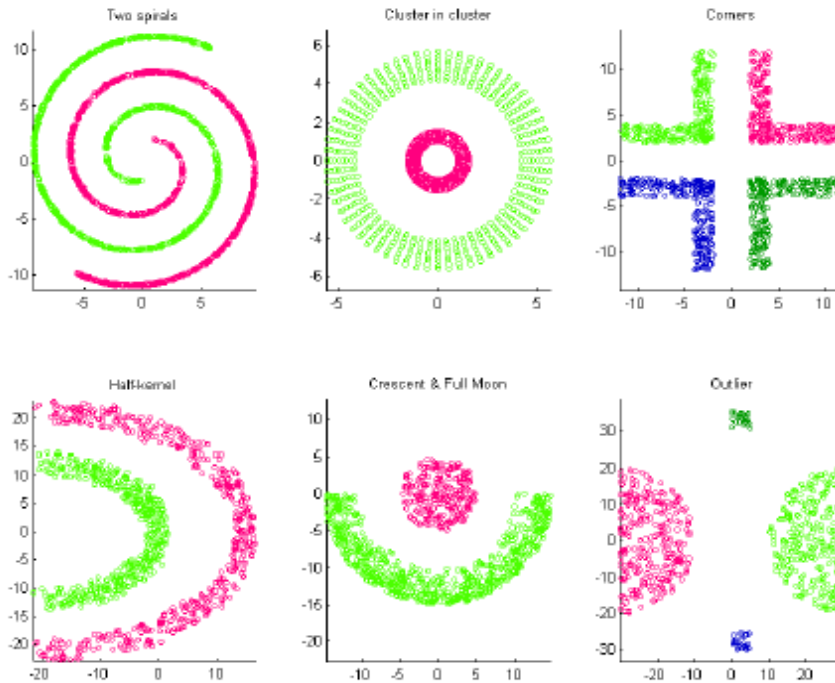
In between



Other (challenging!) clusters to discover

103

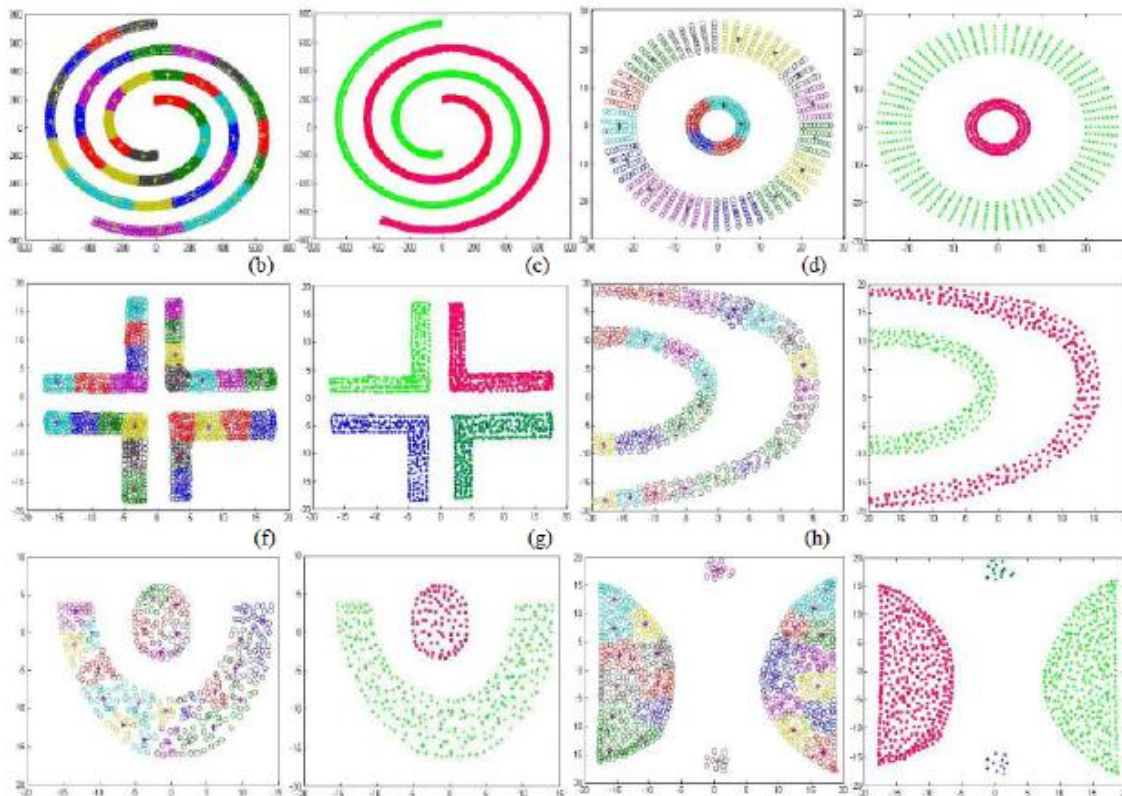
Analysed by your eyes



Other (challenging!) clusters to discover

104

Analysed by clustering algorithms



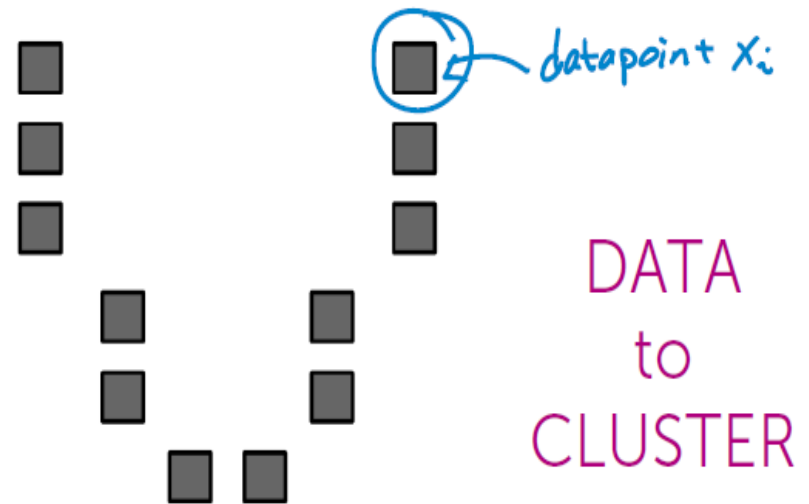
k-means clustering algorithm

k-means clustering algorithm

106

Assume

- Score = distance to cluster center
(smaller better)

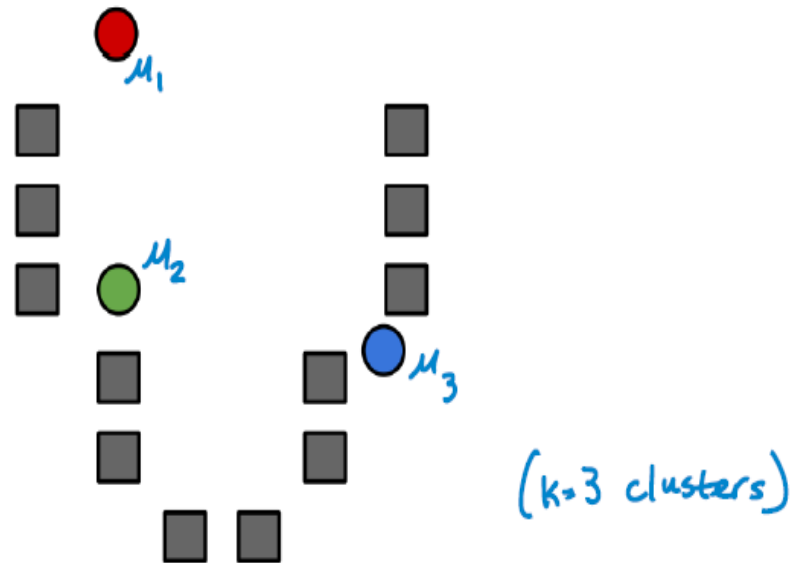


k-means clustering algorithm

107

0. Initialize cluster centers

$$\mu_1, \mu_2, \dots, \mu_k$$



k-means clustering algorithm

108

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

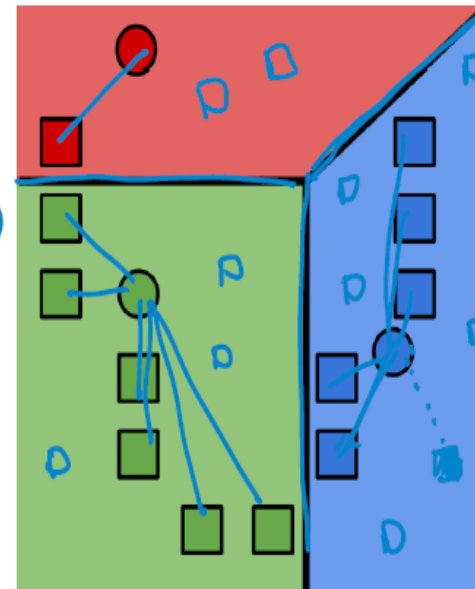
$$z_i \leftarrow \arg \min_j \|\mu_j - \mathbf{x}_i\|_2^2$$

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

j ← j th cluster center (varying)

i ← i th obs. (fixed)

return index j of the cluster whose center is closest to obs x_i (whereas min returning minimum value of $\|\cdot\|_2^2$)



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

k-means clustering algorithm

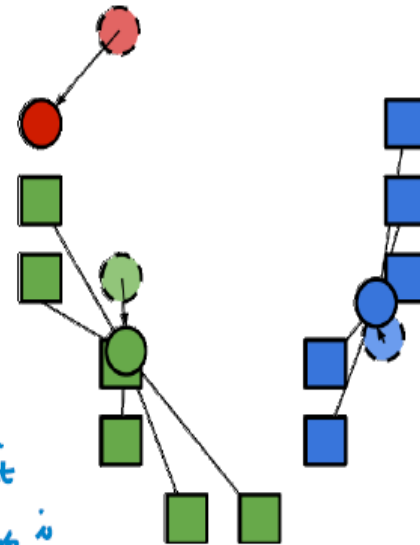
109

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

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

n_j ← # of obs. in cluster j

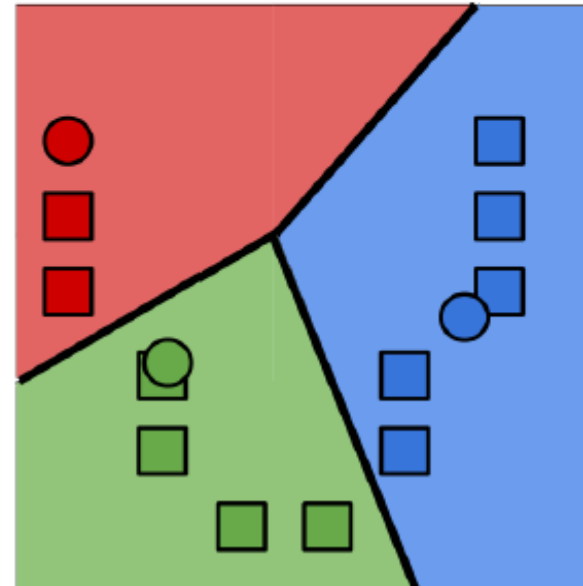
$i: z_i=j$ ← all obs. i such that $z_i=j$ (obs i is in cluster j)



k-means clustering algorithm

110

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

111


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

112

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

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Converges to:

~~- Global optimum~~

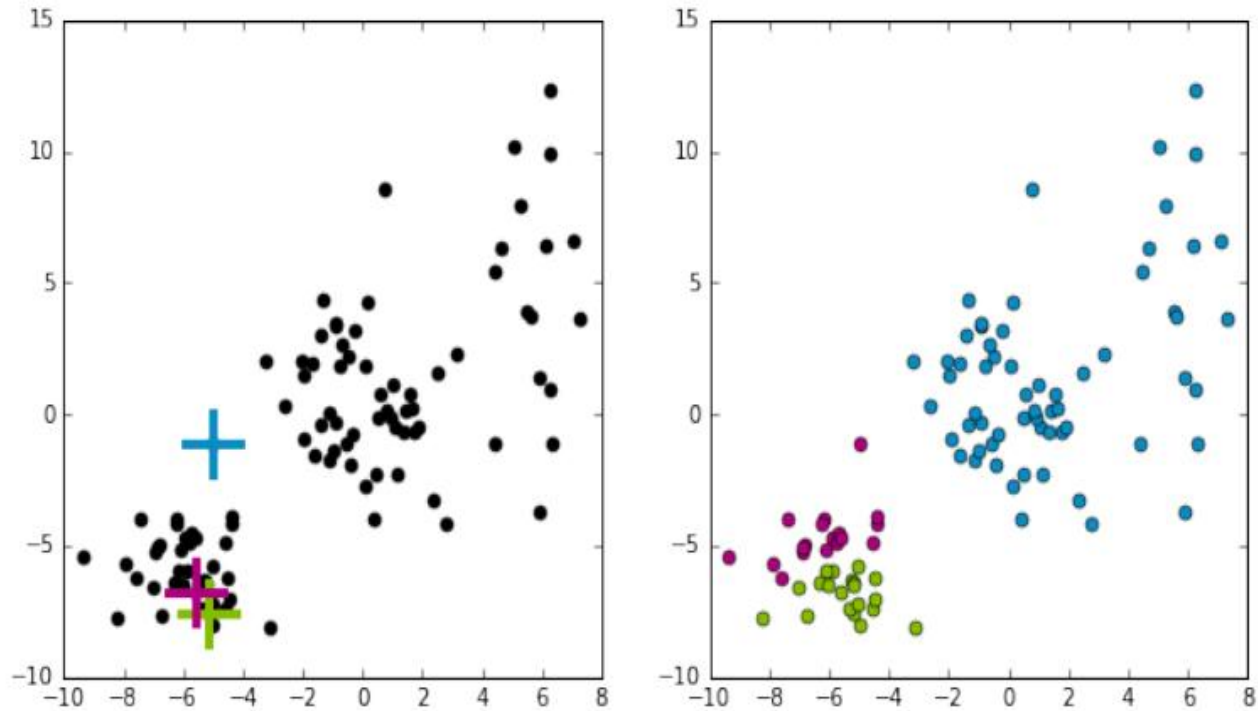
- Local optimum

~~- 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

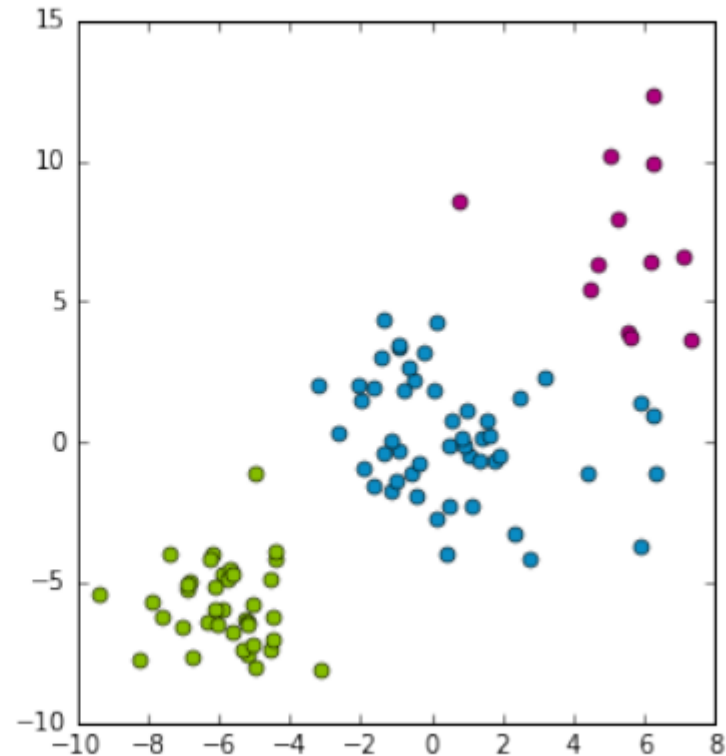
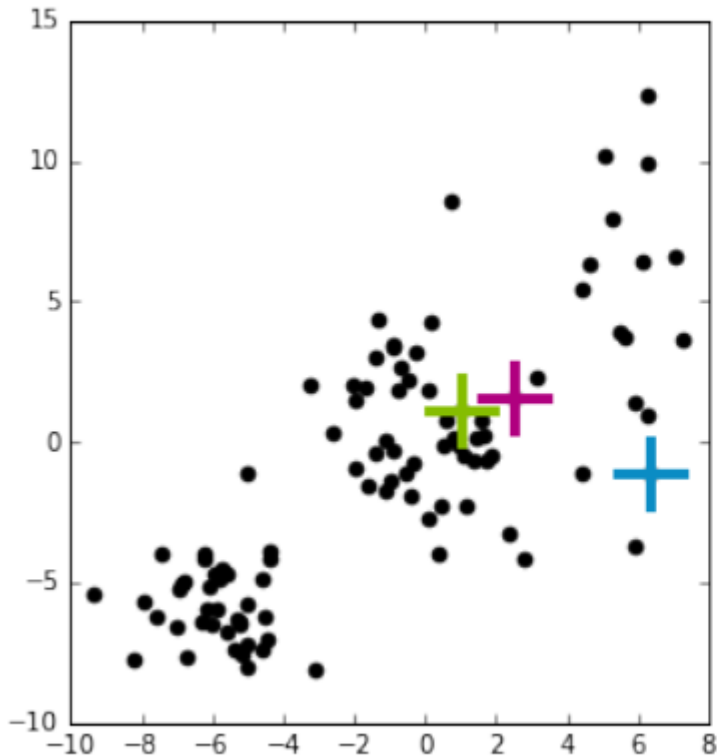
114



Crosses: initialised centers

Convergence of k-mans to local mode

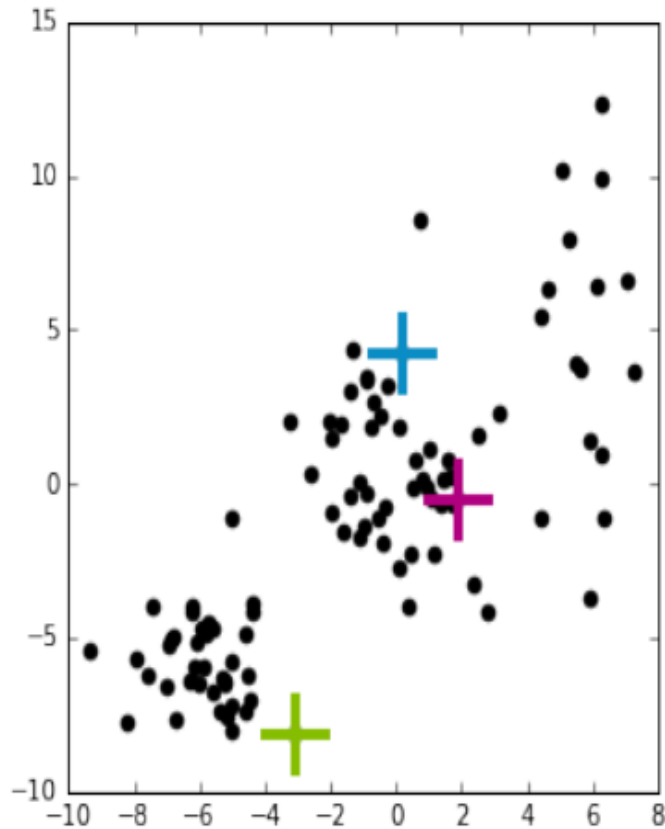
115



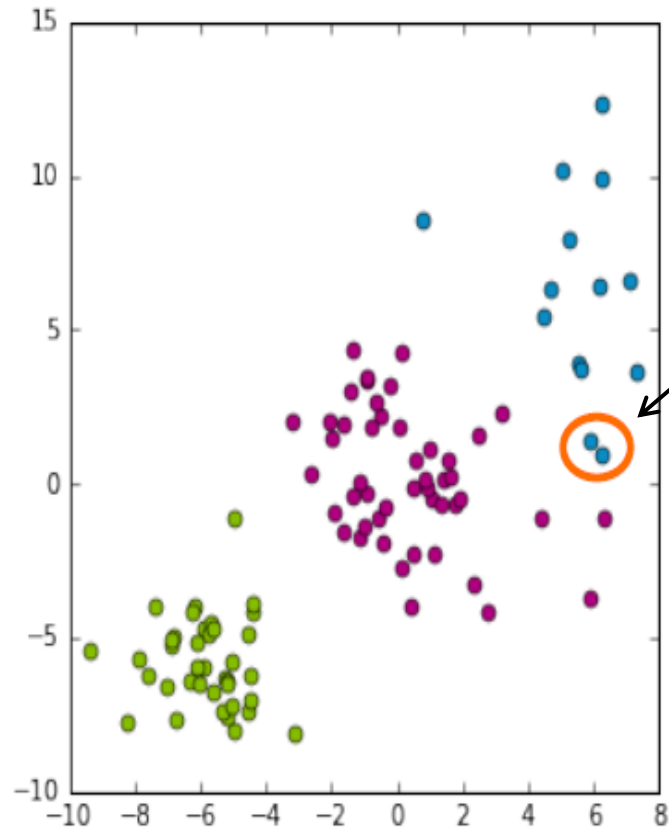
Crosses: initialised centers

Convergence of k-mans to local mode

116



Crosses: initialised centers



Assignment to which group has changed

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

Smart initialization: k-means++ overview

117

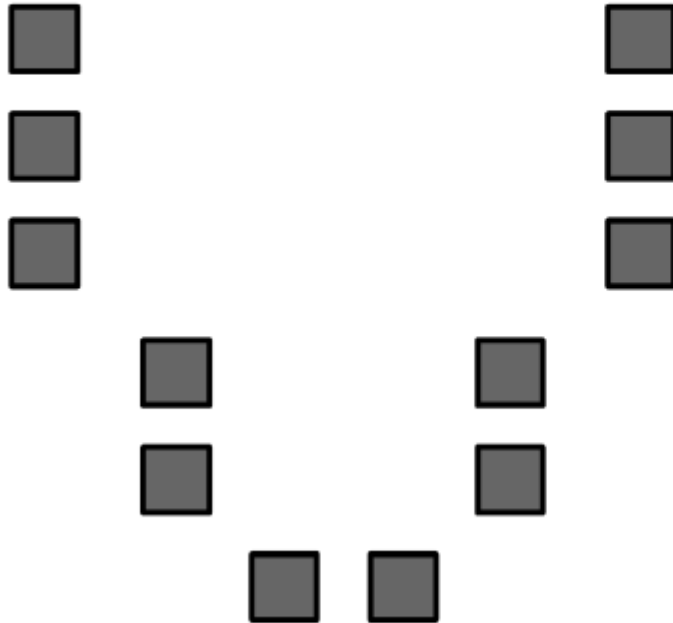
Initialization of k-means algorithm is critical to quality of local optima found

Smart initialization:

