Recap & Look ahead

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What we've learned

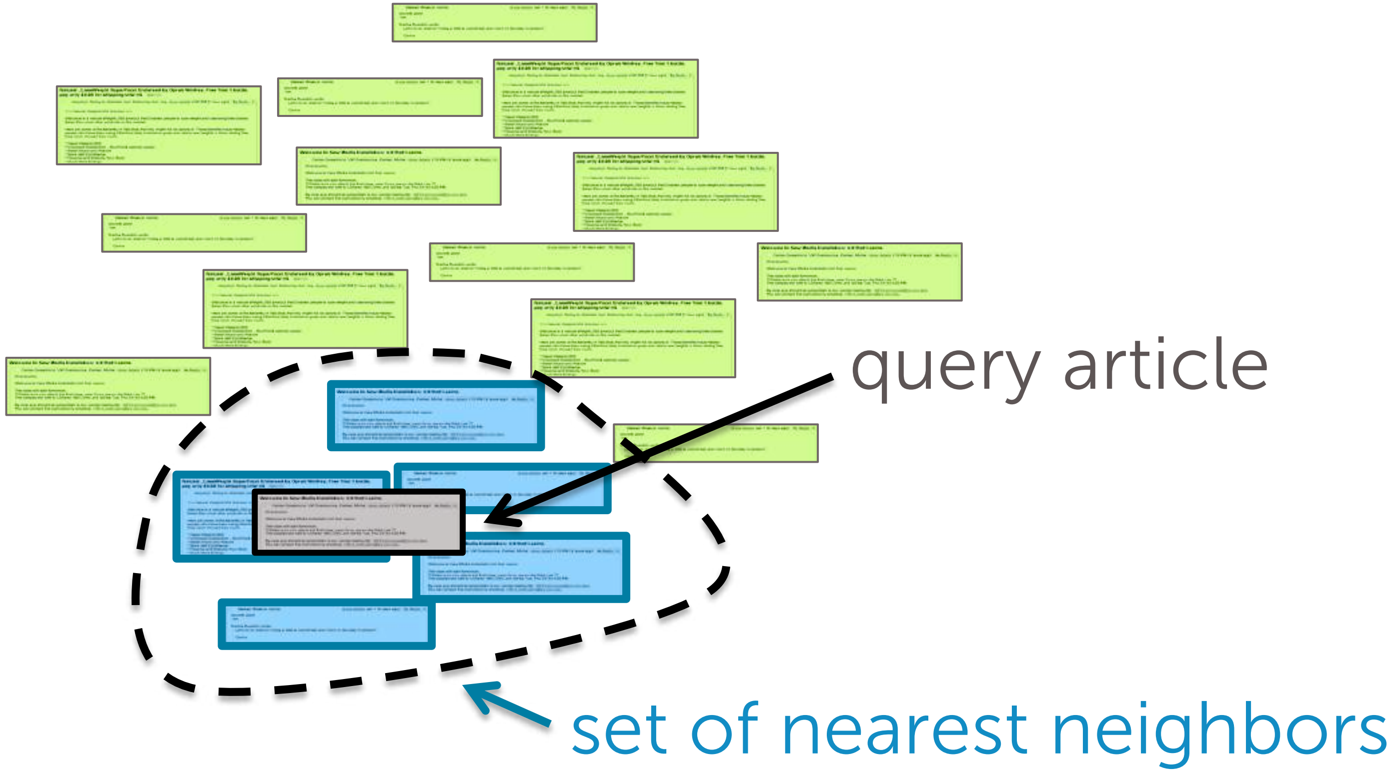
Module 1: Nearest neighbor search

1-NN search

Space of all articles,
organized by similarity of text

k-NN search

Space of all articles,
organized by similarity of text



TF-IDF document representation

Emphasizes important words

- Appears frequently in document (common locally)

  Term frequency = word counts

- Appears rarely in corpus (rare globally)

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

tf * idf

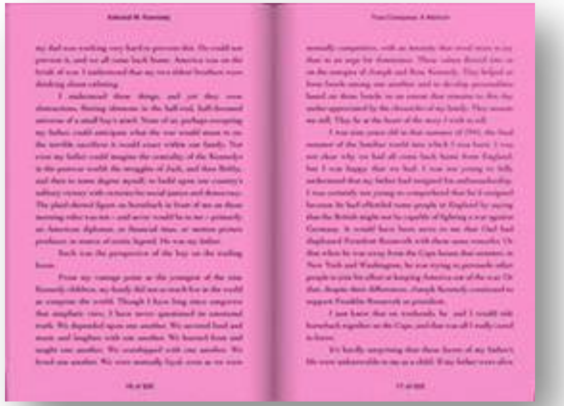
Trade off: local frequency vs. global rarity