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

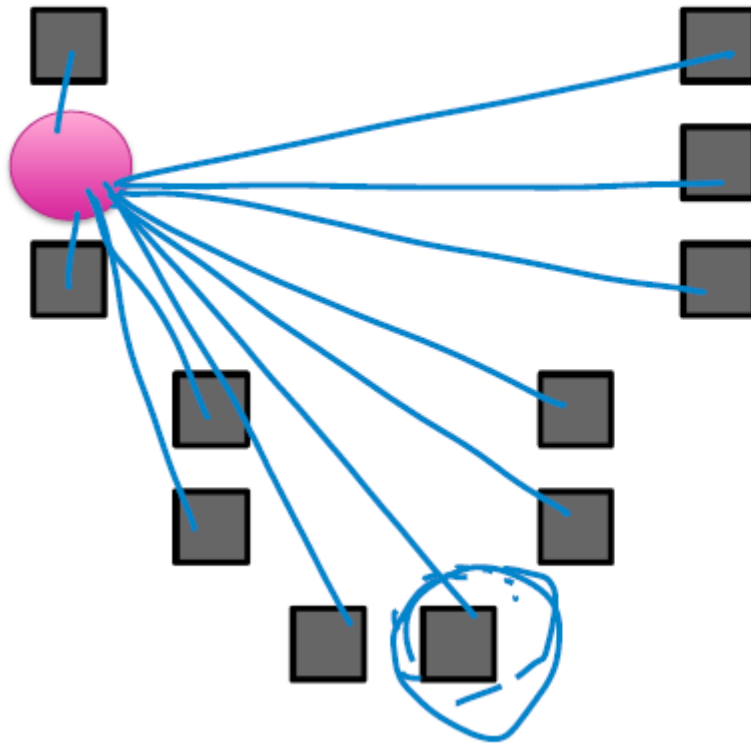
k-means++ visualised

118



k-means++ visualised

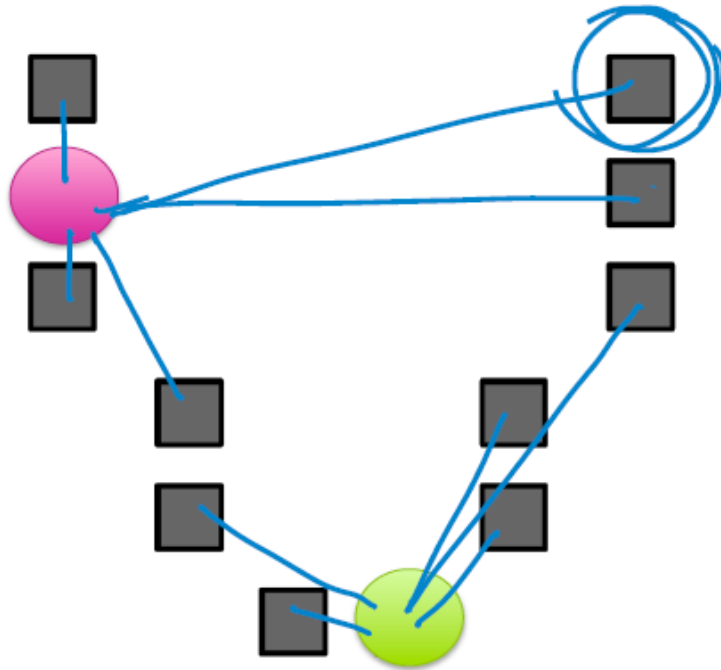
119



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

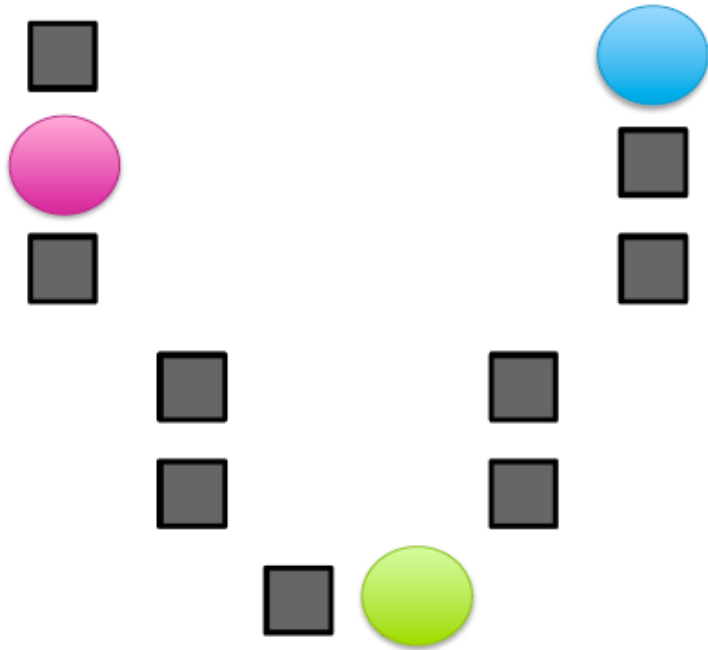
k-means++ visualised

120



k-means++ visualised

121



Smart initialisation: k-means++ overview

122

k-means++ pros/cons

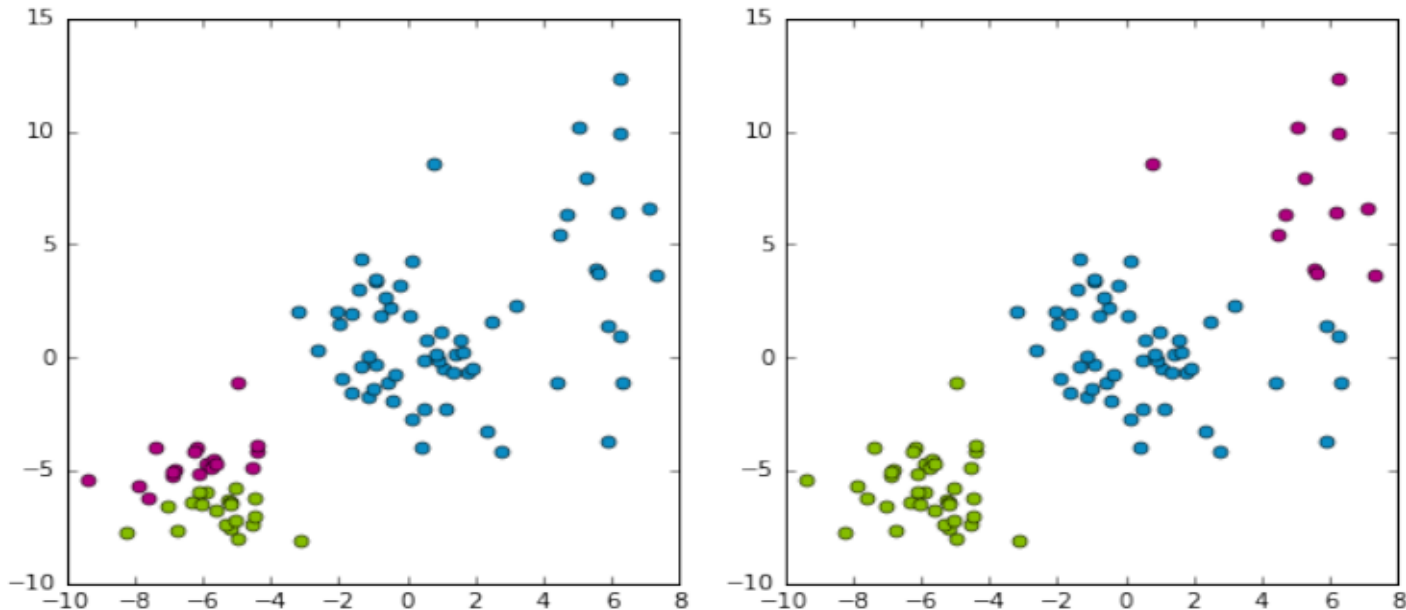
Computationally costly relative to random initialization, but the subsequent k-means often converges more rapidly

Tends to improve quality of local optimum and lower runtime

Assessing quality of the clustering

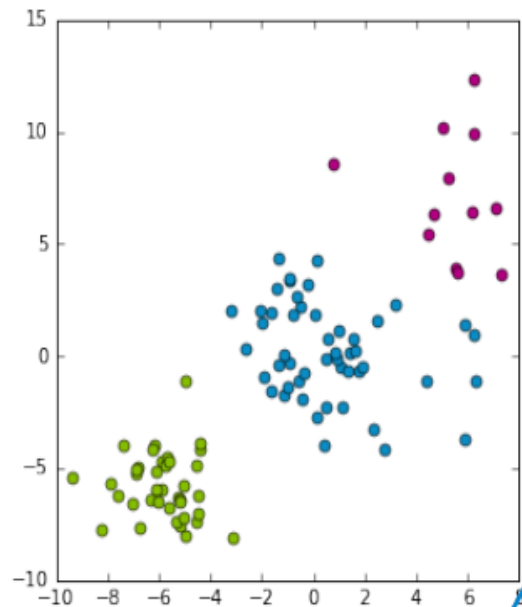
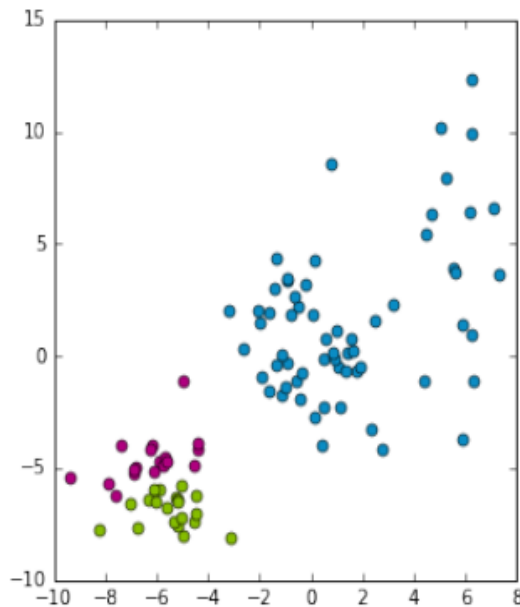
123

Which clustering do I prefer?



k-means objective

124



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

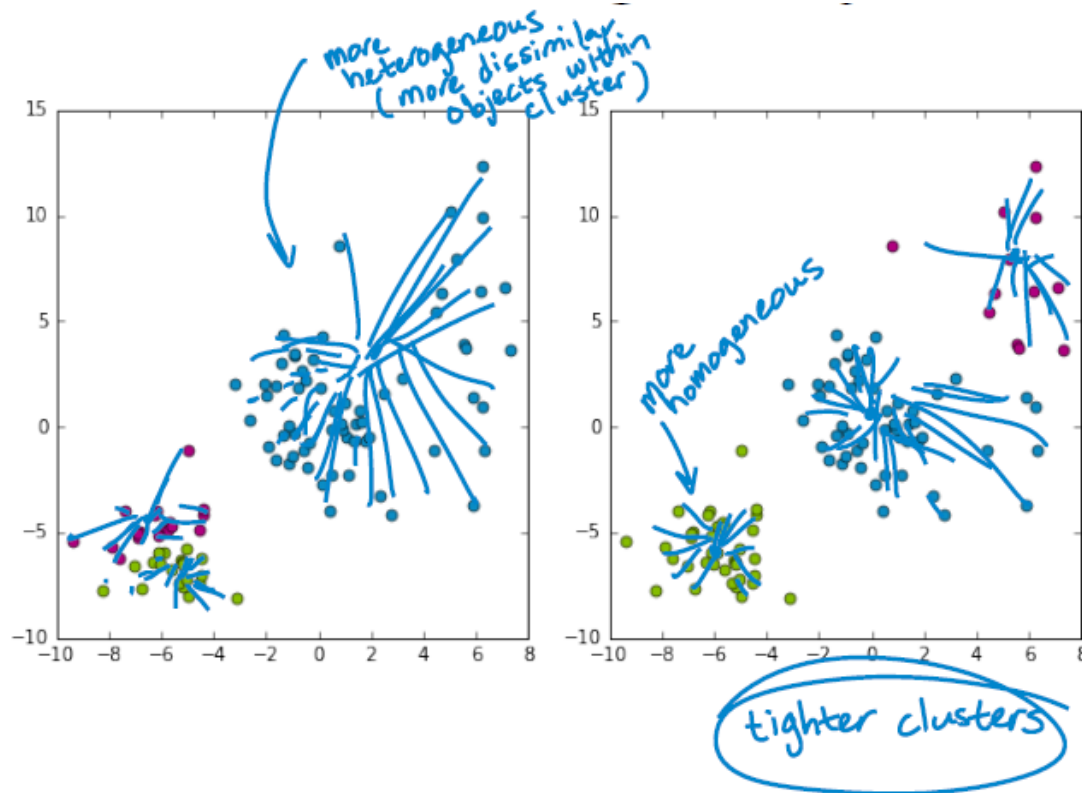
$$\sum_{j=1}^k \sum_{i:z_i=j} \|\mu_j - \mathbf{x}_i\|_2^2$$

sum over all clusters (pointing to k)
sum of squared distances in cluster j (pointing to the inner sum)

Min $\sum_{z_i=j} \|\mu_j - \mathbf{x}_i\|_2^2$

Cluster heterogeneity

125



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?

126

Can refine clusters more and more to the data
→ overfitting!

Extreme case of $k=N$:

- can set each cluster center equal to datapoint
- heterogeneity = 0 !

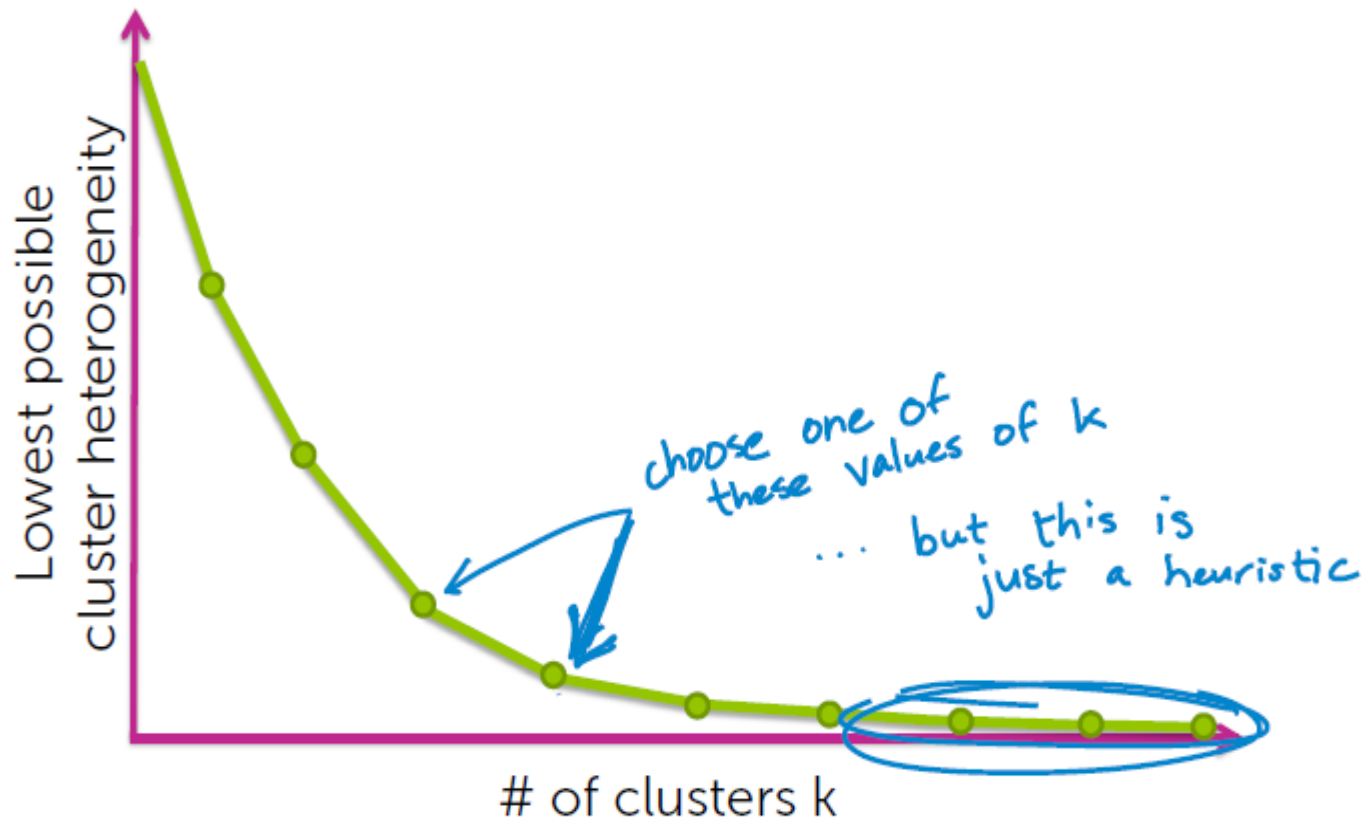
of observations

(all distances to cluster centers are 0)

Lowest possible cluster heterogeneity
decreases with increasing k

How to choose k?

127



MapReduce

Counting words on a single processor

129

(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

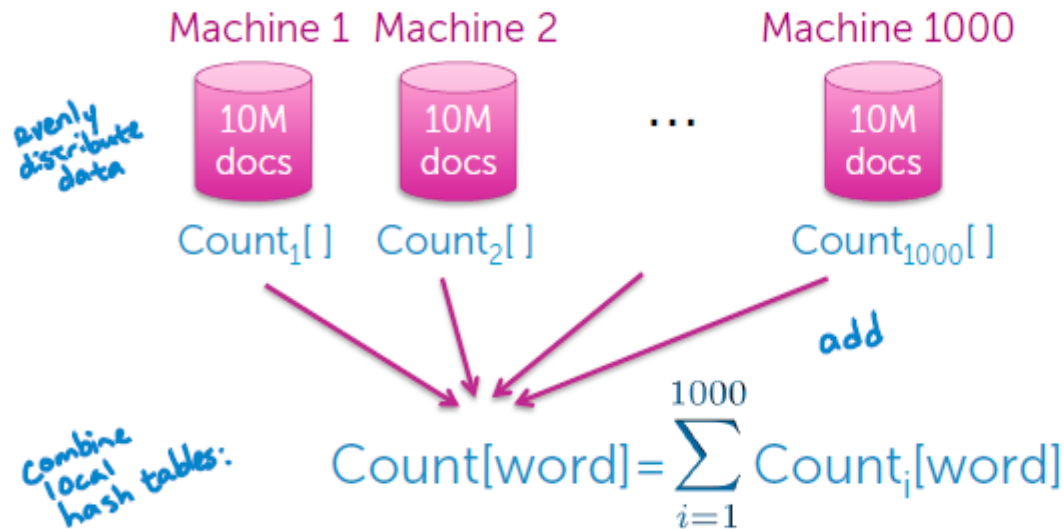
Code:

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

Naive parallel word counting

130

- Word counts are independent across documents (data parallel)
- Count occurrences in sets of documents separately, then merge



How do we do this for all words in vocab?

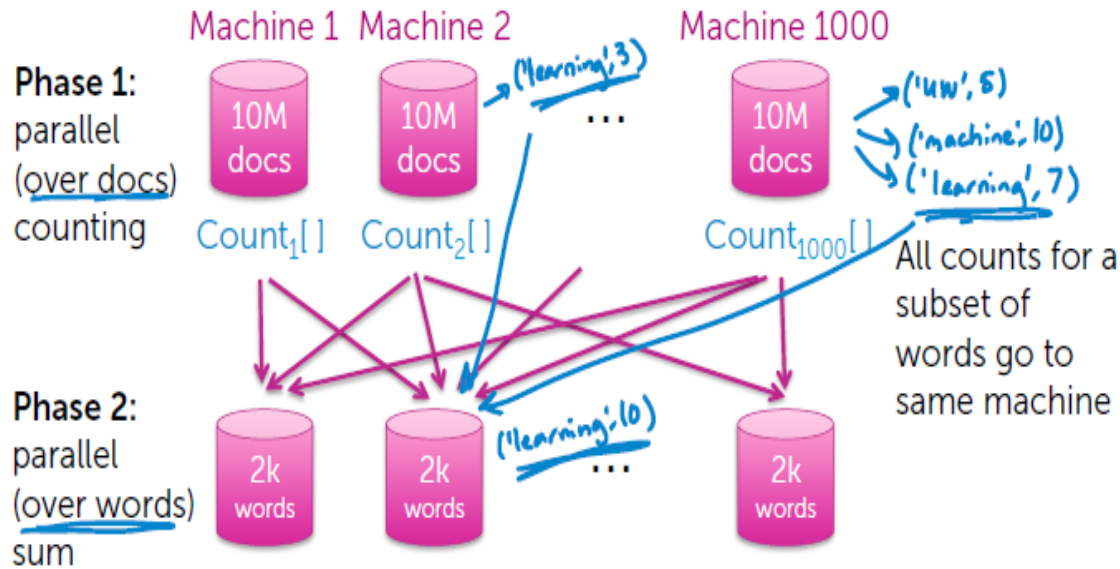
Back to sequential problem to merge counts...

have to cycle through all words in vocab... ugh.

Counting words & merging tables

131

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



Which words go to machine i ?

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

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

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

$h(\text{word index}) \rightarrow \text{machine index}$

MapReduce abstraction

132

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) ...`

Word count example:

```
map(doc)
```

```
for word in doc
```

```
emit(word, 1)
```

↑ key ↑ value

key list of values

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, 1, 0, 0, 1, 2])`
`emit('uw', 3)`

```
reduce(word, counts_list)
```

```
c = 0
```

```
for i in counts_list
```

```
c += counts_list[i]
```

```
emit(word, c)
```

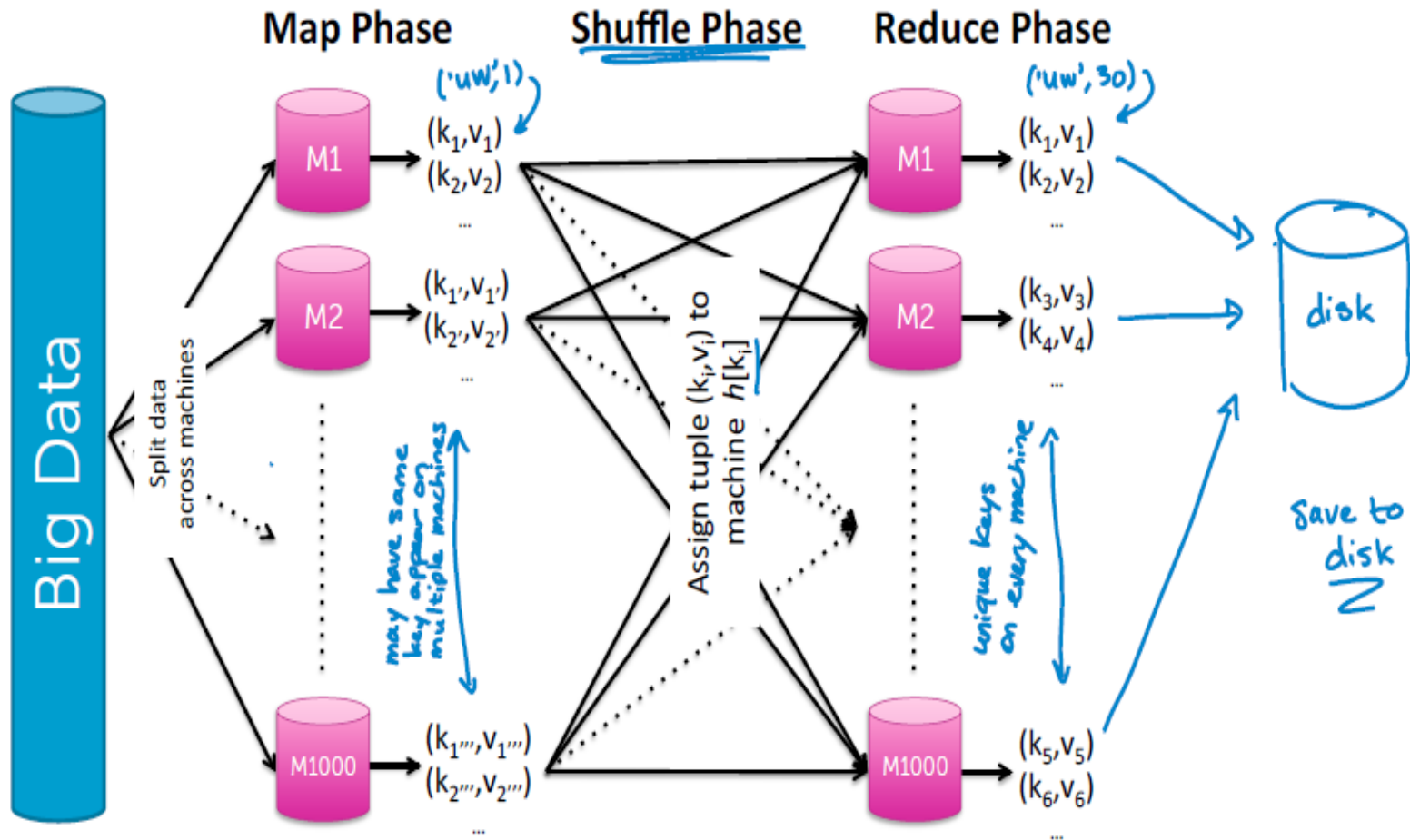
↑ key ↑ value

MapReduce has long history in functional programming

- Popularized by Google, and subsequently by open-source Hadoop implementation from Yahoo!

MapReduce – Execution overview

133

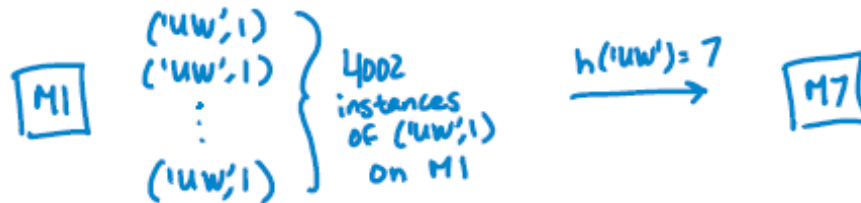


Improving performance

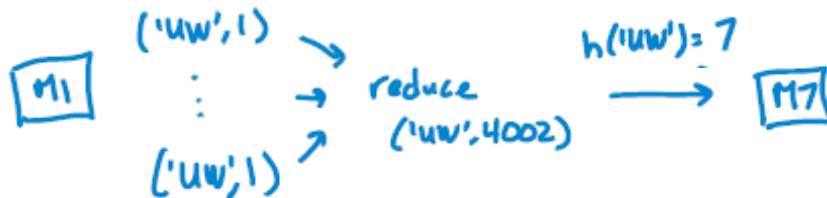
134

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

135

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 ($z_i=k$)

Scaling up k-means via MapReduce

136

Classification step as Map

Classify: Assign observations to closest cluster center

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

$\text{map}([\mu_1, \mu_2, \dots, \mu_k], \mathbf{x}_i)$

set of cluster centers
a datapoint

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

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

cluster label
datapoint

e.g. $\text{emit}(2, [17, 0, 1, 7, 0, 0, 5])$

$z_i=2$ (assigned to cluster 2)
datapoint \mathbf{x}_i

Scaling up k-means via MapReduce

137

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)
`reduce(j, x_in_clusterj : [x1, x3, ...,])`
datapoints assigned to cluster j (have key j)
`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* *total mass to total # obs*

Scaling up k-means via MapReduce

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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

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Map: **classification step**;
data parallel over data points

Reduce: **recompute means**;
data parallel over centers

What you can do now ...

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- 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

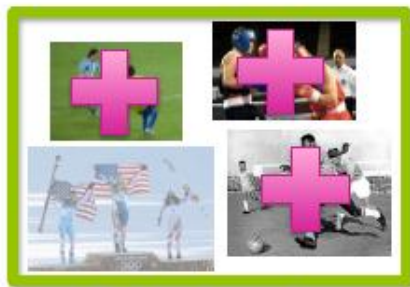
Probabilistic approach: mixture model

Why probabilistic approach?

142

Learn user preferences

Set of clustered documents read by user



Cluster 1



Cluster 2



Cluster 3



Cluster 4

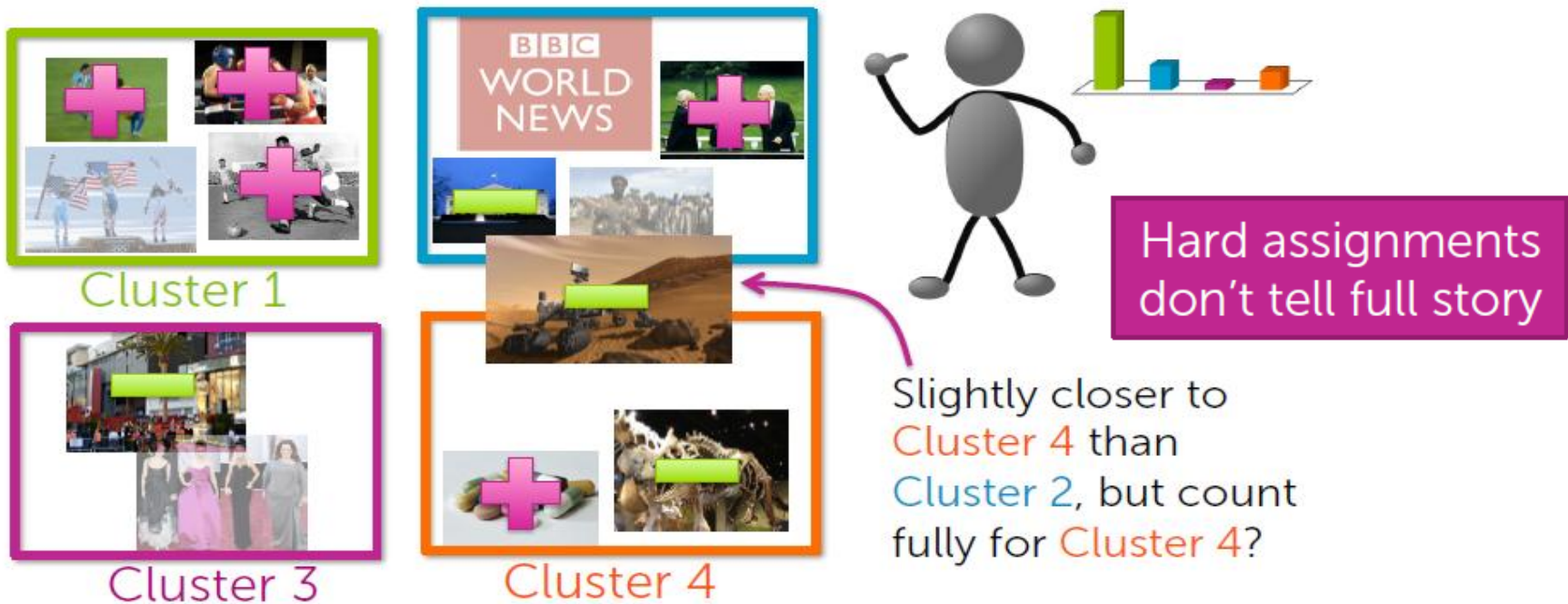


Use feedback
to learn user
preferences
over topics

Why probabilistic approach?

143

Uncertainty in cluster assignments



Why probabilistic approach?

144

Other limitations of k-means

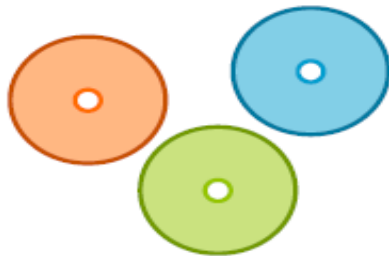
Assign observations to closest cluster center

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

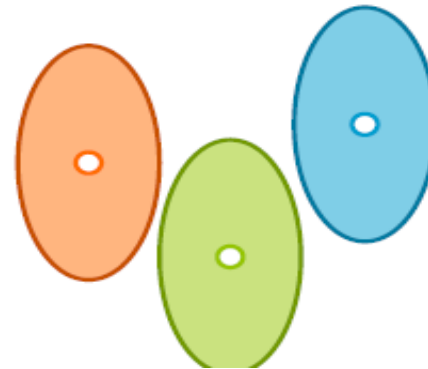
Can use weighted Euclidean, but requires *known* weights

Only center matters

Equivalent to assuming spherically symmetric clusters



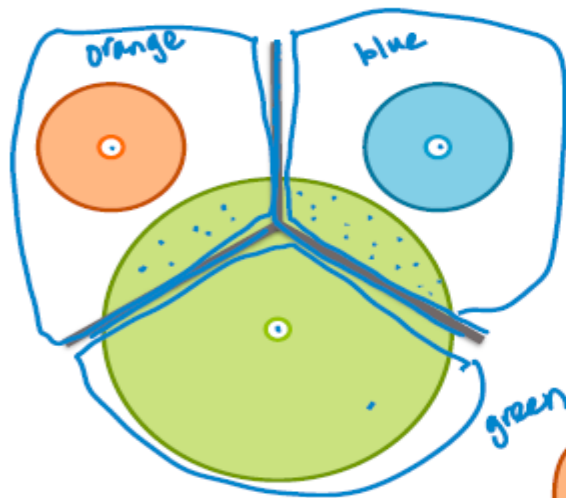
Still assumes all clusters have the same axis-aligned ellipses



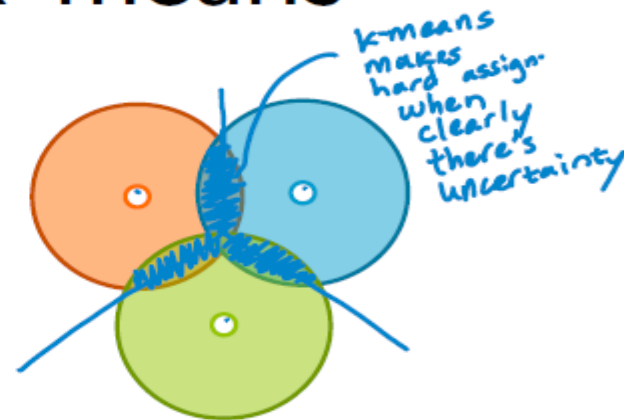
Why probabilistic approach?

145

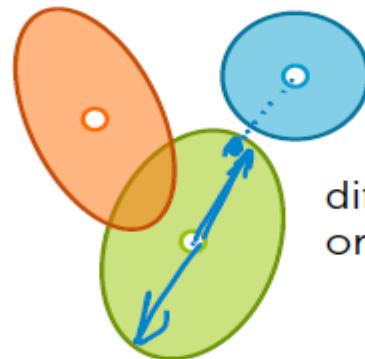
Failure modes of k-means



disparate cluster sizes



overlapping clusters



different shaped/
oriented clusters

Mixture models

146

- 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

147

Discover groups of similar images

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



Application: clustering images

148

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]

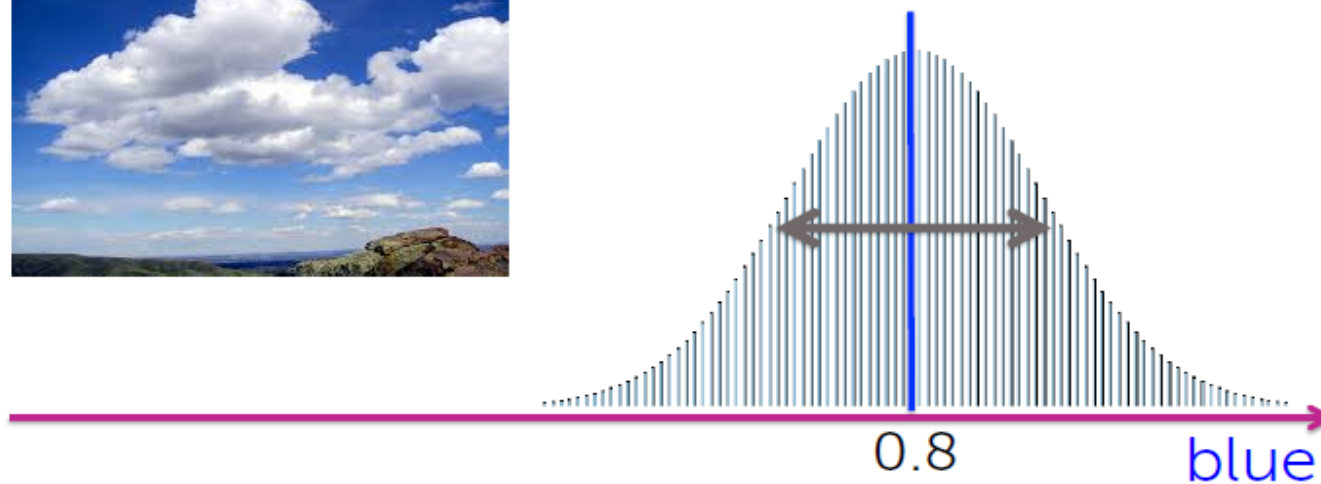
Single RGB vector per image

Application: clustering images

149

Distribution over all **cloud** images

Let's look at just the **blue** dimension

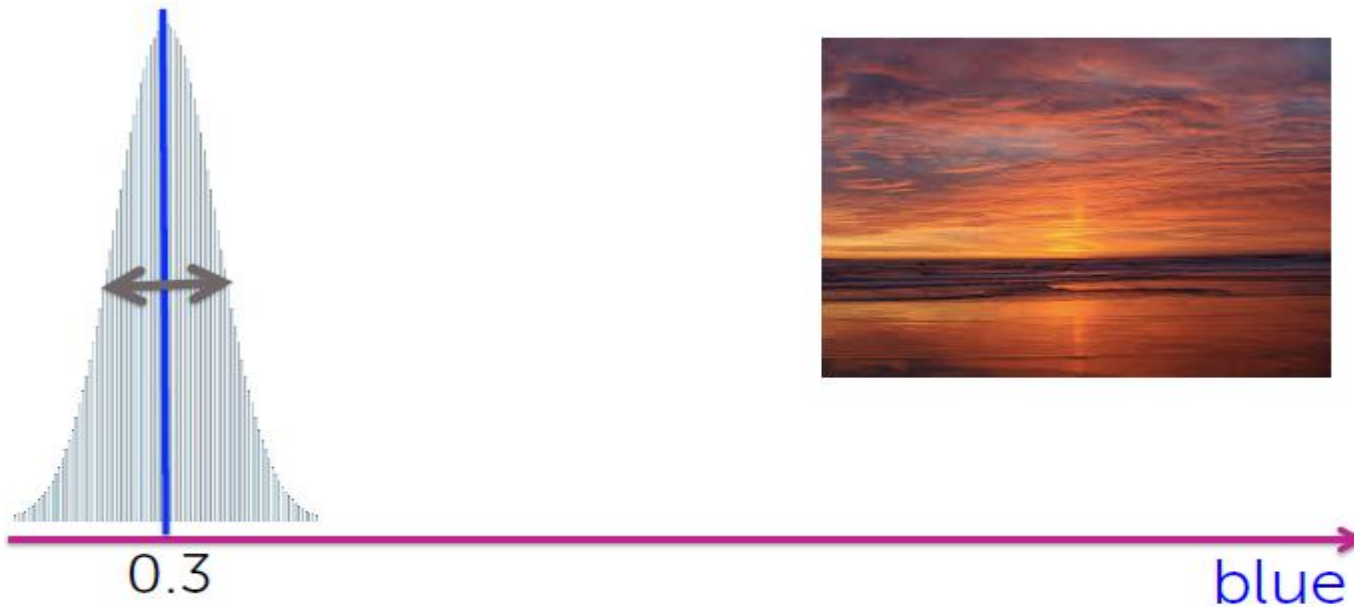


Application: clustering images

150

Distribution over all sunset images

Let's look at just the blue dimension

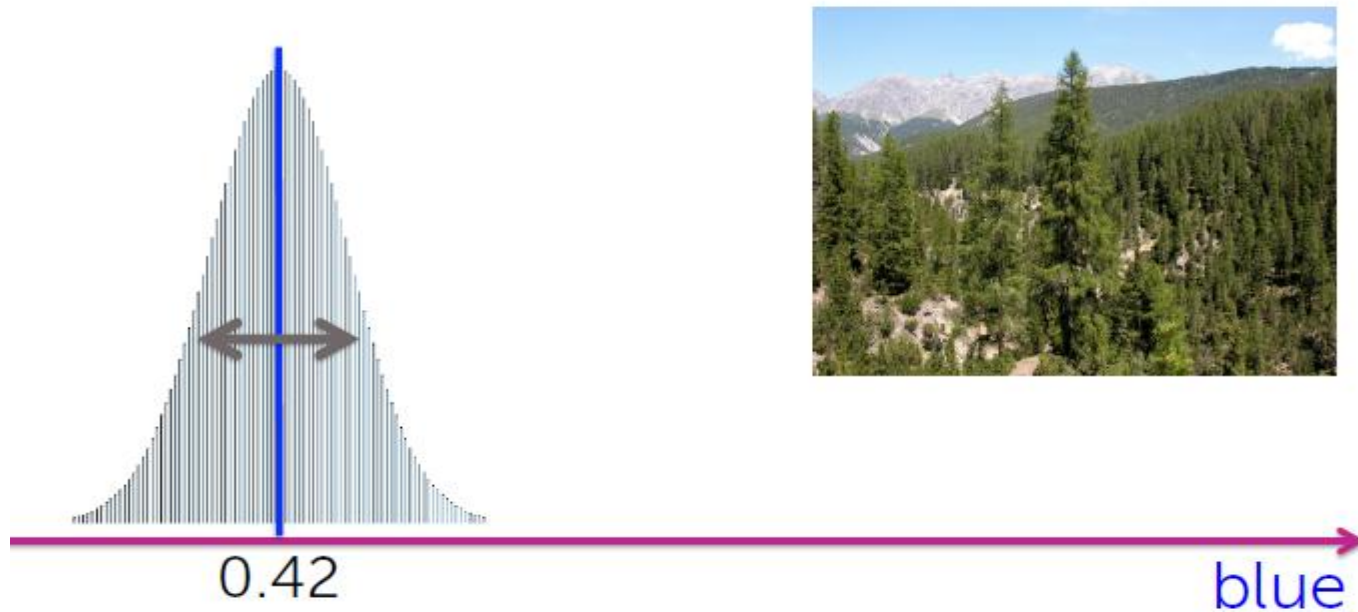


Application: clustering images

151

Distribution over all forest images

Let's look at just the blue dimension



Application: clustering images

152

Distribution over **all** images

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



Application: clustering images

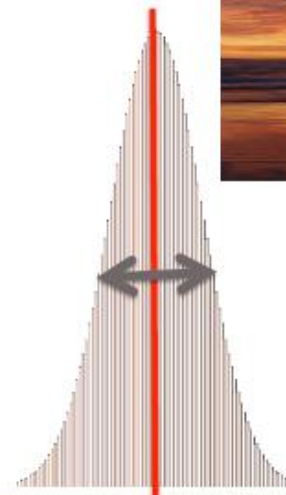
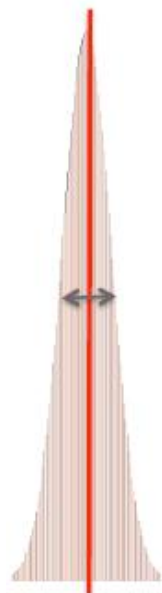
153