Scaled Euclidean distance

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

weight on each feature

title
abstract
main body
conclusion

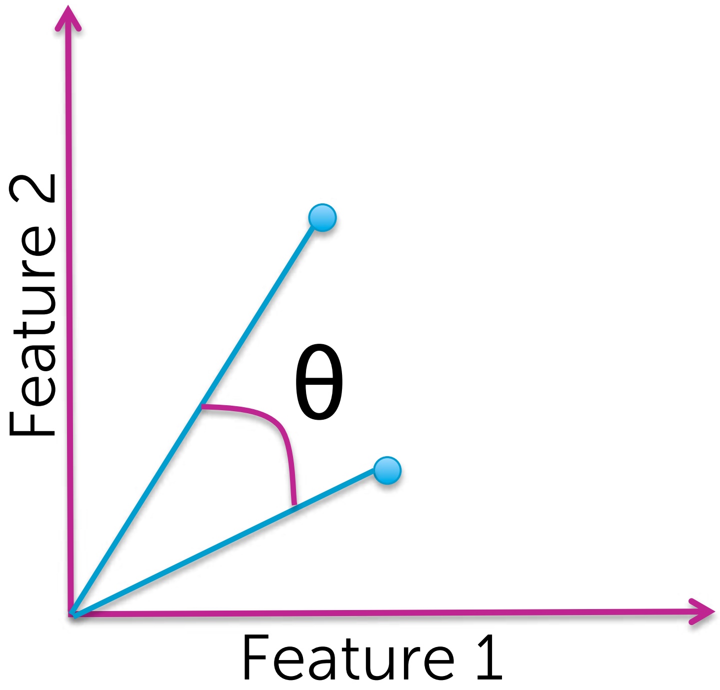


Cosine similarity – normalize

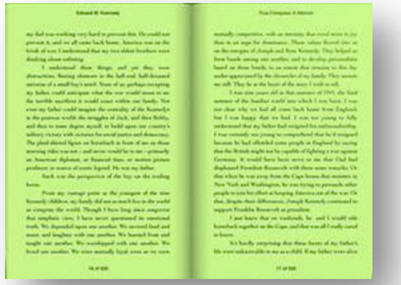
Similarity =
$$\frac{\sum_{j=1}^{d} \mathbf{x}_i[j]\, \mathbf{x}_q[j]}{\sqrt{\sum_{j=1}^{d} (\mathbf{x}_i[j])^2}\sqrt{\sum_{j=1}^{d} (\mathbf{x}_q[j])^2}}$$

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

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



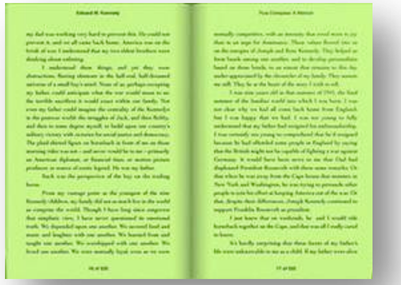
To normalize or not?



long document

short tweet

Normalizing can make dissimilar objects appear more similar



long document

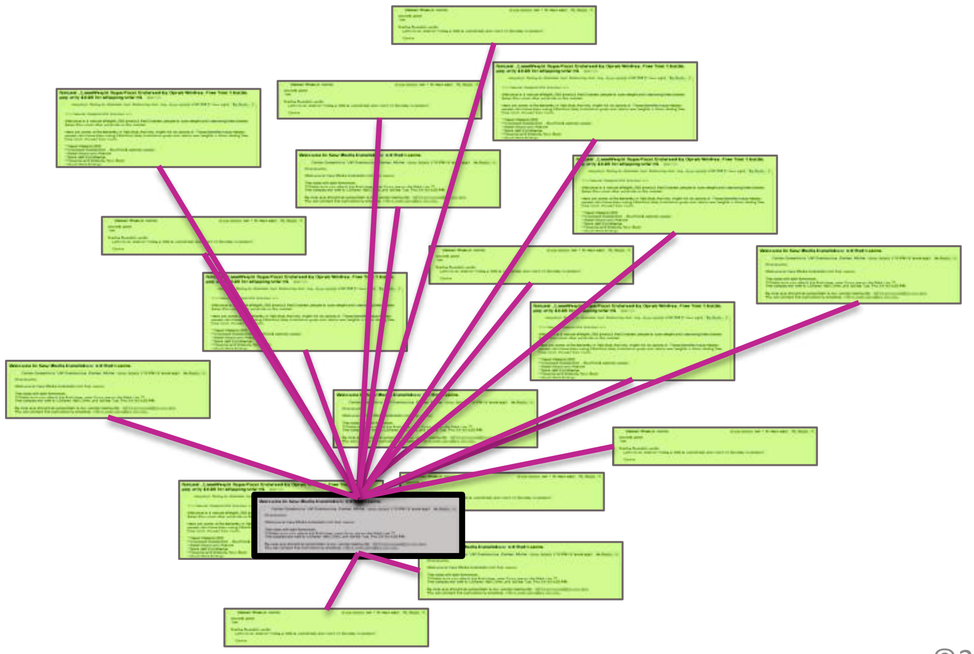
long document

Common compromise:
Just cap maximum word counts

Complexity of brute-force search

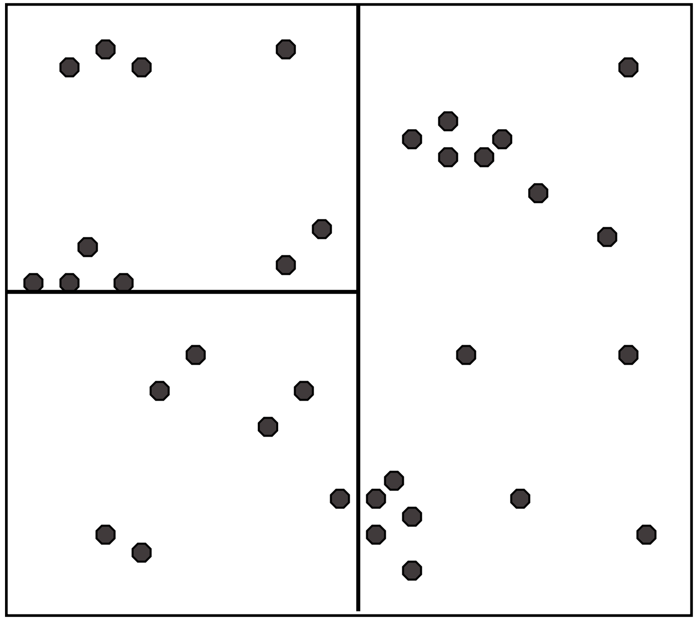
Given a query point, scan through each point