Can be distinguished along other dim

Now look at the **red** dimension



**In this dimension
separable groups!**



0.05

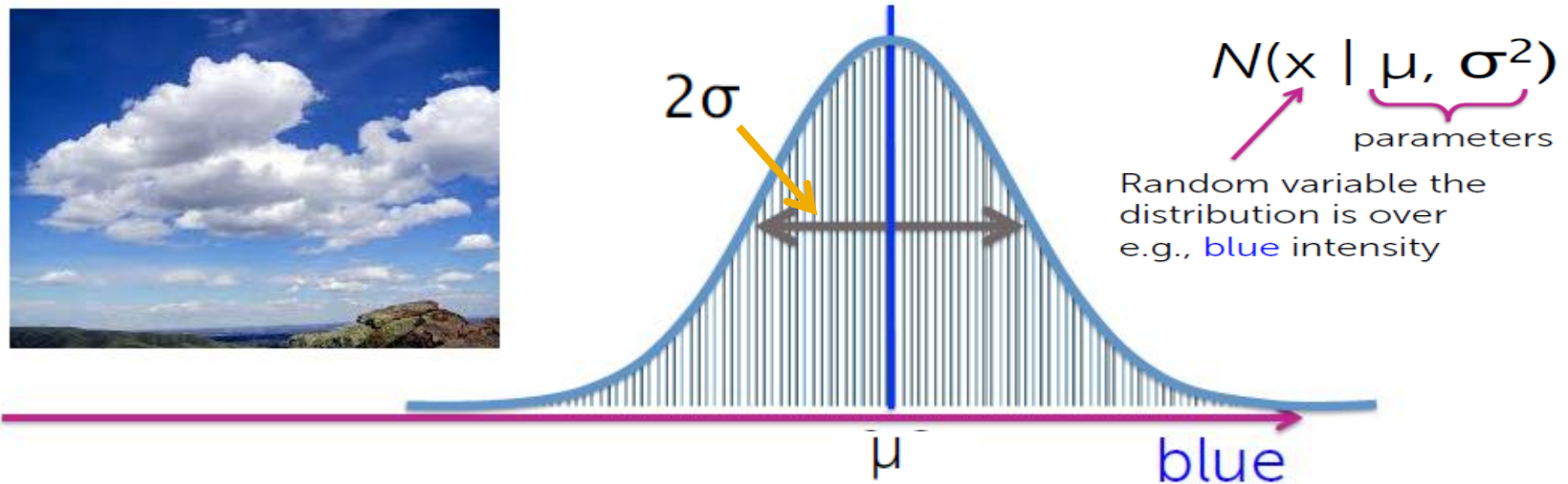
0.9

red

Model for a given image type

154

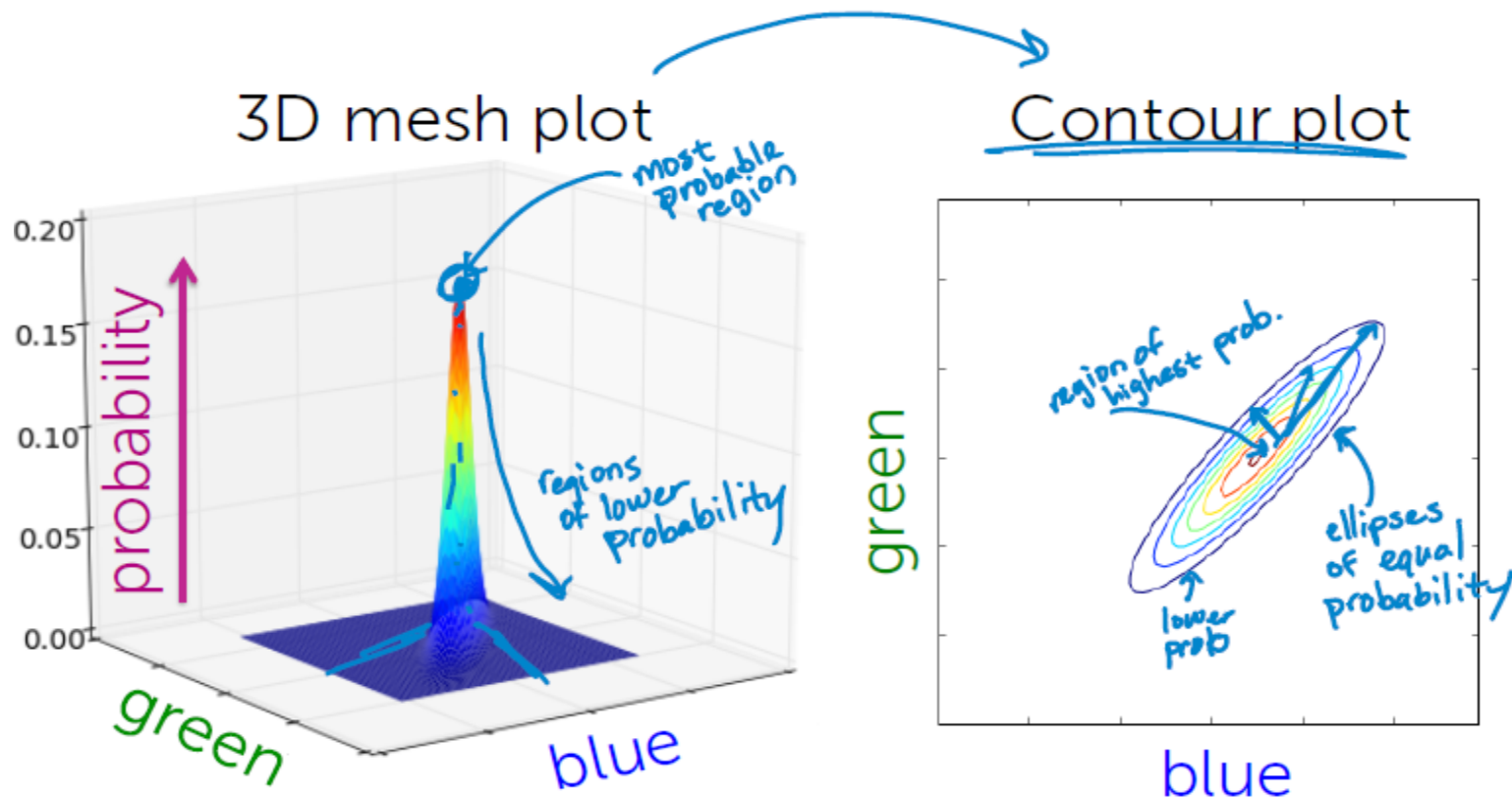
For **each dimension** of the [R, G, B] vector,
and **each image type**, assume a
Gaussian distribution over color intensity



Model for a given image type

155

2D Gaussians – Bird's eye view



Application: clustering images

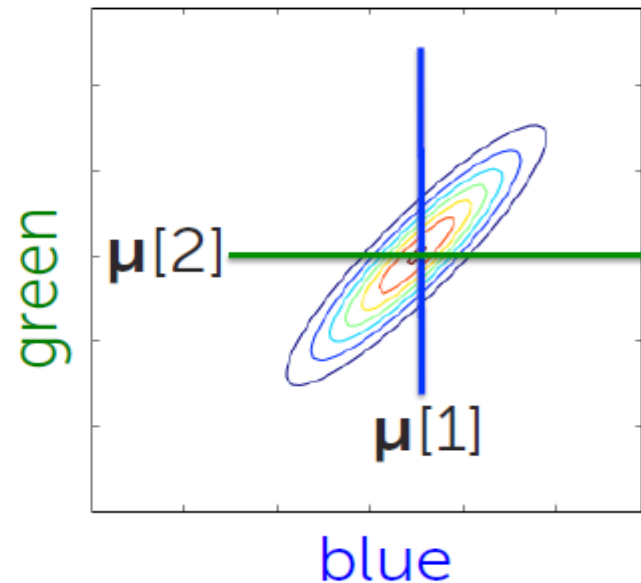
156

2D Gaussians – Parameters

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

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

mean centers the
distribution in 2D



Application: clustering images

157

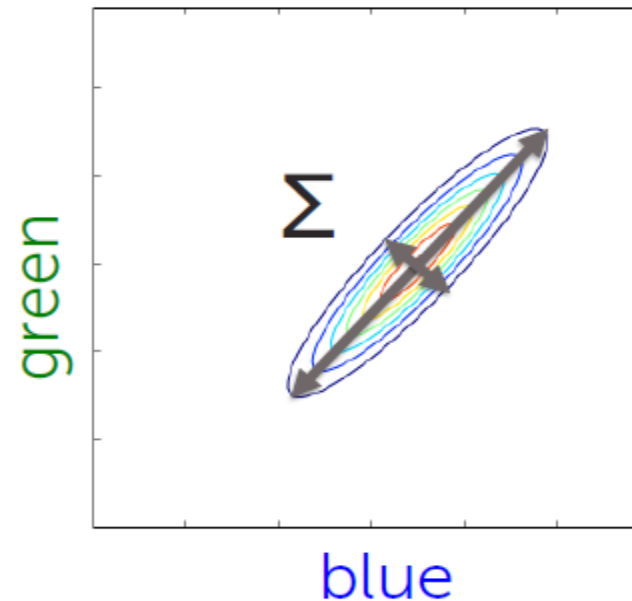
2D Gaussians – Parameters

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

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

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

covariance determines
orientation + spread

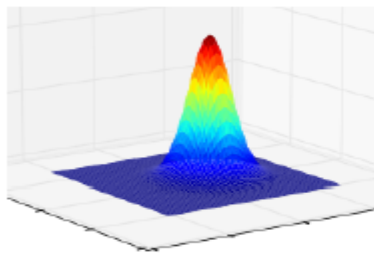
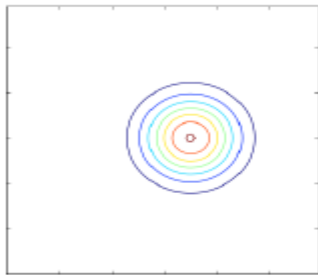


Application: clustering images

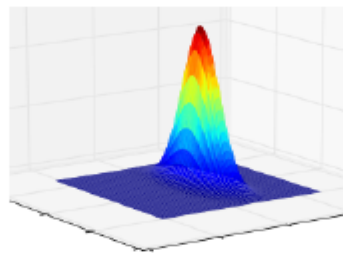
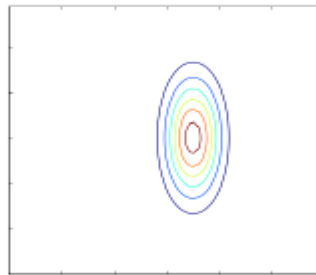
158

Covariance structures

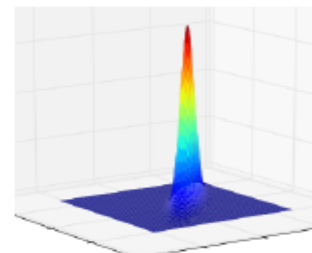
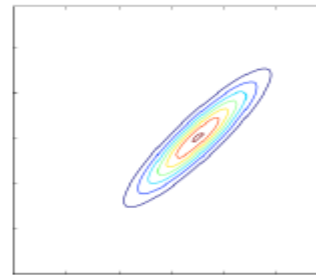
$$\Sigma = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix}$$



$$\Sigma = \begin{pmatrix} \sigma_B^2 & 0 \\ 0 & \sigma_G^2 \end{pmatrix}$$



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



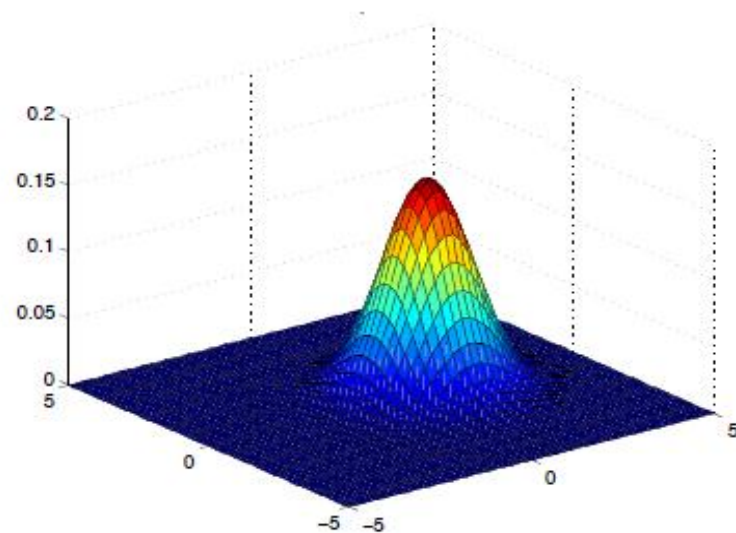
Application: clustering images

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Notating a multivariate Gaussian

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

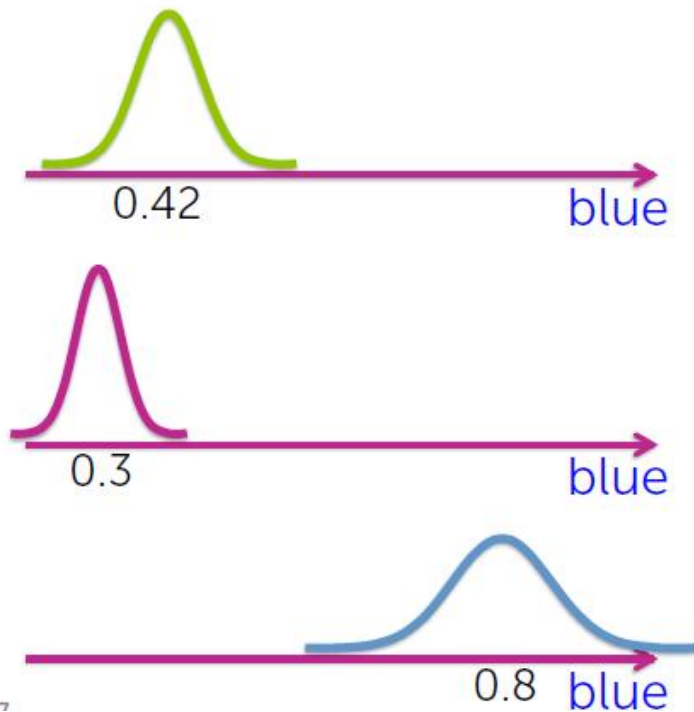
Random vector
e.g., [R, G, B] intensities



Mixture of Gaussians

160

Model as Gaussian per category/cluster

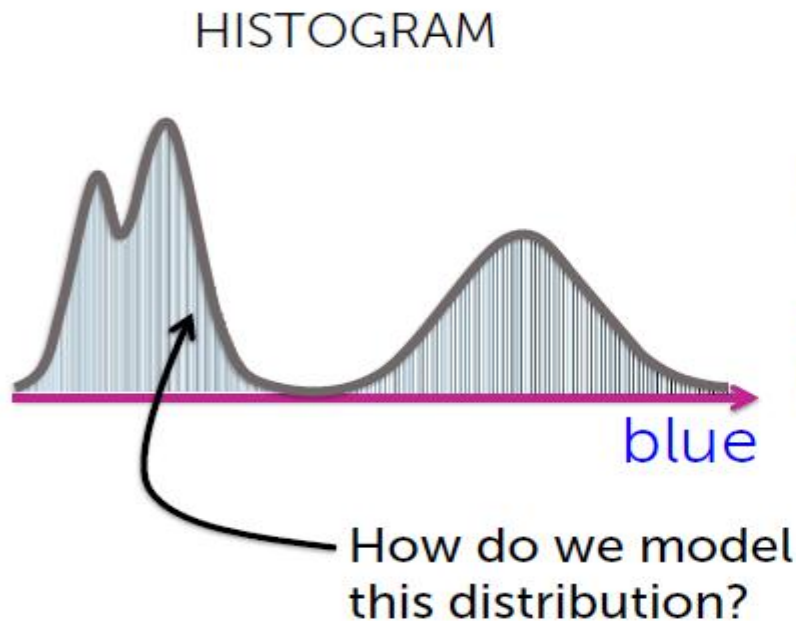


27

Mixture of Gaussians

161

Jumble of unlabeled images

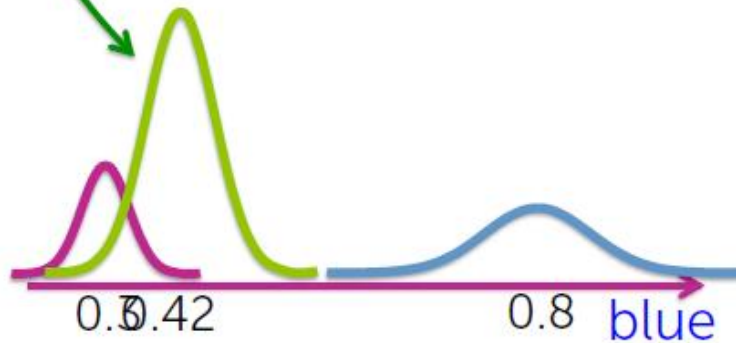


Mixture of Gaussians

162

What if image types not equally represented?

e.g., forest images are very likely in the collection

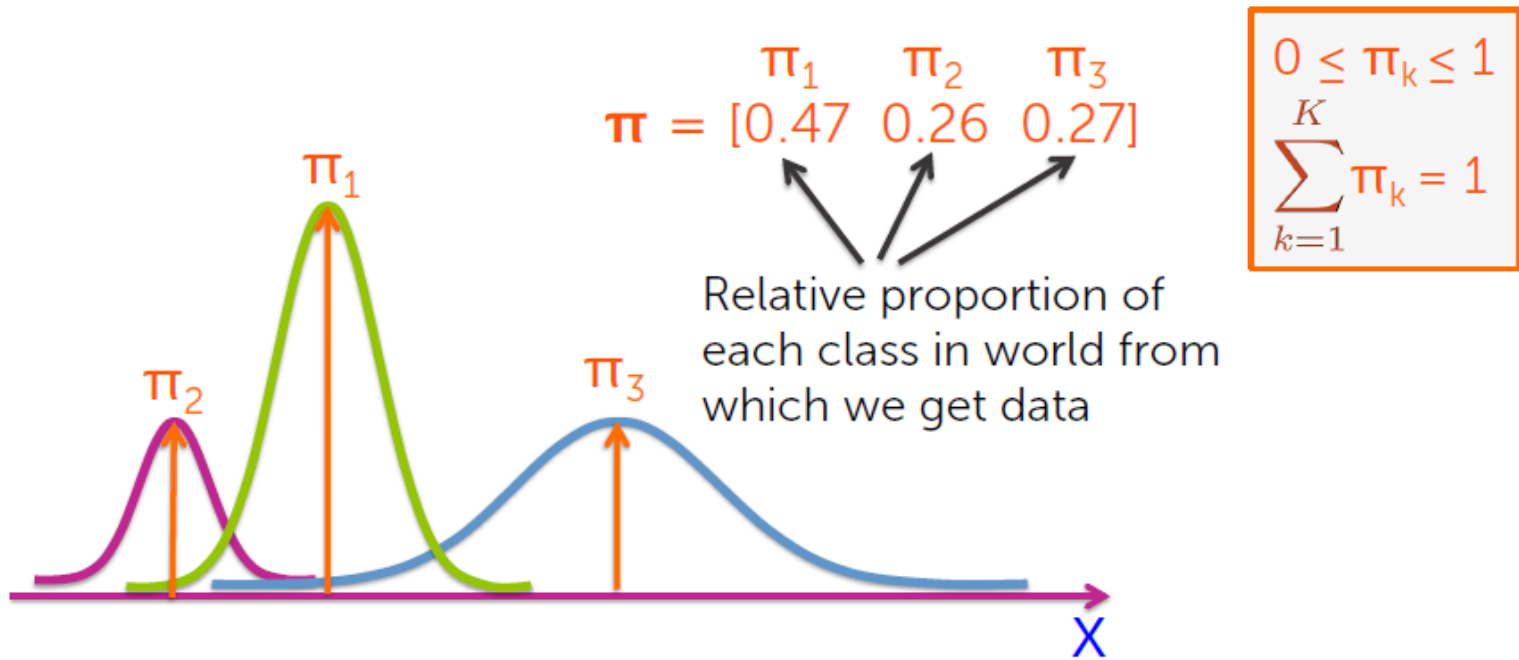


Mixture of Gaussians

163

Combination of weighted Gaussians

Associate a weight π_k with each Gaussian component



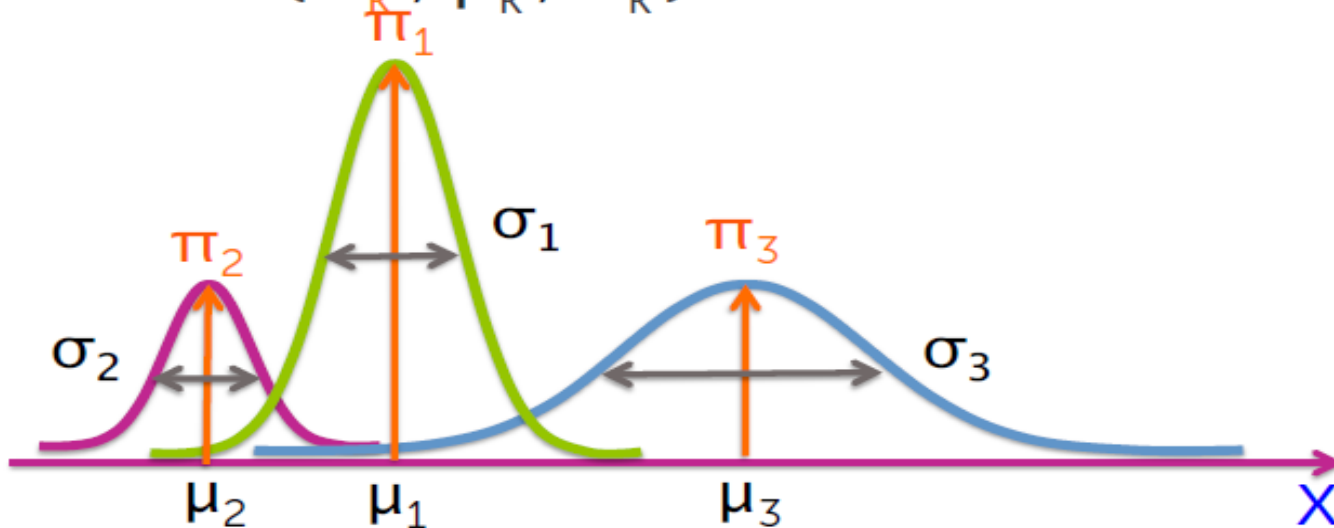
Mixture of Gaussians

164

Mixture of Gaussians (1D)

Each mixture component represents a unique cluster specified by:

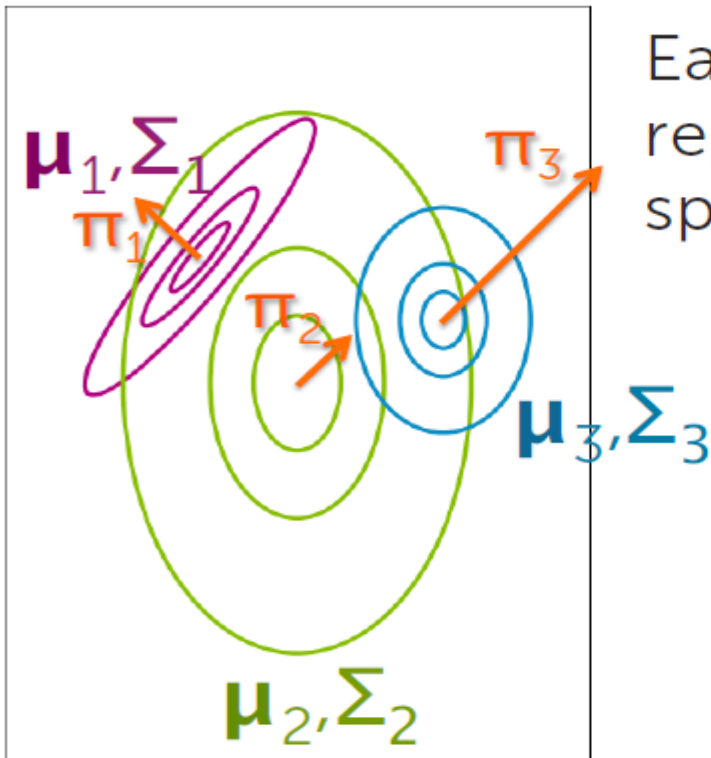
$$\{\pi_k, \mu_k, \sigma_k\}^2$$



Mixture of Gaussians

165

Mixture of Gaussians (general)



Each mixture component represents a unique cluster specified by:

$$\{\pi_k, \mu_k, \Sigma_k\}$$

Application: clustering documents

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Discover groups of related documents



Application: clustering documents

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Document representation



$x_i =$

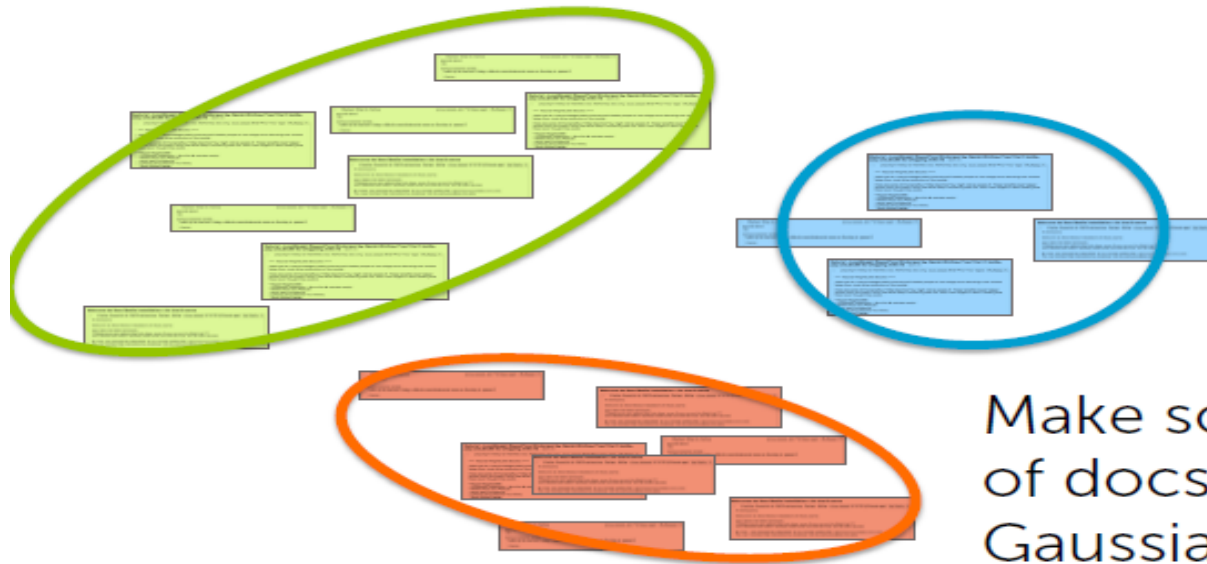


Application: clustering documents

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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

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Counting parameters

Each cluster has $\{\pi_k, \mu_k, \Sigma_k\}$



In 2D:

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

Application: clustering documents

171

Counting parameters

Each cluster has $\{\pi_k, \mu_k, \Sigma_k\}$



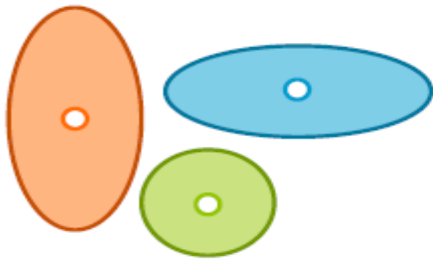
In V (vocab size) dims:

$$\Sigma = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{V(V+1)}{2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Application: clustering documents

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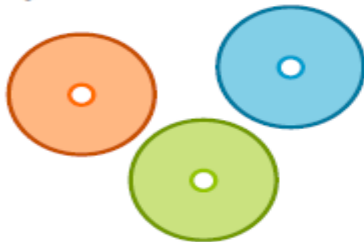
Restrictive assumption, but...



- 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...

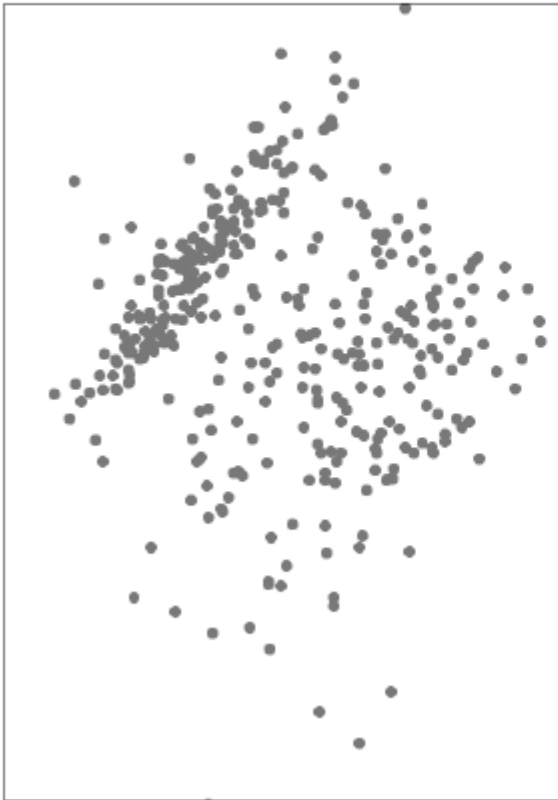
All clusters have same axis-aligned ellipses

Inferring soft assignments with expectation maximization (EM)

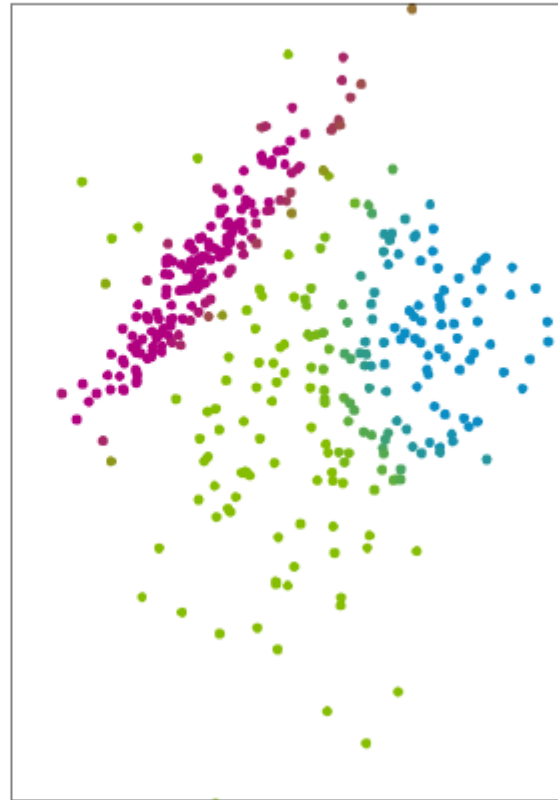
Inferring cluster labels

175

Data



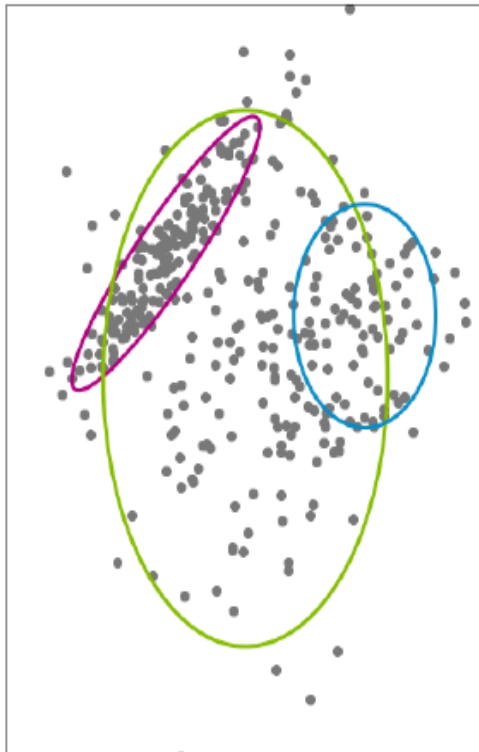
Desired soft assignments



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

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Compute responsibilities



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

Responsibility cluster k takes for observation i

$r_{ik} = p(\underbrace{z_i = k}_{\text{random variable}} \mid \underbrace{\{\pi_j, \mu_j, \Sigma_j\}_{j=1}^K}_{\text{fixed values defining the distribution}}, \underbrace{x_i}_{\text{given}})$

probability of assignment to cluster k

given model parameters and observed value

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

177

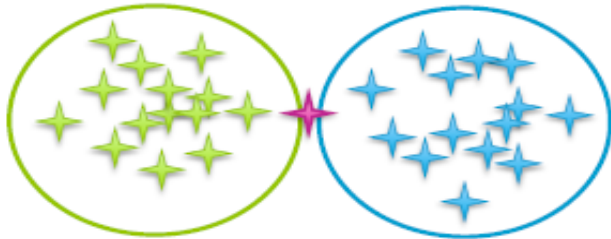
Responsibilities in pictures



Green cluster
takes more
responsibility



Blue cluster
takes more
responsibility



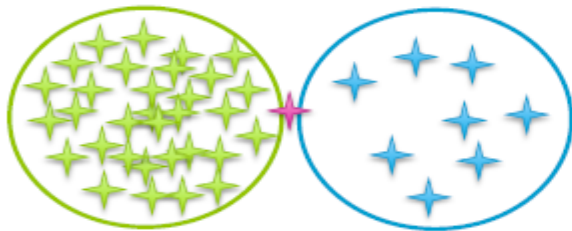
Uncertain...
split
responsibility

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

178

Responsibilities in pictures

Need to weight by cluster probabilities, not just cluster shapes

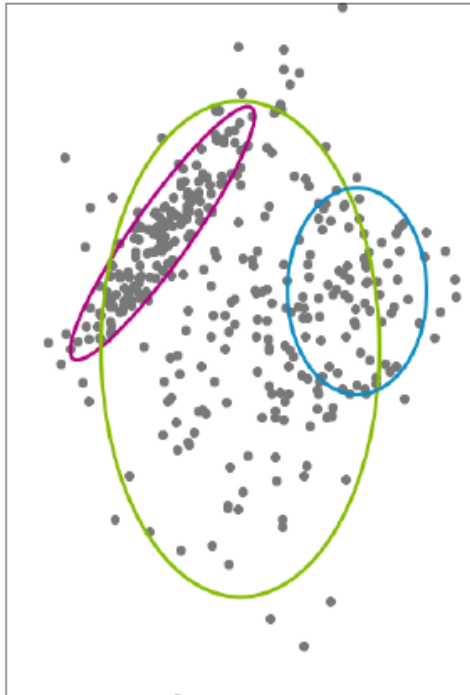


Still **uncertain**,
but **green** cluster seems
more probable...
takes more responsibility

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

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Responsibilities in equations



Responsibility cluster k takes for observation i

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

Initial probability of being from cluster k

How likely is the observed value x_i under this cluster assignment?

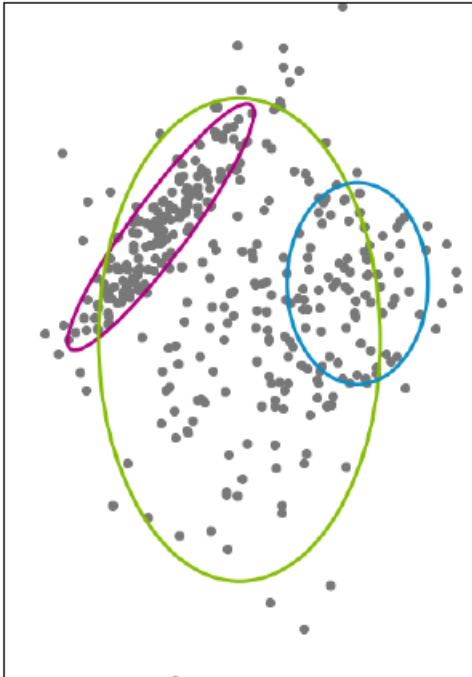
very unlikely under the green cluster, even though the prior on green is higher

A diagram showing two clusters: a green one on the left and a blue one on the right. A red dot representing a point is located within the blue cluster. A red arrow points from the red dot to the handwritten text below.

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

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Responsibilities in equations



Responsibility cluster k takes for observation i

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

Normalized over all possible cluster assignments

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

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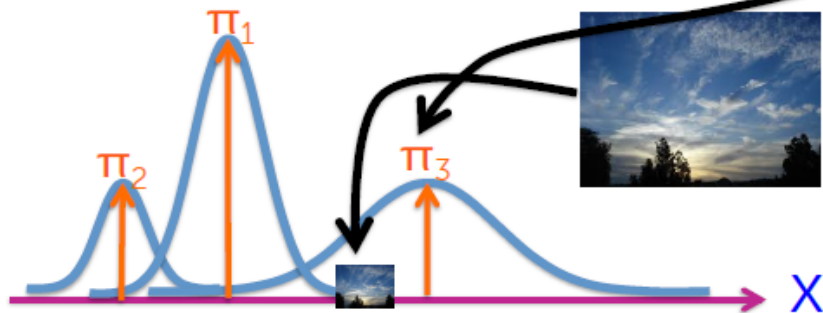
Recall: According to the model...

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")

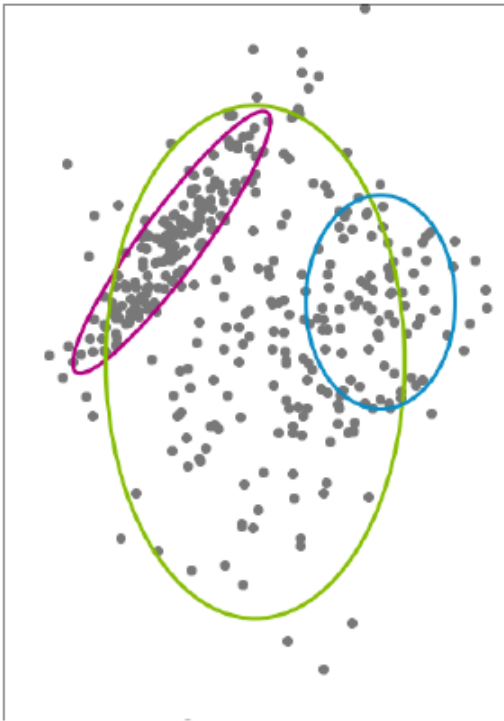
$$p(x_i | z_i = k, \mu_k, \Sigma_k) = N(x_i | \mu_k, \Sigma_k)$$



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

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Part 1: Summary



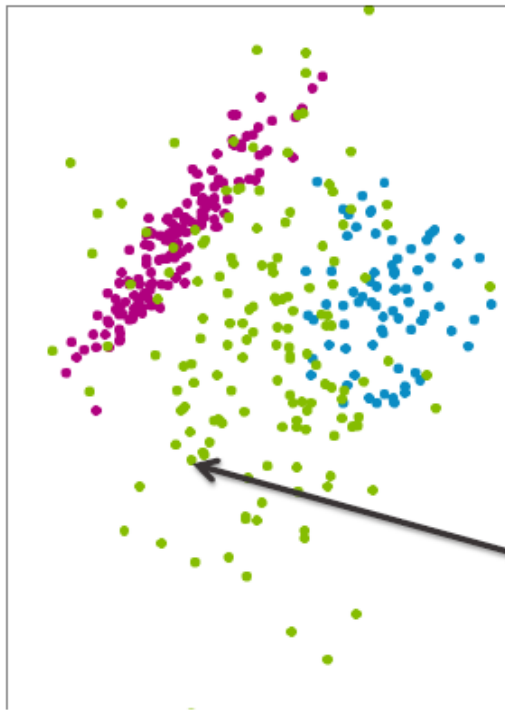
Desired soft assignments (responsibilities) are **easy** to compute when cluster parameters $\{\pi_k, \mu_k, \Sigma_k\}$ are known

But, we don't know these!

Imagine we knew the cluster
(hard) assignments z_i

183

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

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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

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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 $\{\pi_k, \mu_k, \Sigma_k\}$
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

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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

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

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

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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

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

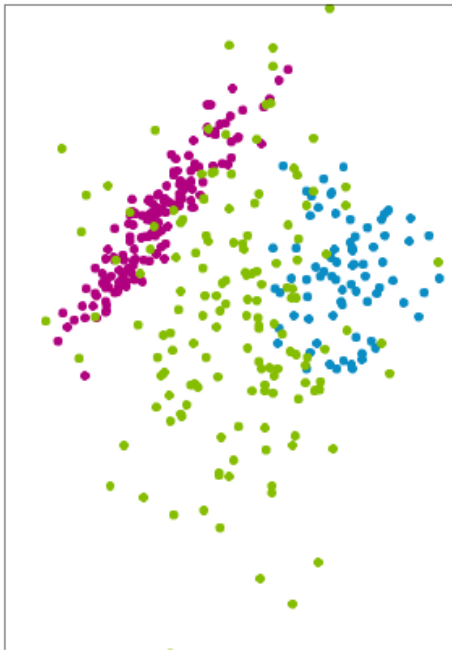
total # of obs

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

Imagine we knew the cluster
(hard) assignments z_i

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Part 2a : Summary



needed to compute soft assignments



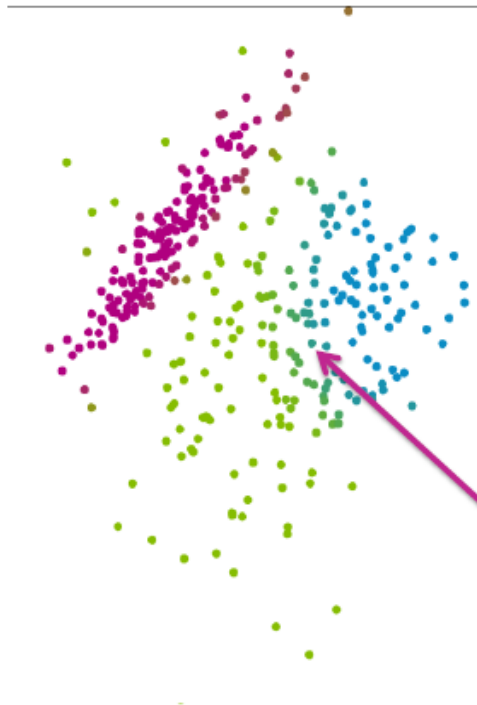
Cluster parameters are simple
to compute if we know the
cluster assignments

But, we don't know these!

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

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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}

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

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

191

Maximum likelihood estimation from soft assignments

R	G	B	Cluster 1 weights		
$x_1[1]$	$x_1[2]$	$x_1[3]$	0.30		
$x_2[1]$	R	G	B	Cluster 2 weights	
$x_3[1]$					
$x_4[1]$	$x_1[1]$	$x_1[2]$	$x_1[3]$	0.18	
$x_5[1]$	$x_2[1]$	R	G	B	Cluster 3 weights
$x_6[1]$	$x_3[1]$				
	$x_4[1]$	$x_1[1]$	$x_1[2]$	$x_1[3]$	0.52
	$x_5[1]$	$x_2[1]$	$x_2[2]$	$x_2[3]$	0.73
	$x_6[1]$	$x_3[1]$	$x_3[2]$	$x_3[3]$	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} ?

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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

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

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

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

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} ?

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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

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

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

Total weight in cluster k
= effective # obs

Total weight
in cluster:

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

Total weight
in dataset:

6

datapoints N

Estimate cluster
proportions from
relative weights

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

194

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} ?

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Equating the estimates...

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

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

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

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Part 2b: Summary



Still straightforward to compute cluster parameter estimates from soft assignments

Expectation maximization (ME)

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An iterative algorithm

Motivates an iterative algorithm:

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

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

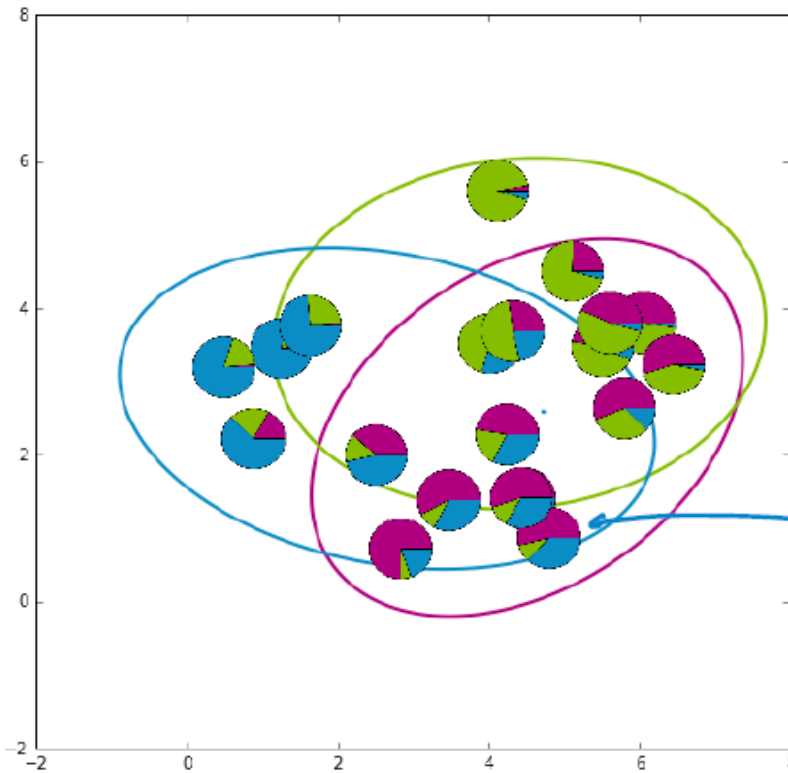
2. **M-step:** maximize likelihood over parameters given current responsibilities

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

Expectation maximization (EM)

198

EM for mixtures of Gaussians in pictures – initialization



Initialize
iter counter
 $\{\pi_k^{(0)}, \mu_k^{(0)}, \Sigma_k^{(0)}\}$

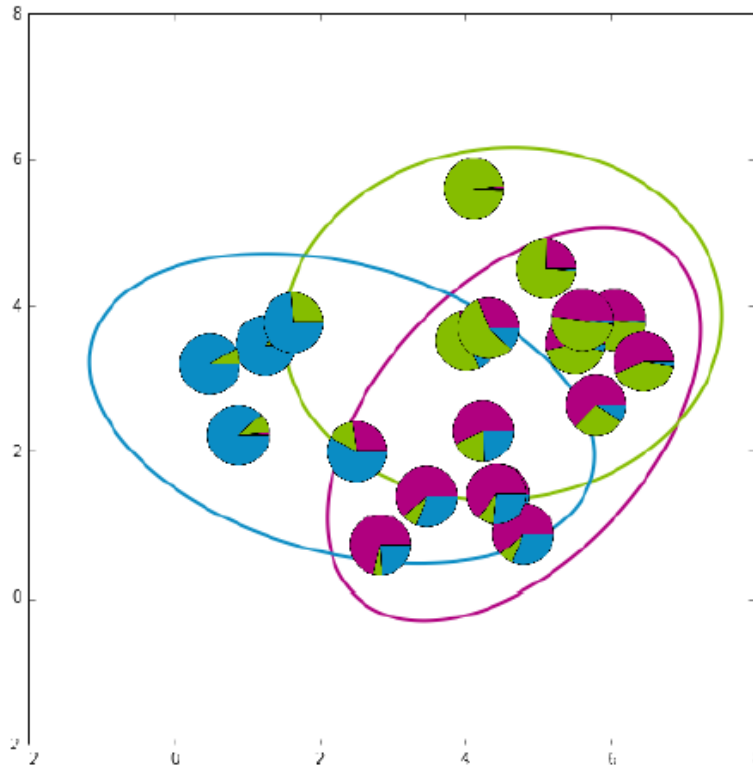
Then compute
 $\hat{r}_{ik}^{(1)}$

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

Expectation maximization (EM)