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

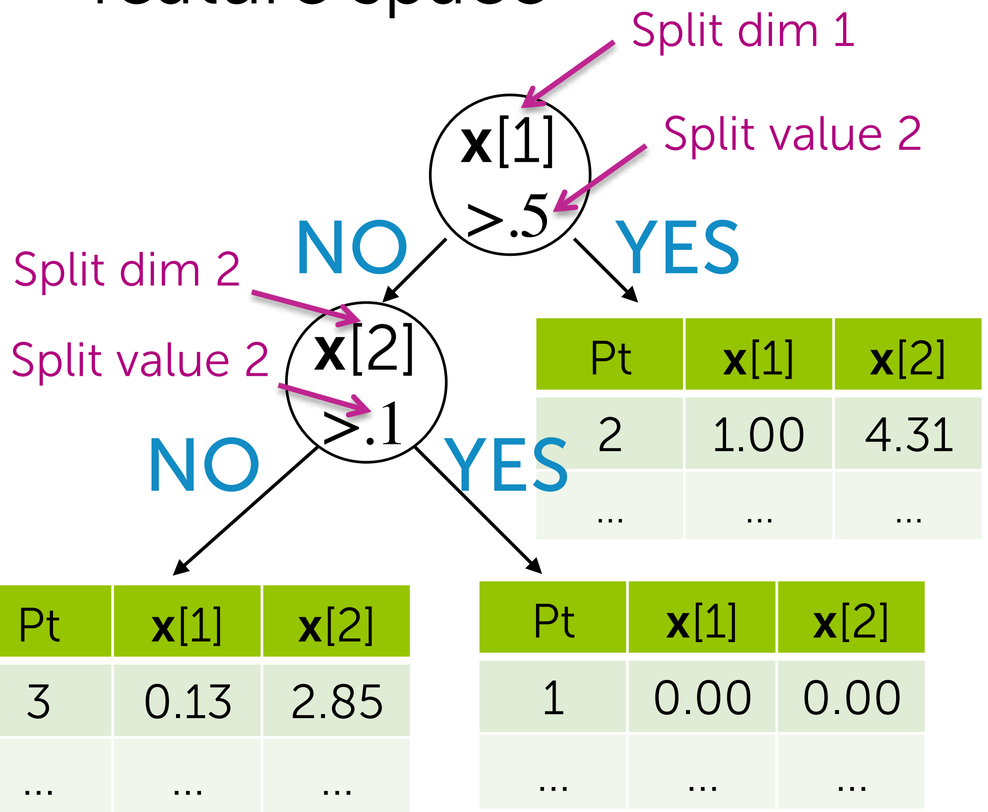


What if N is huge???
(and many queries)