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



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

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

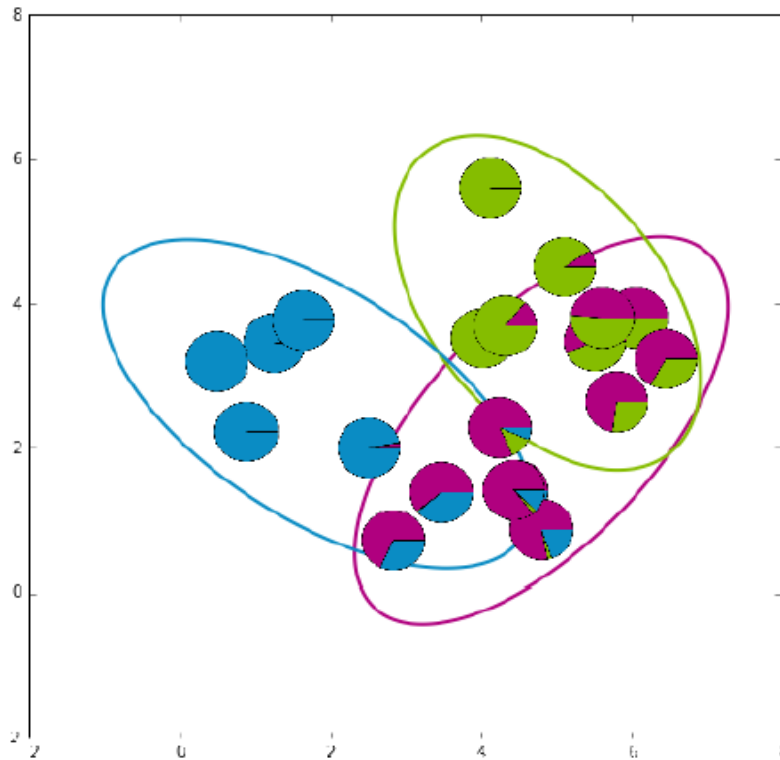
Then recompute responsibilities

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

Expectation maximization (EM)

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

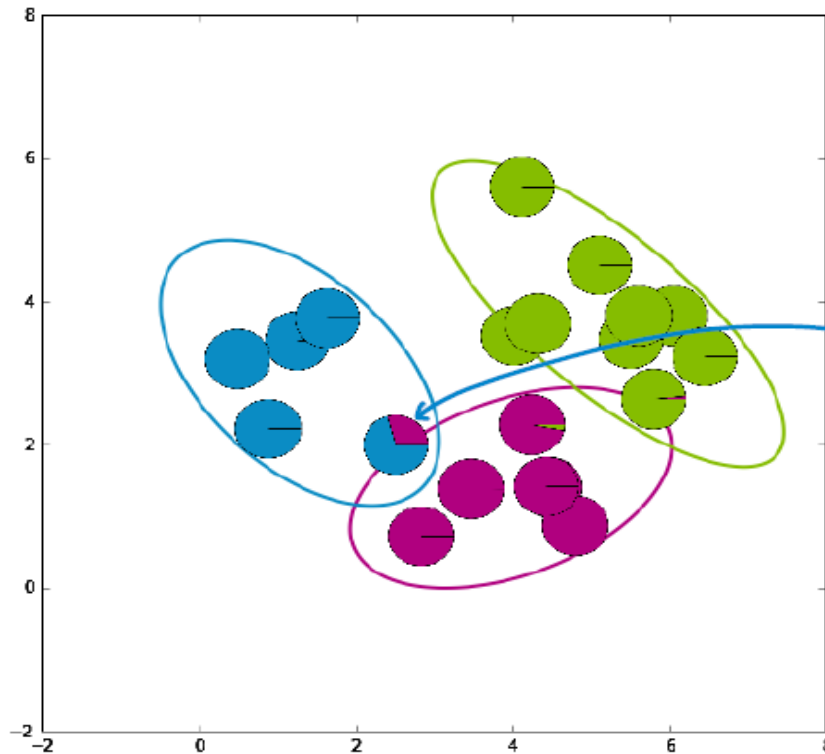


*rinse
+
repeat
until convergence*

Expectation maximization (EM)

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EM for mixtures of Gaussians in pictures – converged solution

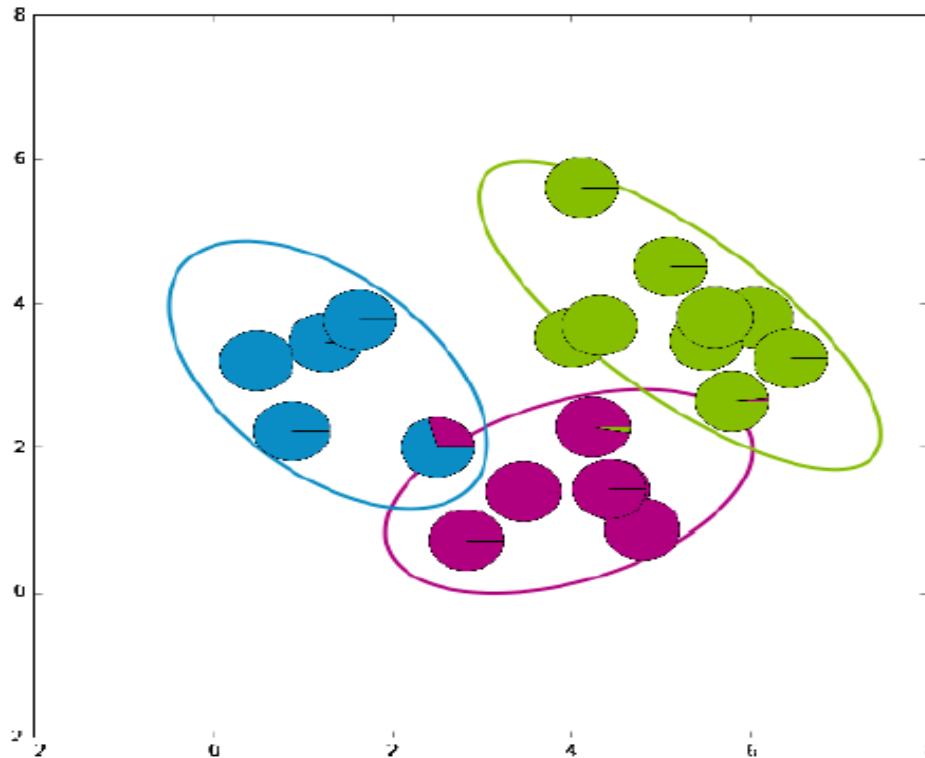


Clearly see
uncertainty in
assignment of obs.
to blue or fuchsia
cluster, even in
final assignments.

Expectation maximization (EM)

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EM for mixtures of Gaussians
in pictures - [replay](#)



Expectation maximization (ME)

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Convergence of EM

- EM is a **coordinate-ascent algorithm**
 - Can equate E-and M-steps with alternating maximizations of an objective function
- Converges to a **local mode**
- We will assess via (log) likelihood of data under current parameter and responsibility estimates

Expectation maximization (ME)

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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 centroid 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)

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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)

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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 $\mu_k[w] = \mathbf{x}_i[w]$ and $\sigma_{w,k}^2 = 0$

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

Expectation maximization (ME)

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Simple regularization of M-step for mixtures of Gaussians

Simple fix: Don't let variances $\rightarrow 0$!

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.

Expectation maximization (ME)

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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 $\rightarrow 0$, **likelihood ratio becomes 0 or 1**
- Responsibilities weigh in cluster proportions, but dominated by likelihood disparity

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

Expectation maximization (ME)

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Infinitesimally small variance EM = k-means

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

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

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 ...

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- 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

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So far, clustered articles into groups



Clustering goal: discover groups of related docs

Clustering model

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Are documents about just one thing?



Is this article
just about
science?



Clustering model

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Soft assignments capture uncertainty



Soft assignments

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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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^bDepartment of Neurology, University of Pennsylvania, Philadelphia, PA

^cDepartment of Statistics, University of Washington, Seattle, WA

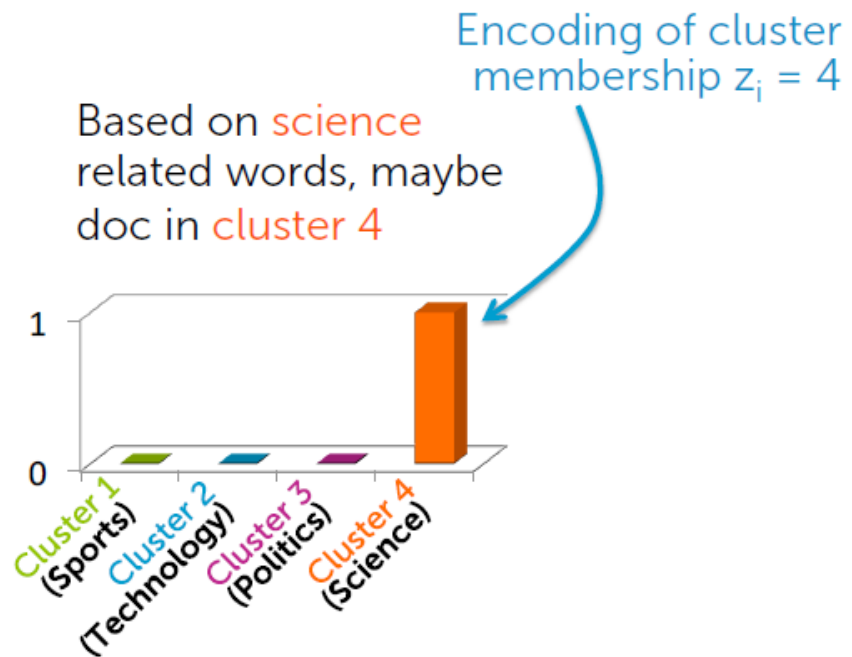
Abstract

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



Soft assignments

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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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^bDepartment of Neurology, University of Pennsylvania, Philadelphia, PA

^cDepartment of Statistics, University of Washington, Seattle, WA

Abstract

Patients with epilepsy can manifest short, sub-clinical epileptic “bursts” in addition to full-blown seizures. We 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.

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

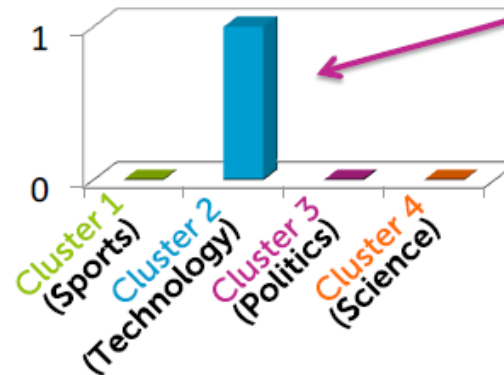
1. Introduction

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

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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Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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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. We introduce a 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.

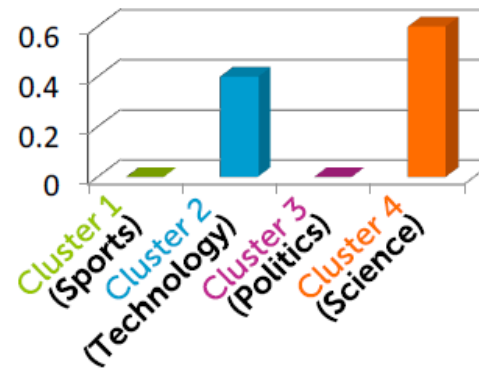
“ z_i ” is both 2 and 4

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

Really, it's about science and technology



Mixed membership models

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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}

^aDepartment of Bioengineering, University of Pennsylvania, Philadelphia, PA

^bDepartment of Neurology, University of Pennsylvania, Philadelphia, PA

^cDepartment 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.

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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

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An alternative document clustering model



(Back to clustering, not mixed membership modeling)

Building an alternative model

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So far, we have considered...

Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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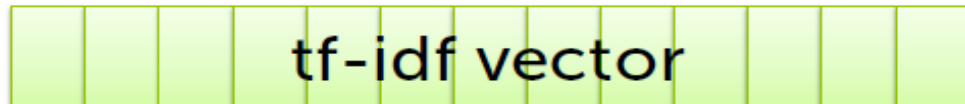
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$x_i =$



Building an alternative model

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Bag-of-words representation

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$\mathbf{X}_i = \{ \text{modeling, complex, epilepsy, modeling, Bayesian, clinical, epilepsy, EEG, data, dynamic...} \}$

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:

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

$\boldsymbol{\pi} = [\pi_1 \ \pi_2 \ \dots \ \pi_k]$
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

Model for „bag-of-words”

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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”

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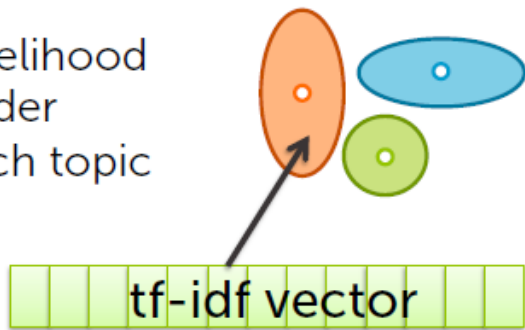
Comparing and contrasting

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	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	
...

{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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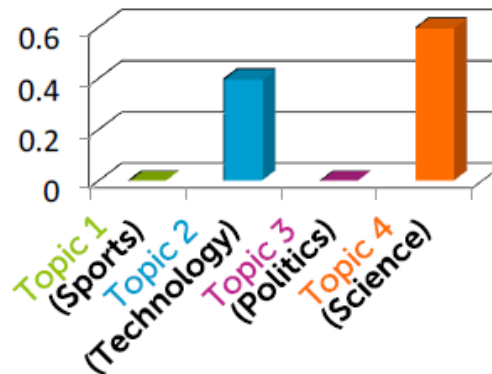
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LDA is a mixed membership model

Want to discover a set of topics



Latent Dirichlet allocation

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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
goal	0.03
injury	0.01
...	...

⋮

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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

$\pi = [\pi_1 \ \pi_2 \ \dots \ \pi_K]$

Latent Dirichlet allocation

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Same topic 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
goal	0.03
injury	0.01
...	...

⋮

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Research on 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 is 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 for 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.

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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

$$\pi_i = [\pi_{i1} \ \pi_{i2} \ \dots \ \pi_{iK}]$$

Inference in LDA models

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
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SPORTS	
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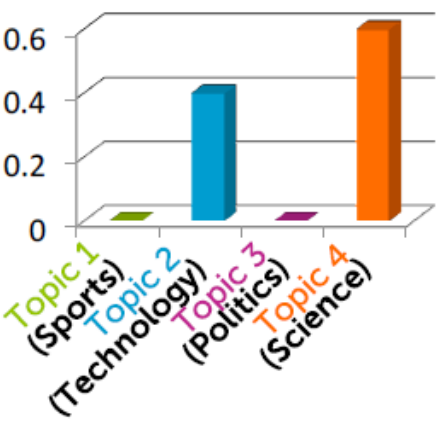
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Document topic proportions:

$$\pi_i = [\pi_{i1} \ \pi_{i2} \ \dots \ \pi_{iK}]$$



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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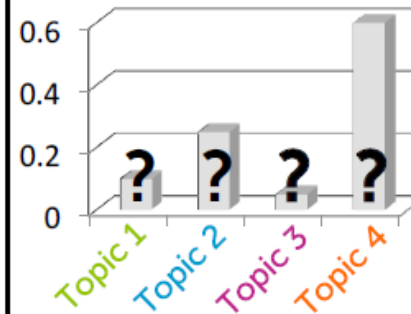
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$$\boldsymbol{\pi}_i = [\pi_{i1} \ \pi_{i2} \ \dots \ \pi_{iK}]$$



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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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LDA inputs:

- Set of words per doc for each doc in corpus

LDA outputs:

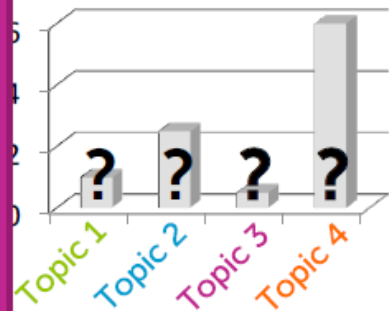
- Corpus-wide topic vocab distributions
- Topic assignments per word
- Topic proportions per doc

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Inference in LDA models

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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
score	0.07
team	0.06
goal	0.03
injury	0.01
...	...

⋮

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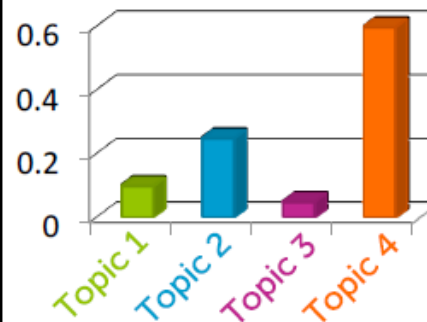
Drausia F. Walsin^a, Emily B. Fox^c, Brian Litt^{a,b}

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Inference in LDA models

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Interpreting LDA outputs

TOPIC 1	
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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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...	...

TOPIC 3	
player	0.15
score	0.07
team	0.06
goal	0.03
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...	...

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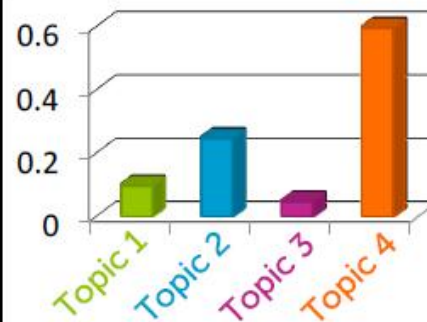
Abstract

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 iEEG (iEEG) data we used 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 graphical model for the innovations process driving the observed dynamics and demonstrate the importance of this modeling in fitting 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 nonparametrics, 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



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,...)

Inference in LDA models

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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
score	0.07
team	0.06
goal	0.03
injury	0.01
...	...

⋮

Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

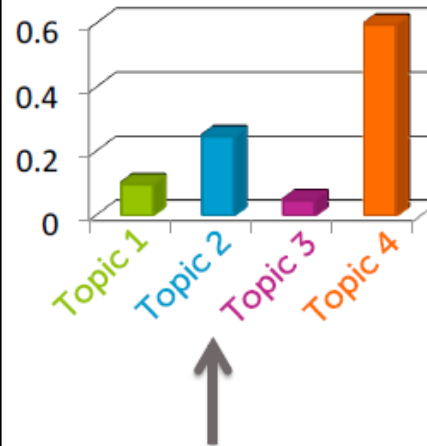
Drausin F. Wulsin^a, Emily B. Fox^a, Brian Litt^{a,b}

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

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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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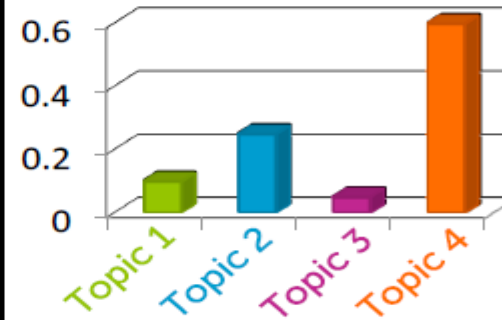
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Typically **not** interested in word assignments

An inference algorithm for LDA: Gibbs sampling

Clustering so far

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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

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

M-step: maximize likelihood over parameters

$$\hat{\pi}_k, \hat{\mu}_k, \hat{\Sigma}_k \mid \{\hat{r}_{ik}, \mathbf{x}_i\}$$

Iterative **soft** assignment to max objective

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

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Part 1: Clustering model

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
...	...

⋮

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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
 $\pi = [\pi_1 \ \pi_2 \ \dots \ \pi_K]$

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

241

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

TECH	
develop	0.18
computer	0.09
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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?

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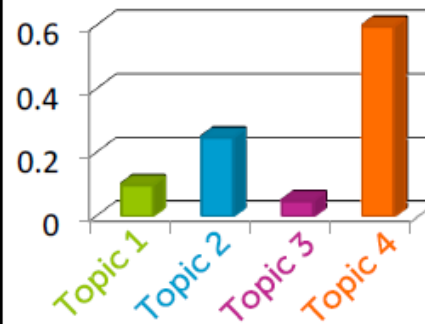
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Can derive EM algorithm, but not common (performs poorly)

An inference algorithms

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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...

Algorithm for Bayesian inference

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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	
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score	0.07
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goal	0.03
injury	0.01
...	...

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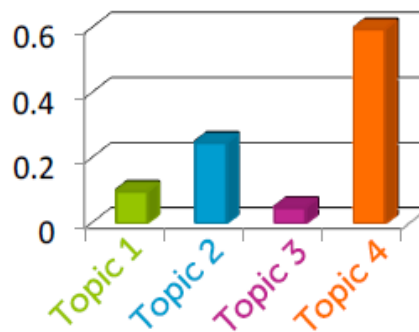
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Current set of assignments

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
team	0.06
goal	0.03
injury	0.01
...	...

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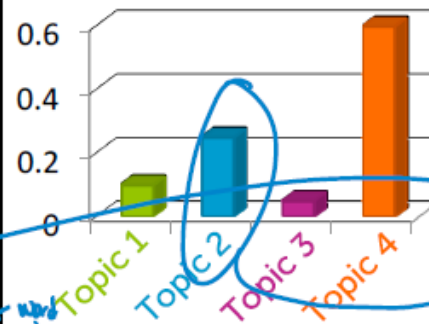
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- Step 1: Randomly reassign all z_{iw} based on**
- doc topic proportions
 - topic vocab distributions

Draw randomly from responsibility vector
 $[r_{i1w} \ r_{i2w} \ \dots \ r_{iKw}]$

$$r_{i2w} = \frac{\pi_{i2} \cdot P(\text{"EEG"} | z_{i2w}=2)}{\sum_{j=1}^K \pi_{ij} \cdot P(\text{"EEG"} | z_{ijw}=j)}$$

↑ prior Prob. of $z_{i2w}=2$
 ↑ prob. of assigning $z_{i2w}=2$

Gibbs sampling for LDA

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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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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
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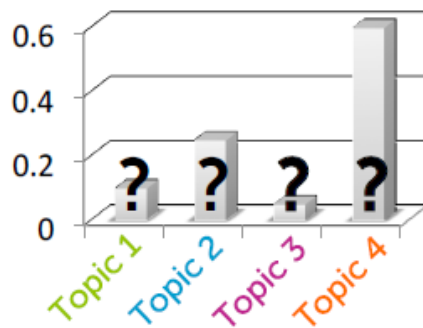
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Step 3: Repeat for all docs

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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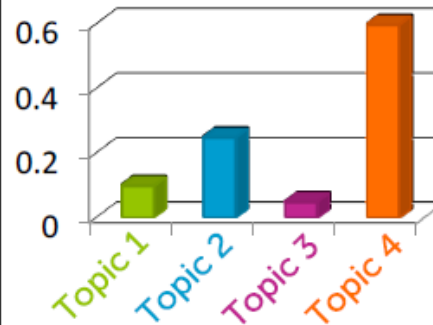
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Step 4: Randomly reassign topic vocab distributions based on assignments $z_{i,w}$ in entire corpus

An inference algorithm: Gibbs sampling

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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
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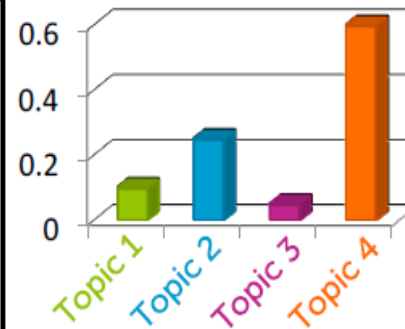
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Repeat Steps 1-4 until max iter reached

An inference algorithm: Gibbs sampling

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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
...	...

⋮

Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

Drausin F. Wulsin^a, Emily B. Fox^c, Brian Litt^{a,b}

^aDepartment of Bioengineering, University of Pennsylvania, Philadelphia, PA
^bDepartment of Neurology, University of Pennsylvania, Philadelphia, PA
^cDepartment of Statistics, University of Washington, Seattle, WA

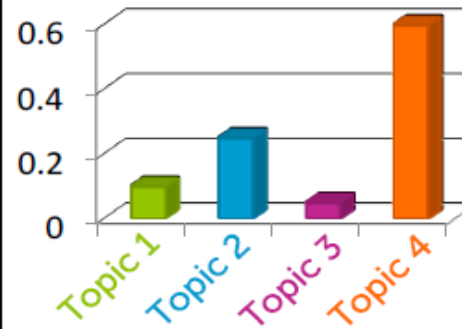
Abstract

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



Current set of assignments

An inference algorithm: Gibbs sampling

252

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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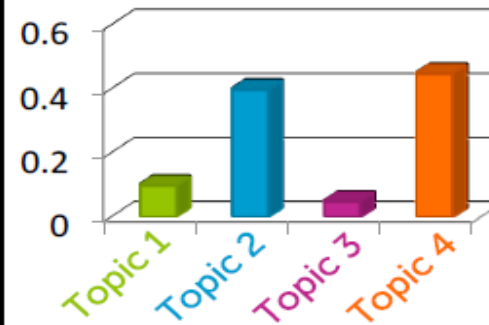
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Current set of assignments

An inference algorithm: Gibbs sampling

253

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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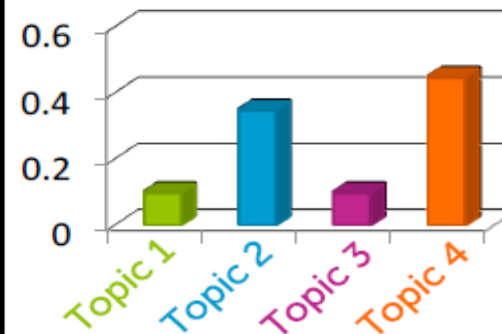
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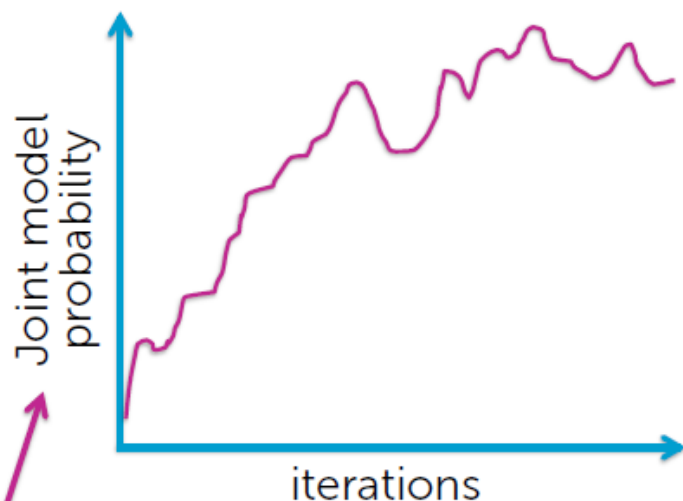
Current set of assignments

An inference algorithm: Gibbs sampling

254

What do we know about this process?

Not an optimization algorithm



Eventually provides "correct" Bayesian estimates...

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

An inference algorithm: Gibbs sampling

255

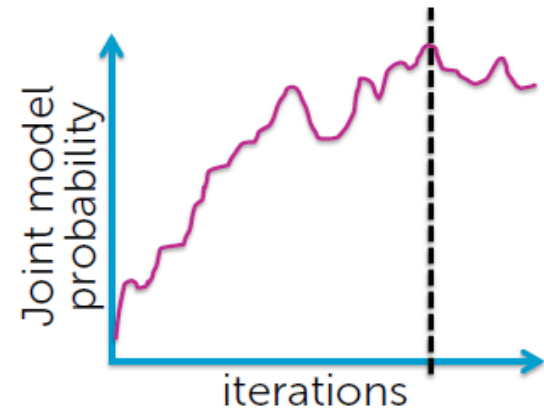
What to do with sampling output?

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

256

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

257

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

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Never draw topic vocab distributions or doc topic proportions

TOPIC 1

experiment	0.1
test	0.1
discover	0.1
hypothesize	0.1
climate	0.1
...	...

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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Topic	Proportion
Topic 1	Low
Topic 2	Medium
Topic 3	Low
Topic 4	High

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

Collapsed Gibbs sampling for LDA

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Select a document

epilepsy	dynamic	Bayesian	EEG	model

5 word document

Collapsed Gibbs sampling for LDA

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Randomly assign topics

3	2	1	3	1
epilepsy	dynamic	Bayesian	EEG	model

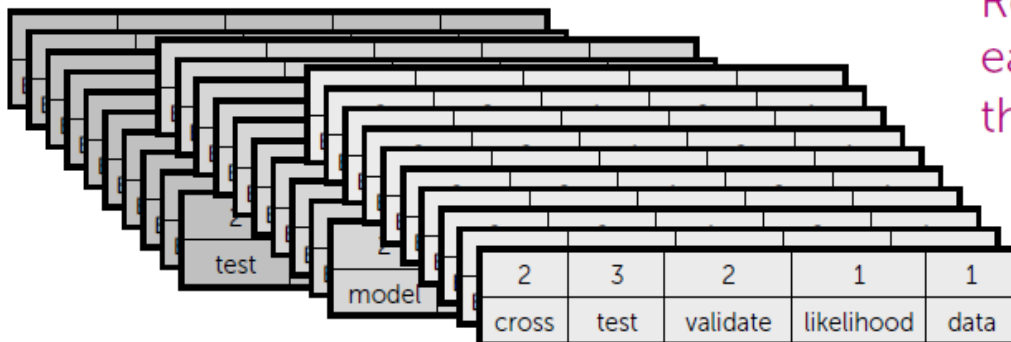
(one possible approach)

Collapsed Gibbs sampling for LDA

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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

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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

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Maintain global statistics

3	2	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	8	1
...			

	Topic 1	Topic 2	Topic 3
Doc i	2	1	2

Total counts from **all** docs

Collapsed Gibbs sampling for LDA

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Randomly reassign topics

3	2	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 1	2

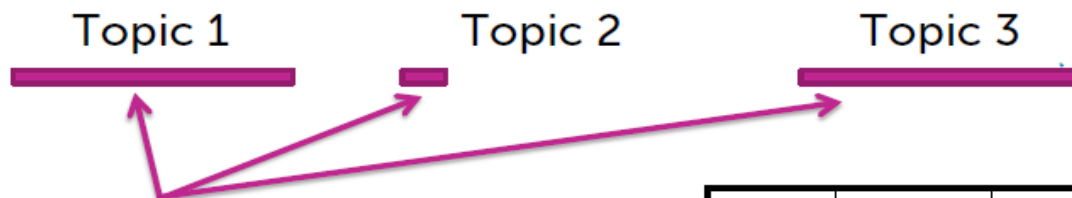
decrementing
counts
after removing
current assignment
 $Z_{iw} = 2$

Collapsed Gibbs sampling for LDA

265

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 $\rightarrow n_{ik} + \alpha$ ← smoothing param from Bayes prior

words in doc i $\rightarrow N_i - 1 + K\alpha$ ← ignore current word

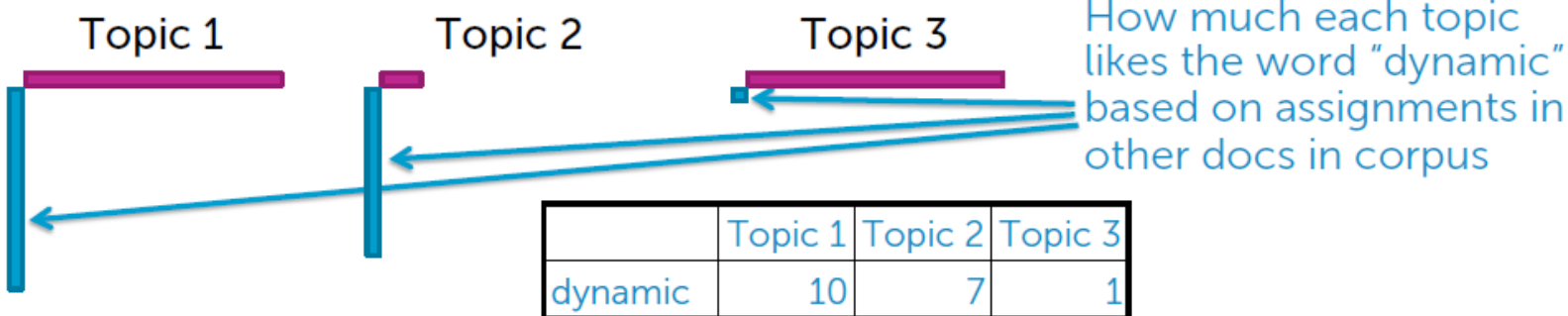
63

Collapsed Gibbs sampling for LDA

266

Probability of new assignment

3	?	1	3	1
epilepsy	dynamic	Bayesian	EEG	model



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

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

$m_{\text{dynamic},k} + \gamma$ ← smoothing param from Bayes prior
 $\sum_{w \in V} m_{w,k} + V\gamma$ ← size of vocab

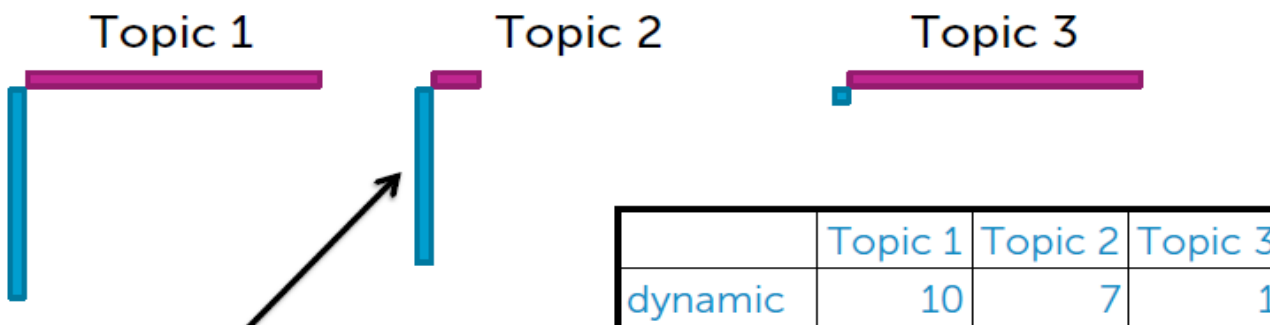
6.1

Collapsed Gibbs sampling for LDA

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Probability of new assignment

3	?	1	3	1
epilepsy	dynamic	Bayesian	EEG	model



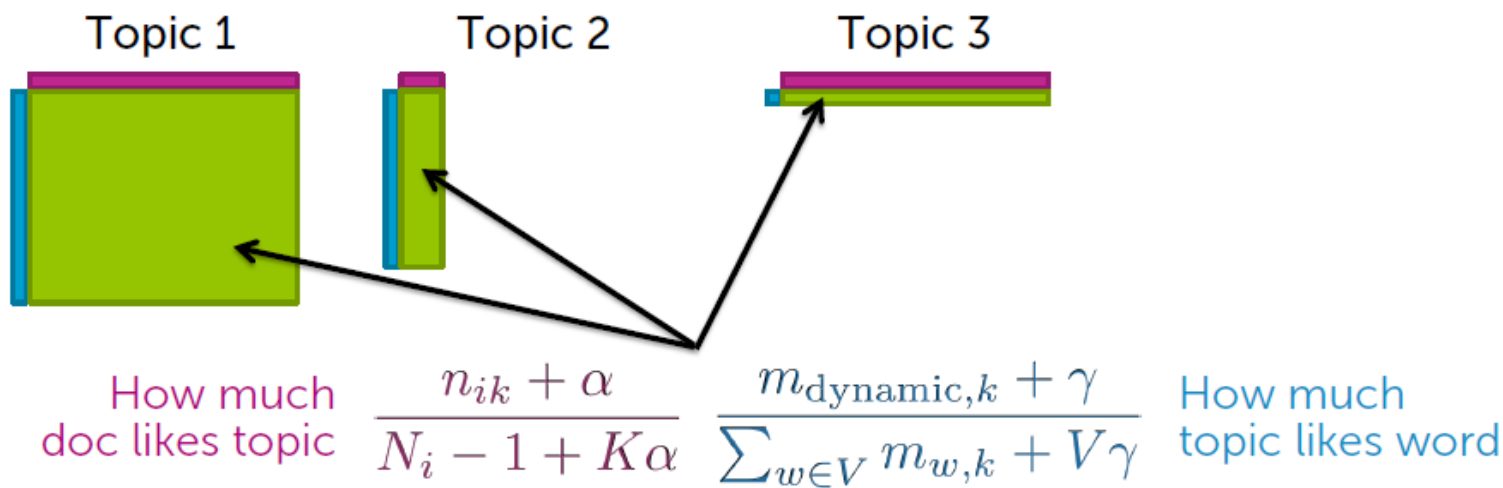
Topic 2 also really likes "dynamic",
but in a different context...
e.g., a topic on fluid dynamics

Collapsed Gibbs sampling for LDA

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Probability of new assignment

3	?	1	3	1
epilepsy	dynamic	Bayesian	EEG	model



Collapsed Gibbs sampling for LDA

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Randomly draw a new topic indicator

3	?	1	3	1
epilepsy	dynamic	Bayesian	EEG	model



How much doc likes topic



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!

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

How much topic likes word

Collapsed Gibbs sampling for LDA

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Update counts

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	11	7	1
...			

	Topic 1	Topic 2	Topic 3
Doc i	3	0	2

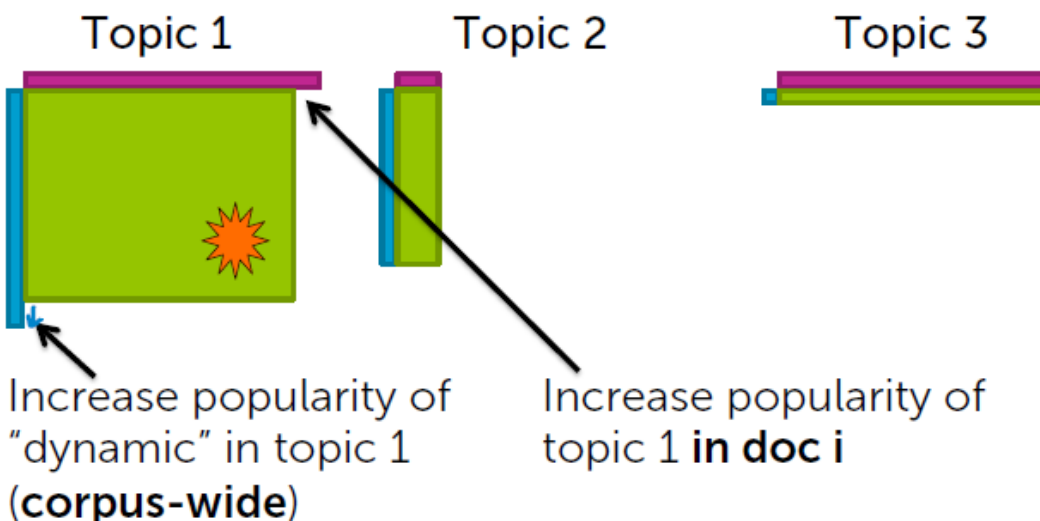
increment counts
based on new
assignment of
 $z_{iw}=1$

Collapsed Gibbs sampling for LDA

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Geometrically...

3	1	1	3	1
epilepsy	dynamic	Bayesian	EEG	model



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Collapsed Gibbs sampling for LDA

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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

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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

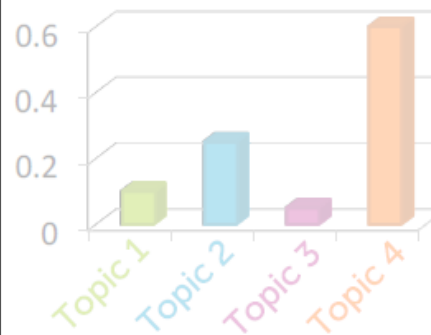
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From “best” sample of $\{z_{i,w}\}$, can infer:

1. Topics from conditional distribution...

need corpus-wide info

Collapsed Gibbs sampling for LDA

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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
...	...

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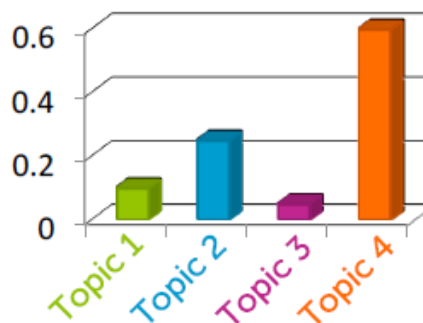
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1. Topics from conditional distribution...
need corpus-wide info
2. Document “embedding”...
need doc info only

Collapsed Gibbs sampling for LDA

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Embedding new documents

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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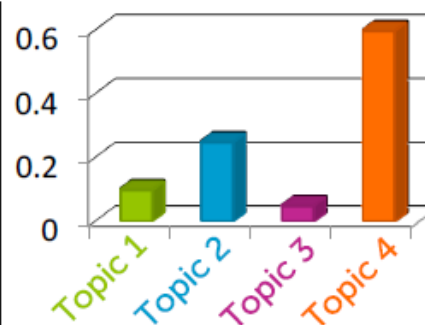
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Simple approach:

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

What you can do now

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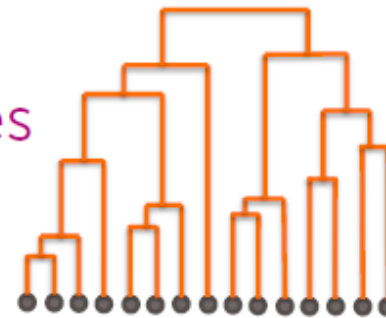
- Compare and contrast clustering and mixed membership models
- Describe a document clustering model for the bag-of-words doc representation
- Interpret the components of the LDA mixed membership model
- Analyze a learned LDA model
 - Topics in the corpus
 - Topics per document
- Describe Gibbs sampling 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

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- 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

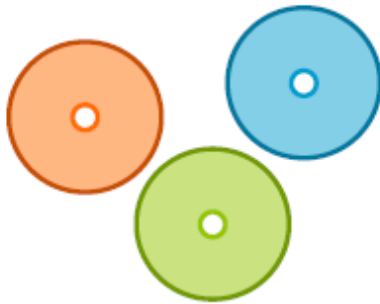


Why hierarchical clustering

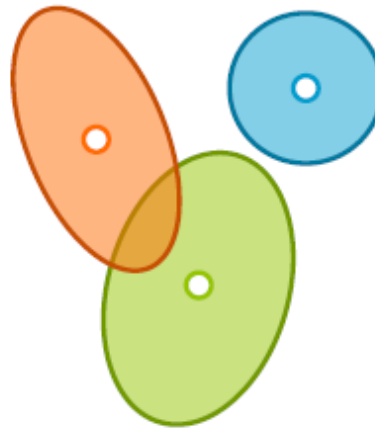
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Can often find more **complex shapes** than k-means or Gaussian mixture models

k-means: spherical clusters



Gaussian mixtures: ellipsoids

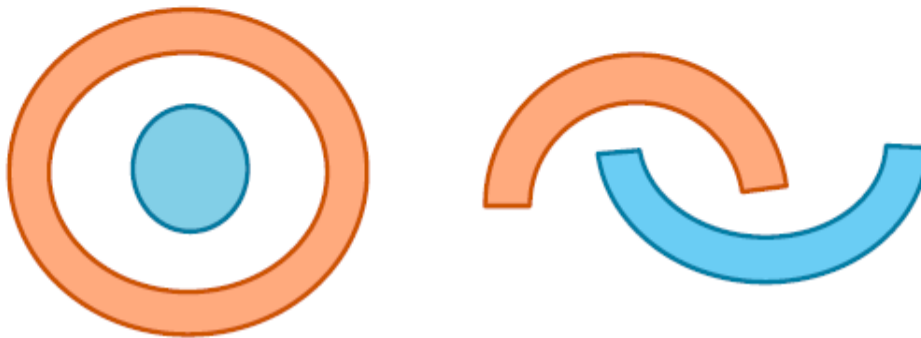


Why hierarchical clustering

280

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

What about these?



Two main types of algorithms

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

- Example: **recursive k-means**

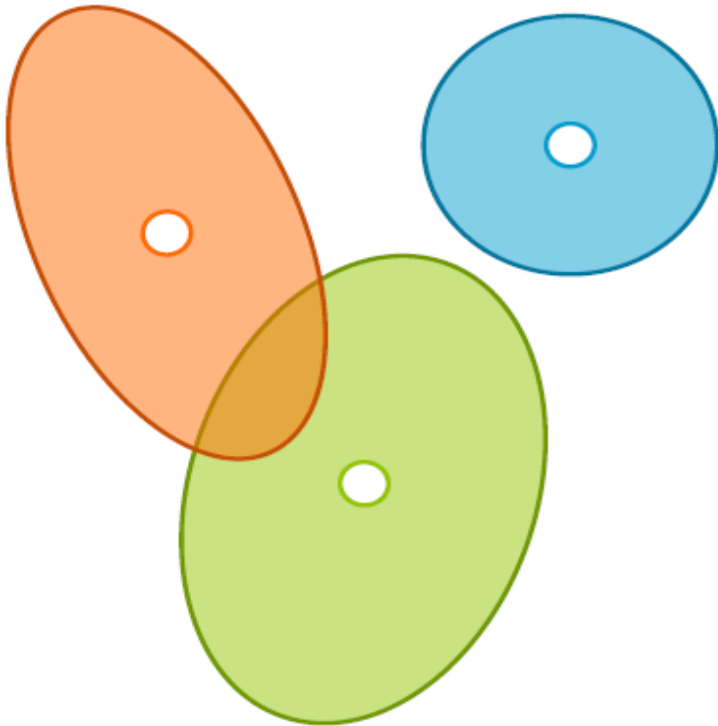
Agglomerative *a.k.a. bottom-up*: Start with each data point as its own cluster. Merge clusters until all points are in one big cluster.