KD-trees



Recursively partition the feature space

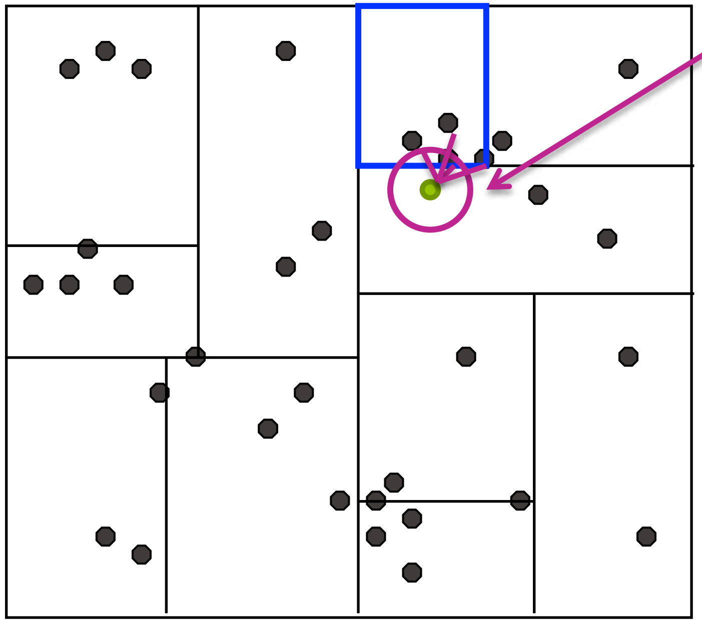


Pt	**x**[1]	**x**[2]
2	1.00	4.31
…	…	…

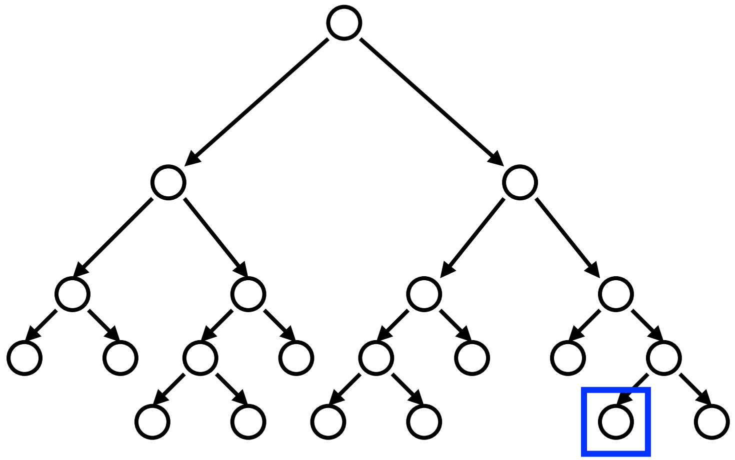
Pt	**x**[1]	**x**[2]
3	0.13	2.85
…	…	…

Pt	**x**[1]	**x**[2]
1	0.00	0.00
…	…	…

Nearest neighbor with KD-trees

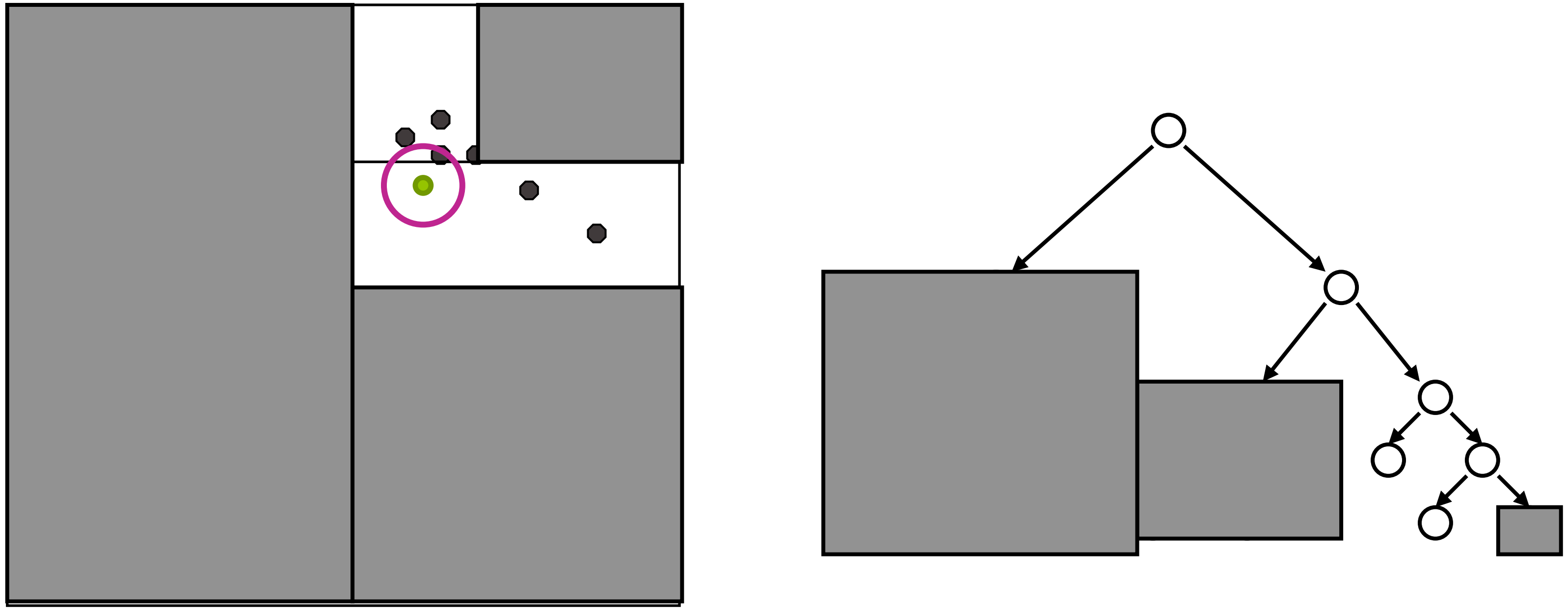


Update distance bound when new nearest neighbor is found



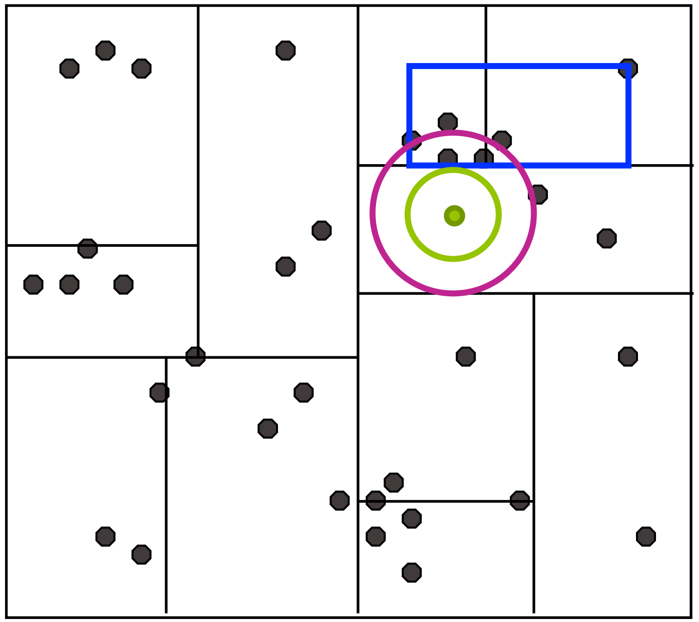
1. Start by exploring leaf node containing query point
2. Compute distance to each other point at leaf node
3. Backtrack and try other branch at each node visited

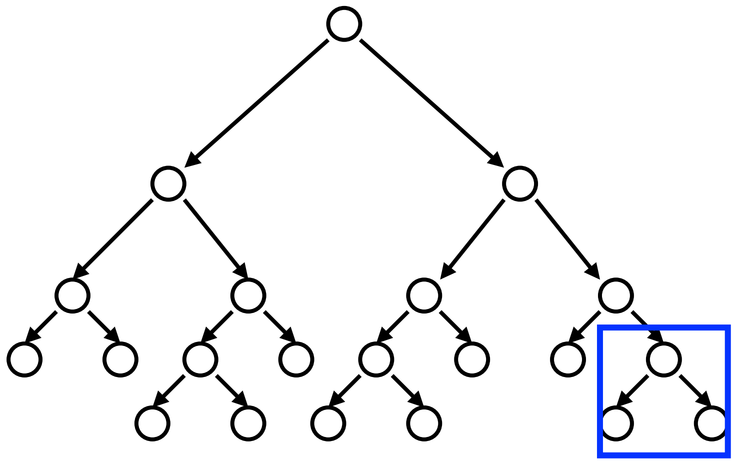
Nearest neighbor with KD-trees



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

Approximate k-NN with KD-trees





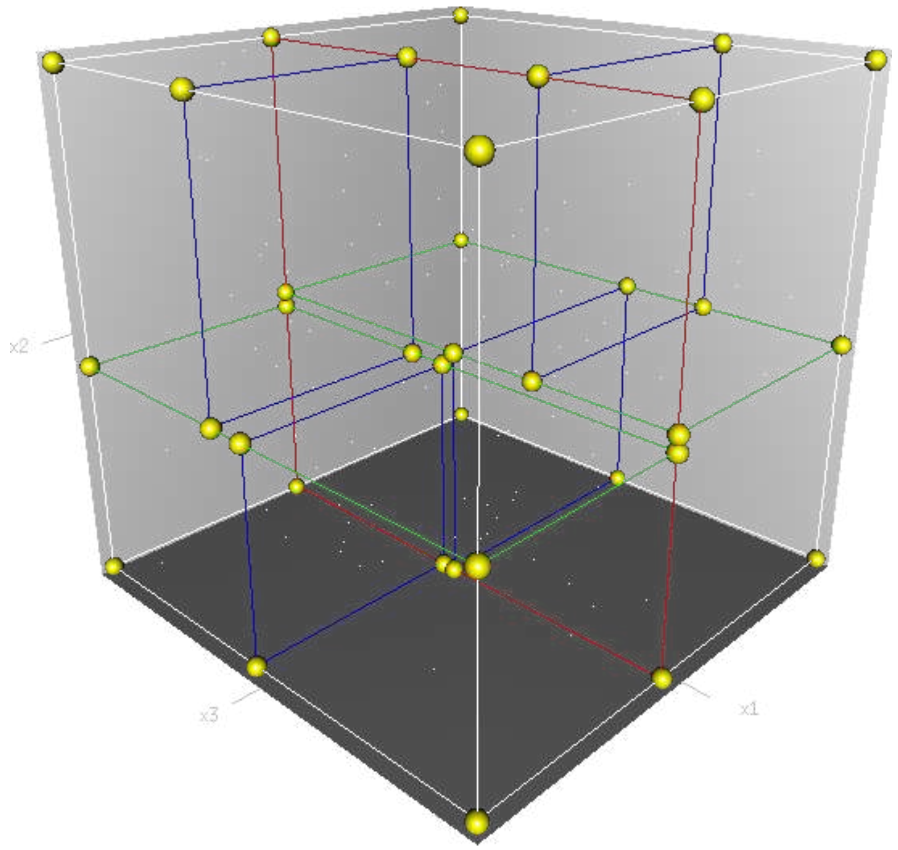
Before: Prune when distance to bounding box > r

Now: Prune when distance to bounding box > r/α

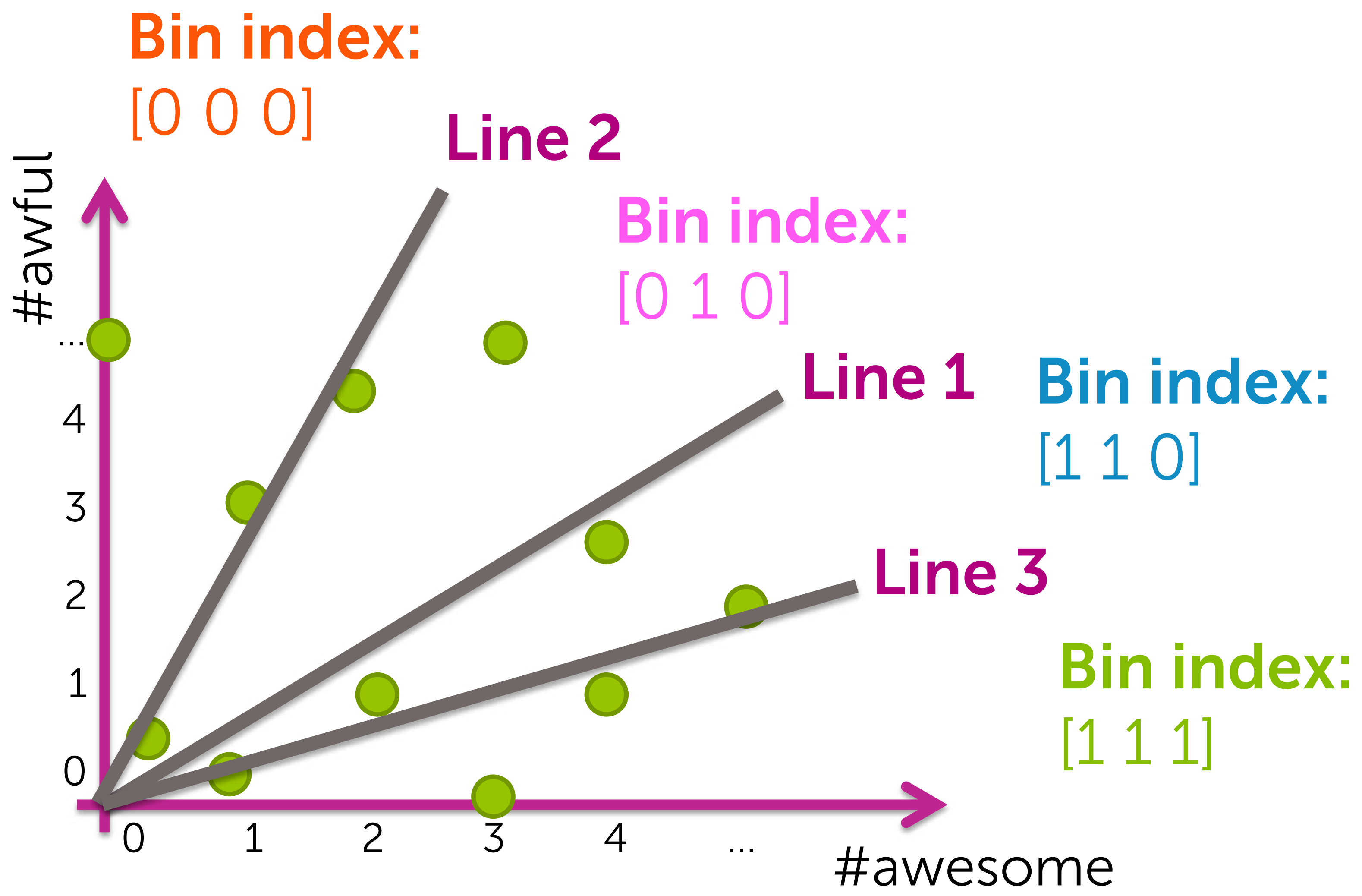
Saves lots of search time at little cost in quality of NN!