- Example: **single linkage**

Divisive clustering

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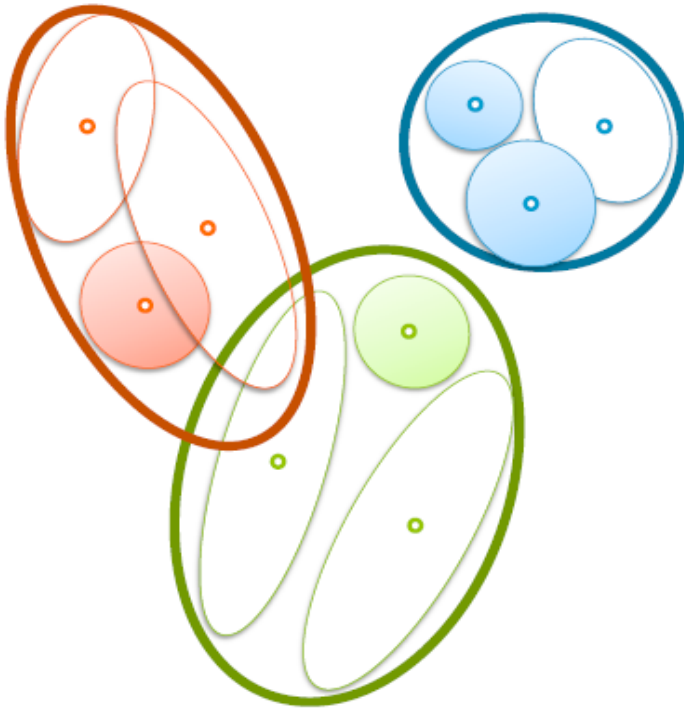
Divisive in pictures – level 1



Divisive clustering

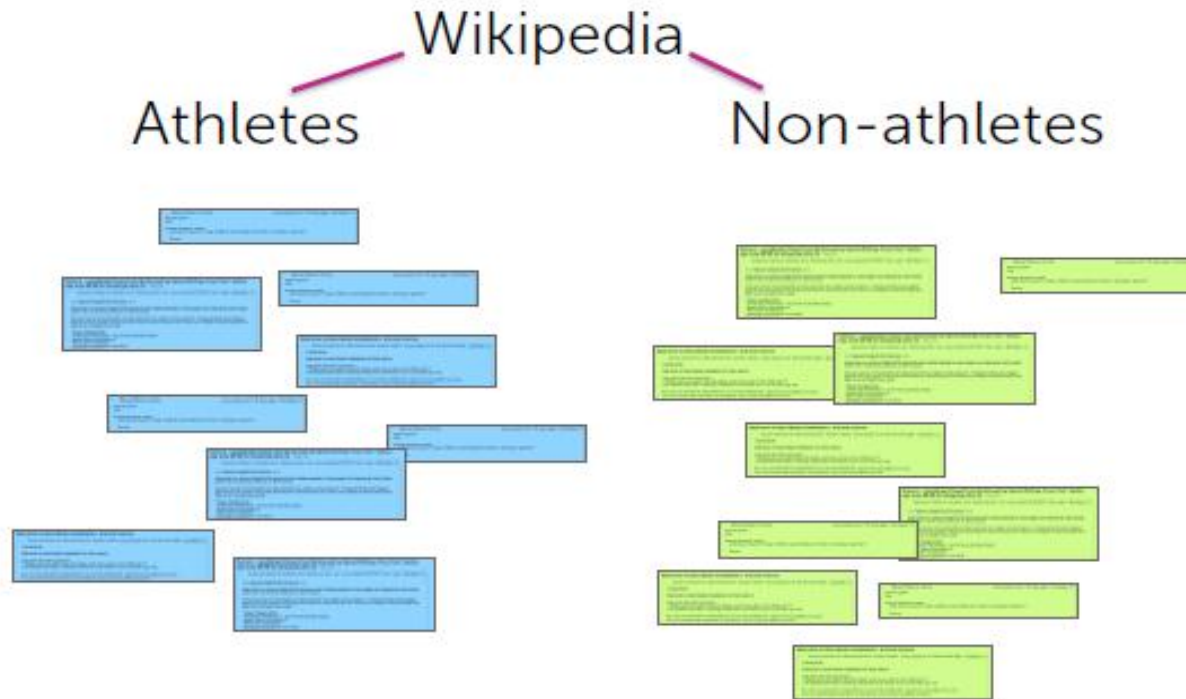
283

Divisive in pictures – level 2



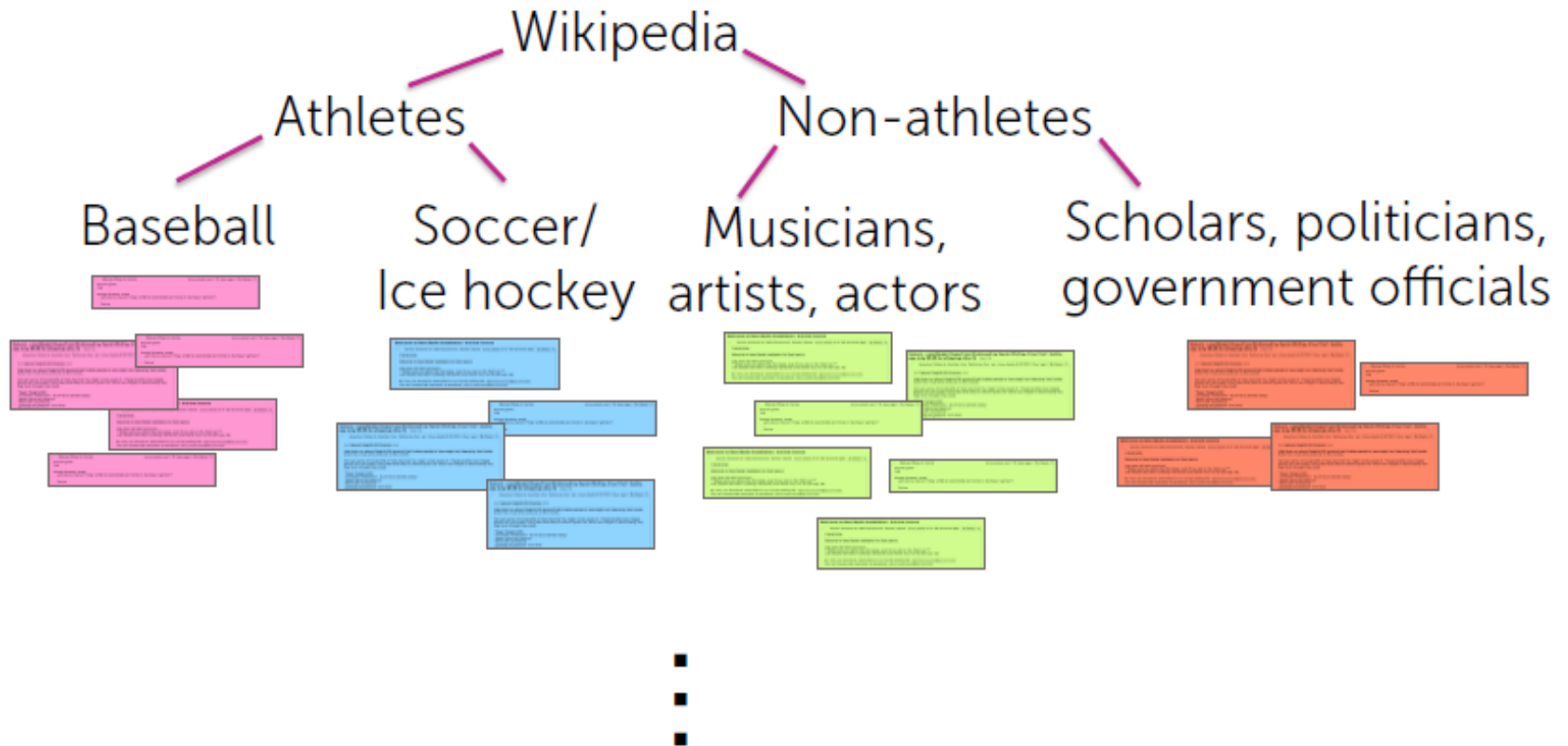
Divisive: Recursive k-means

284



Divisive: Recursive k-means

285



Divisive: choices to be made

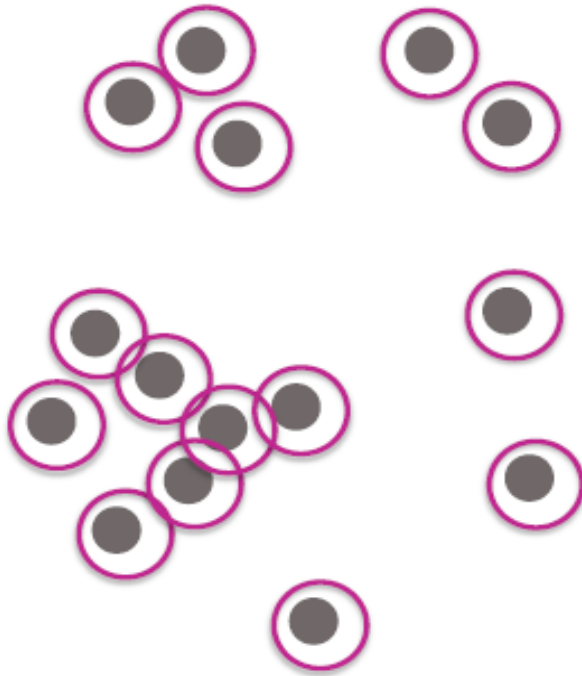
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- Which algorithm to recurse
- How many clusters per split
- When to split vs. stop
 - **Max cluster size:**
number of points in cluster falls below threshold
 - **Max cluster radius:**
distance to furthest point falls below threshold
 - **Specified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

Aglomerative: Single linkage

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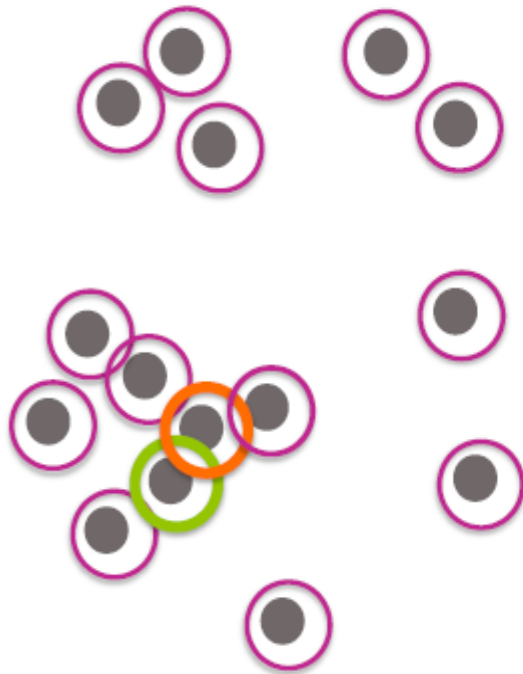
1. Initialize each point to be its own cluster



Aglomerative: Single linkage

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2. Define distance between clusters to be:



$$\text{distance}(C_1, C_2) =$$

$$\min_{\substack{x_i \in C_1, \\ x_j \in C_2}} d(x_i, x_j)$$

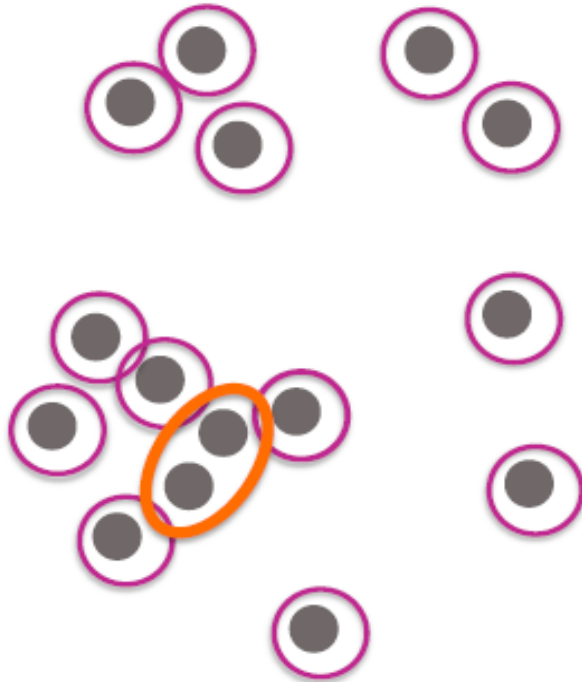
specified pairwise
distance function

Linkage criteria

Aglomerative: Single linkage

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3. Merge the two closest clusters



Aglomerative: Single linkage

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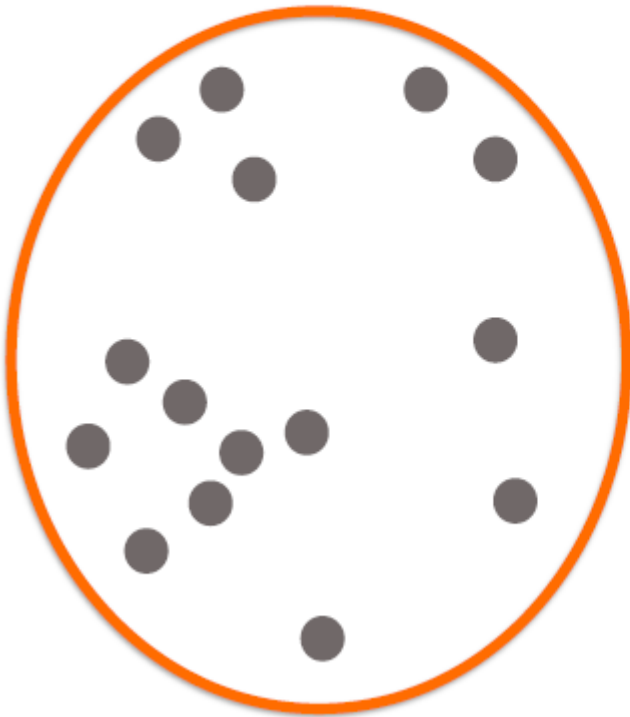
4. Repeat step 3 until all points are in one cluster



Aglomerative: Single linkage

291

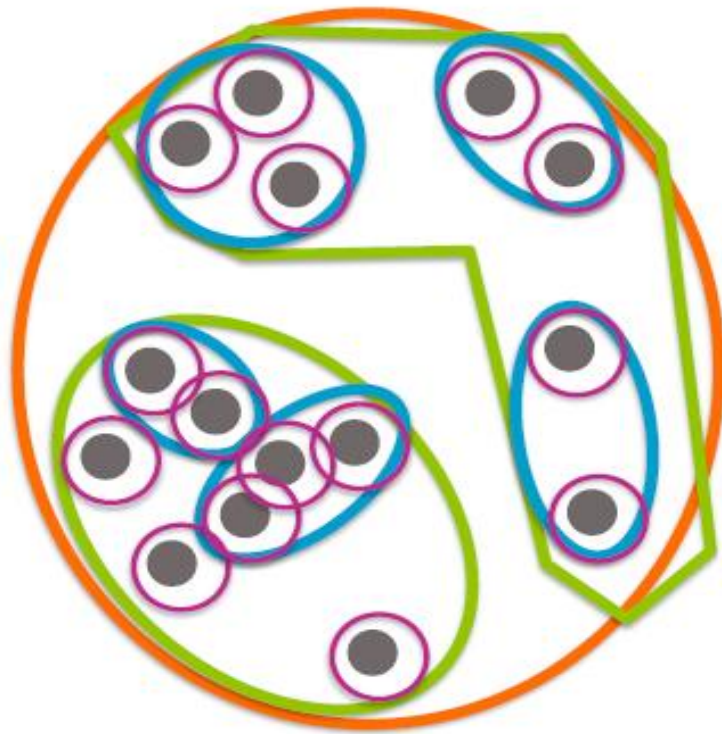
4. Repeat step 3 until all points are in one cluster



Cluster of clusters

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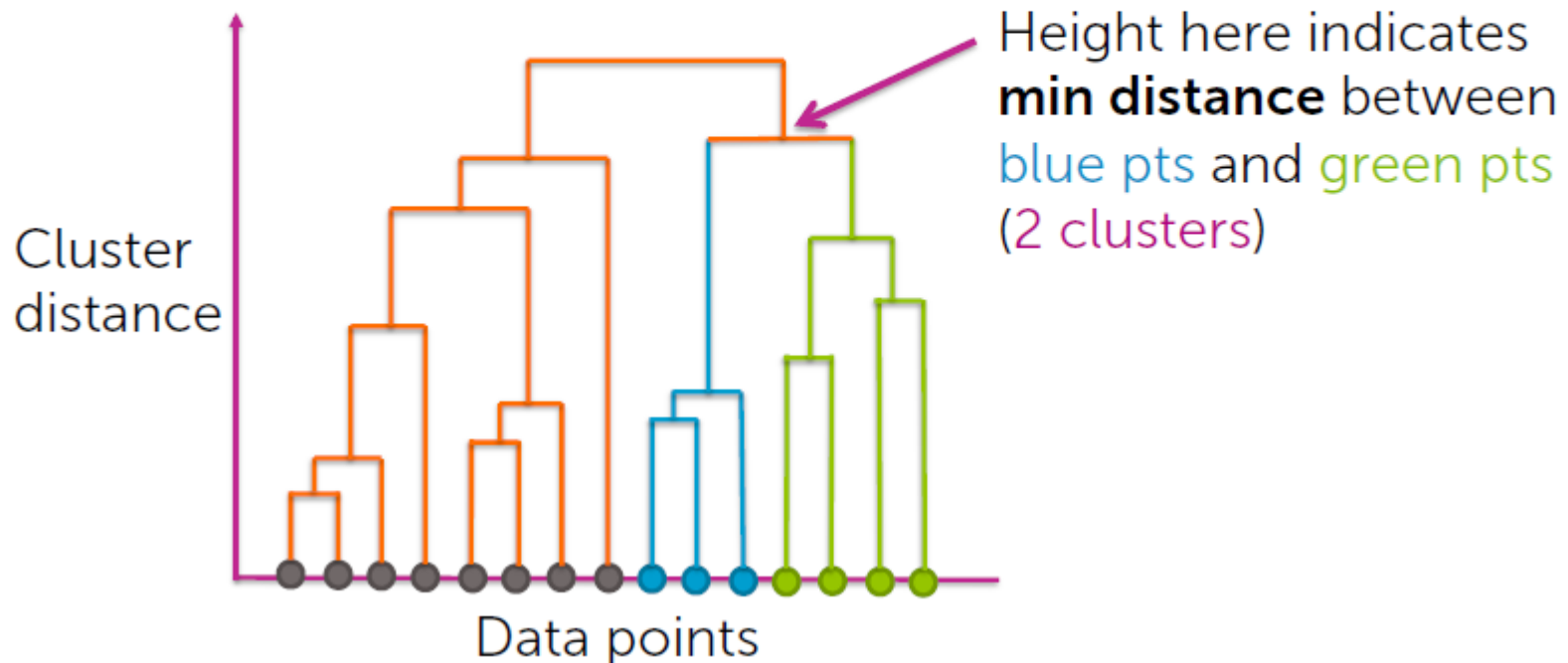
Just like our picture for divisive clustering...



The dendrogram

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

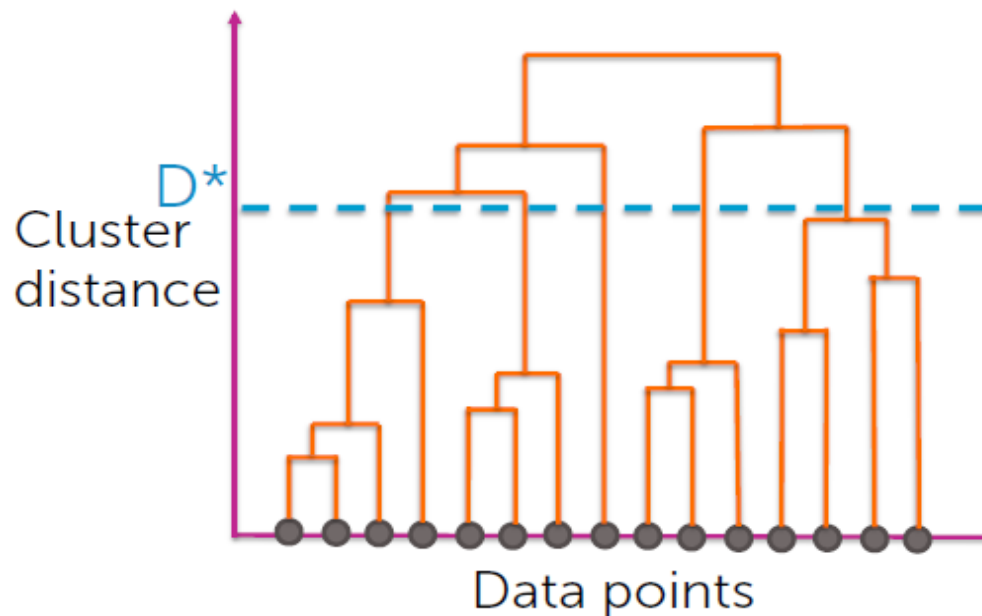


Extracting a partition

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Choose a distance D^* at which to cut dendrogram

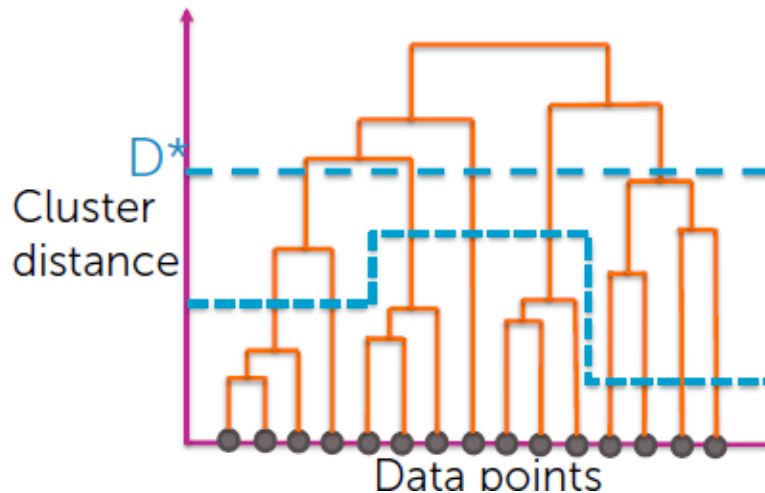
Every branch that crosses D^* becomes a separate cluster



Agglomerative: choices to be made

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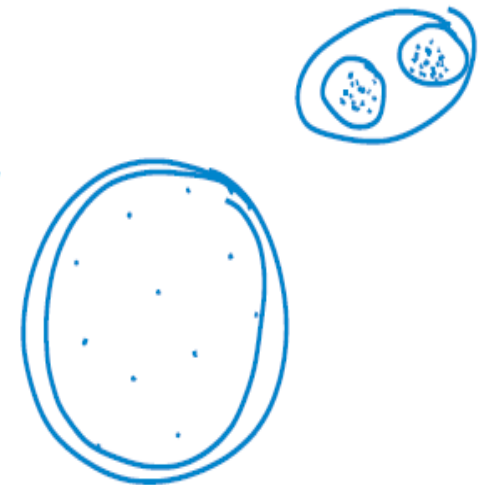
- Distance metric: $d(\mathbf{x}_i, \mathbf{x}_j)$
- Linkage function: e.g., $\min_{\substack{\mathbf{x}_i \in C_1, \\ \mathbf{x}_j \in C_2}} d(\mathbf{x}_i, \mathbf{x}_j)$
- Where and how to cut dendrogram



More on cutting dendrogram


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- 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

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- 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 $O(N^2)$