Limitations of KD-trees

- Difficult to implement
- Don't tend to perform well in high dimensions
  - Under some conditions, visit at least 2^d nodes



Locality sensitive hashing

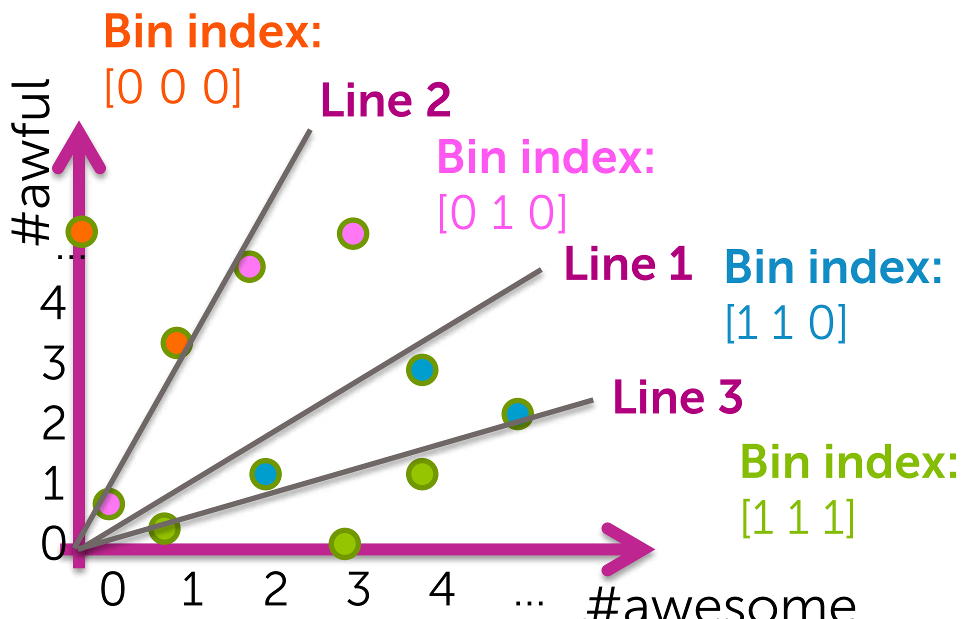


LSH for approximate NN search

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?

Next closest bins (flip 1 bit)



Module 2: k-means and MapReduce

Module 2: k-means and MapReduce

Discover *clusters* of related documents

Cluster 1

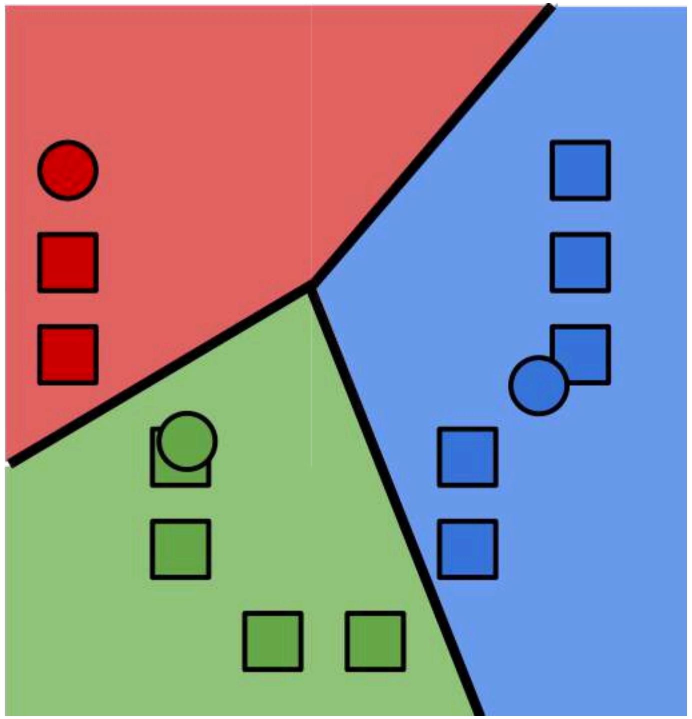
Cluster 2

Cluster 3

Cluster 4

k-means algorithm

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



A coordinate descent algorithm

1. Assign observations to closest cluster center

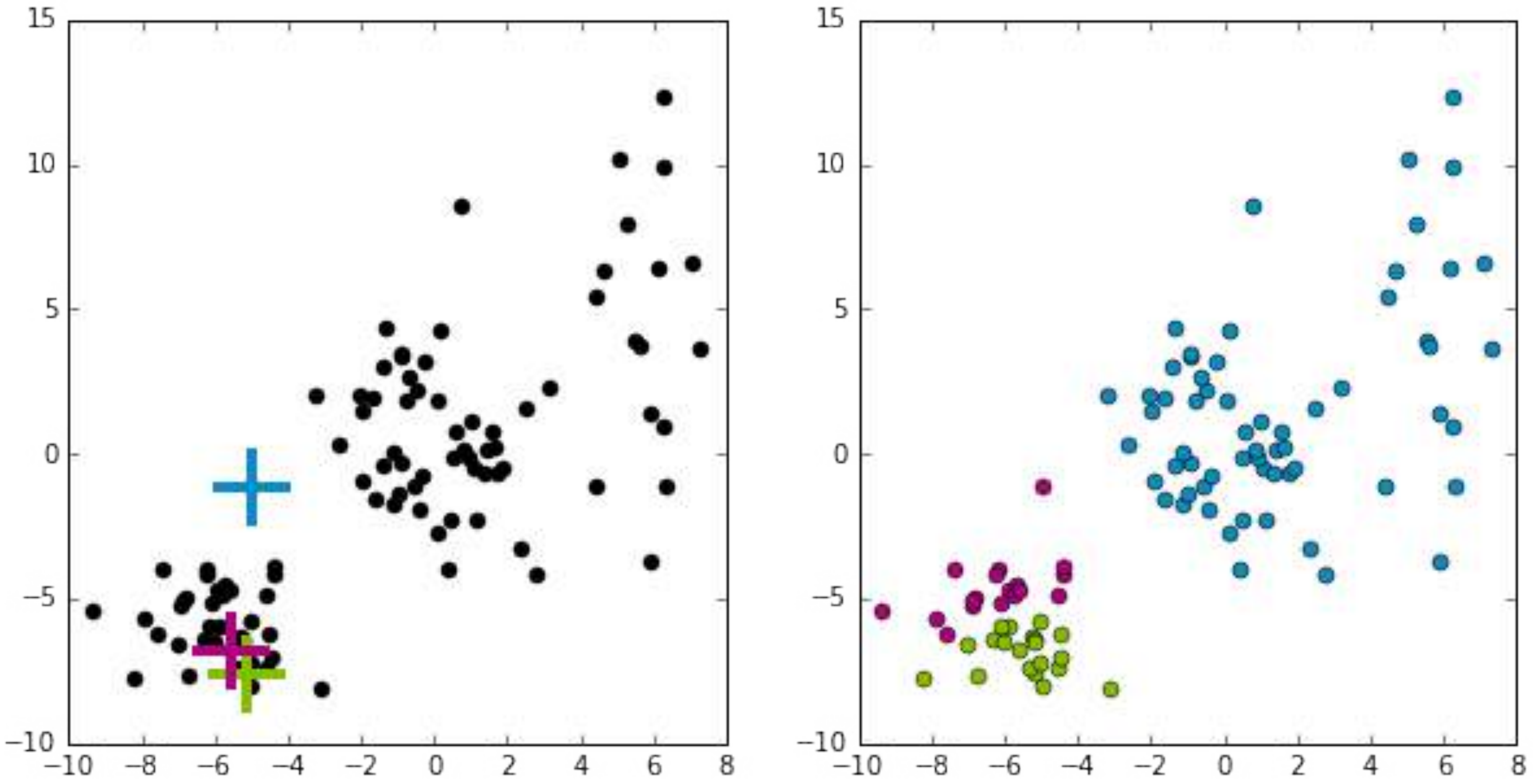
$$z_i \leftarrow \arg\min_j ||\mu_j - \mathbf{x}_i||_2^2$$

2. Revise cluster centers as mean of assigned observations

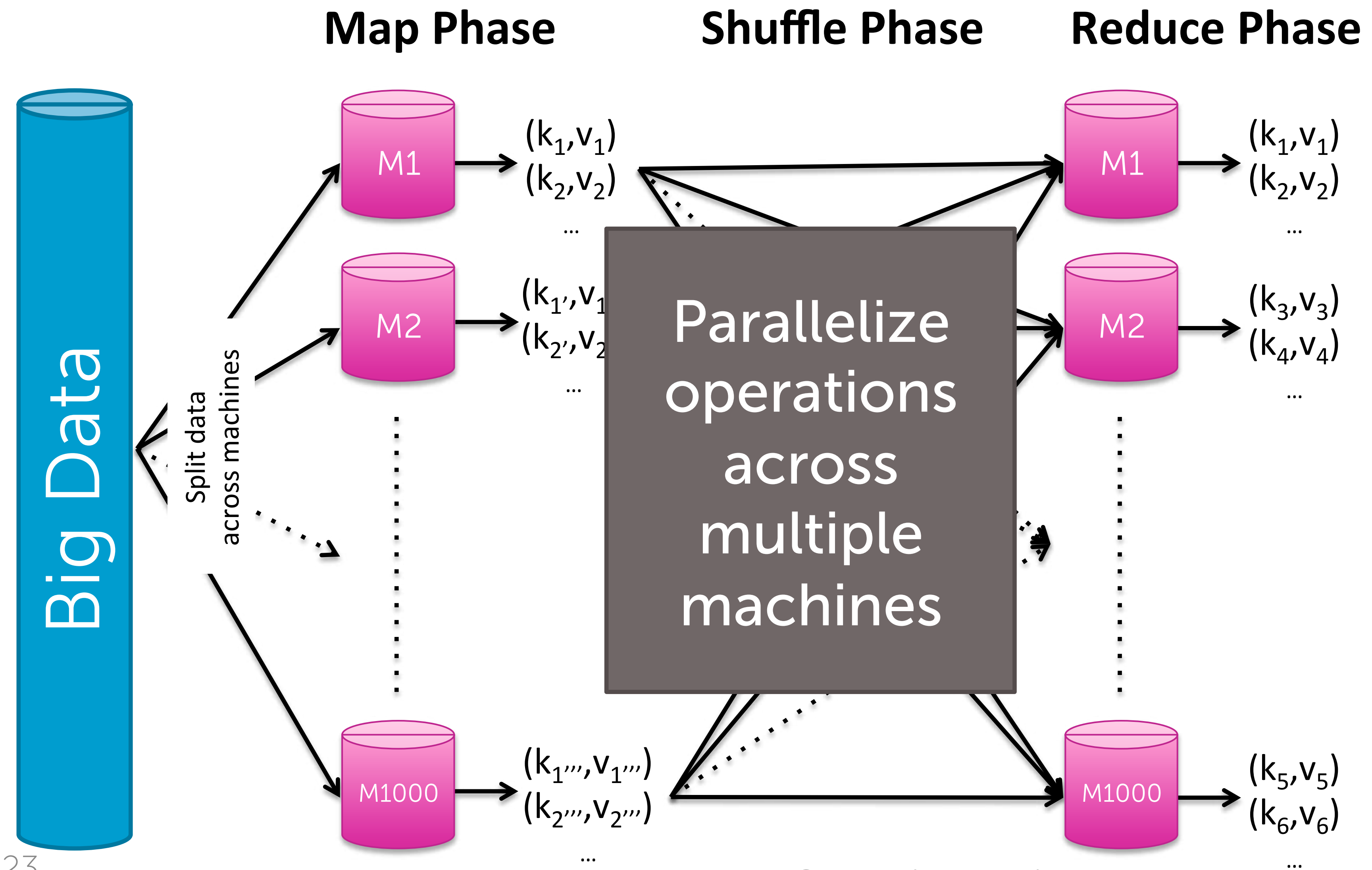
$$\mu_j \leftarrow \arg\min_\mu \sum_{i:z_i=j} ||\mu - \mathbf{x}_i||_2^2$$

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

Convergence of k-means to local mode



MapReduce framework



MapReduce abstraction

Map:

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

Word count example:

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

Reduce:

- Aggregate values for each key
- Must be commutative-associative operation
- Data-parallel over keys
- Generate (key,value) pairs

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

MapReduce has long history in functional programming

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

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)

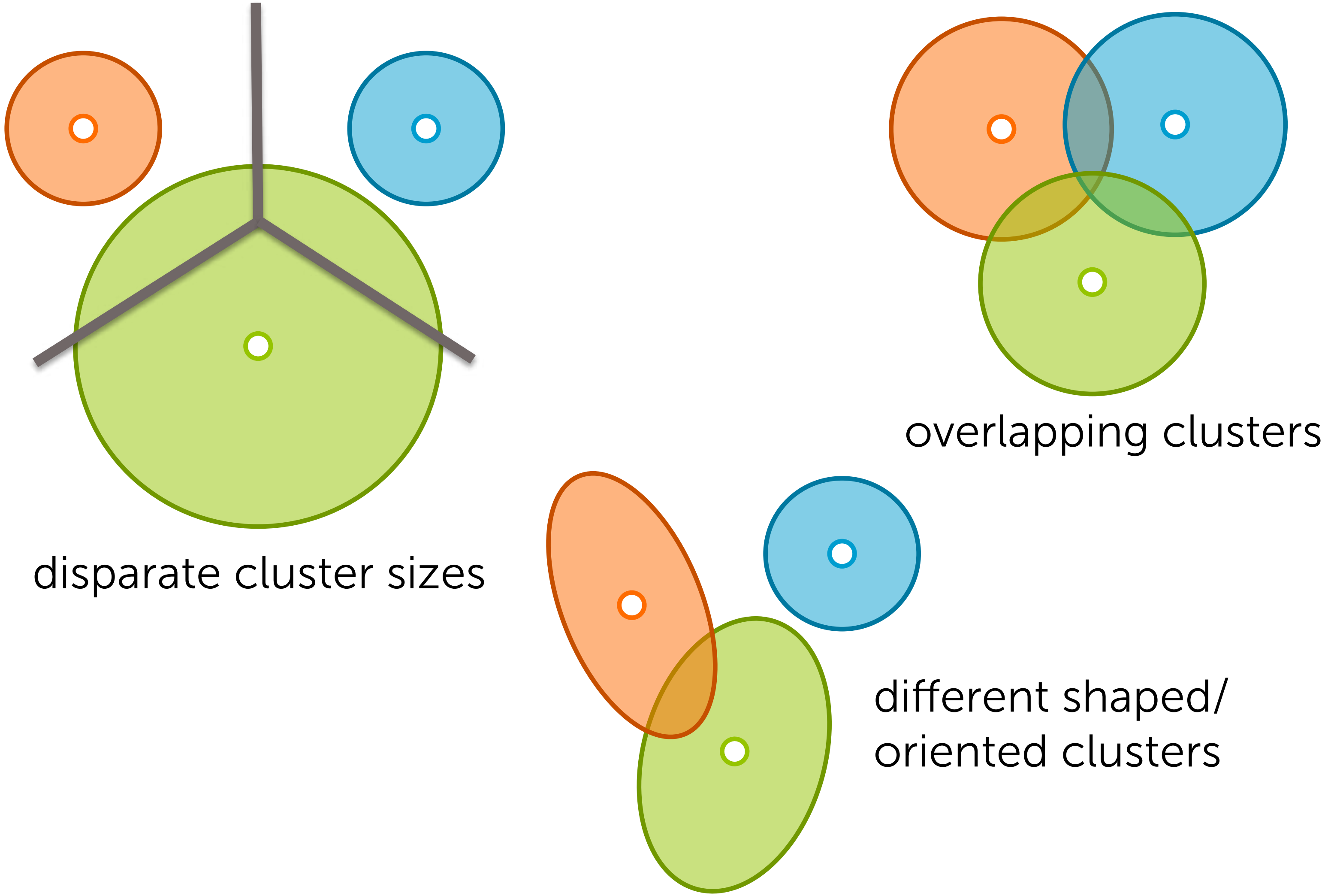
Module 3: Mixture models

Mixture models

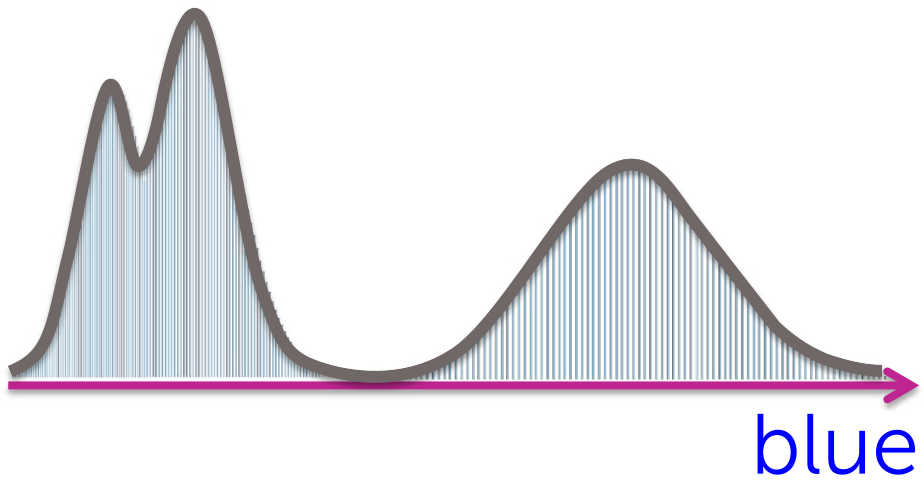
Probabilistic clustering model

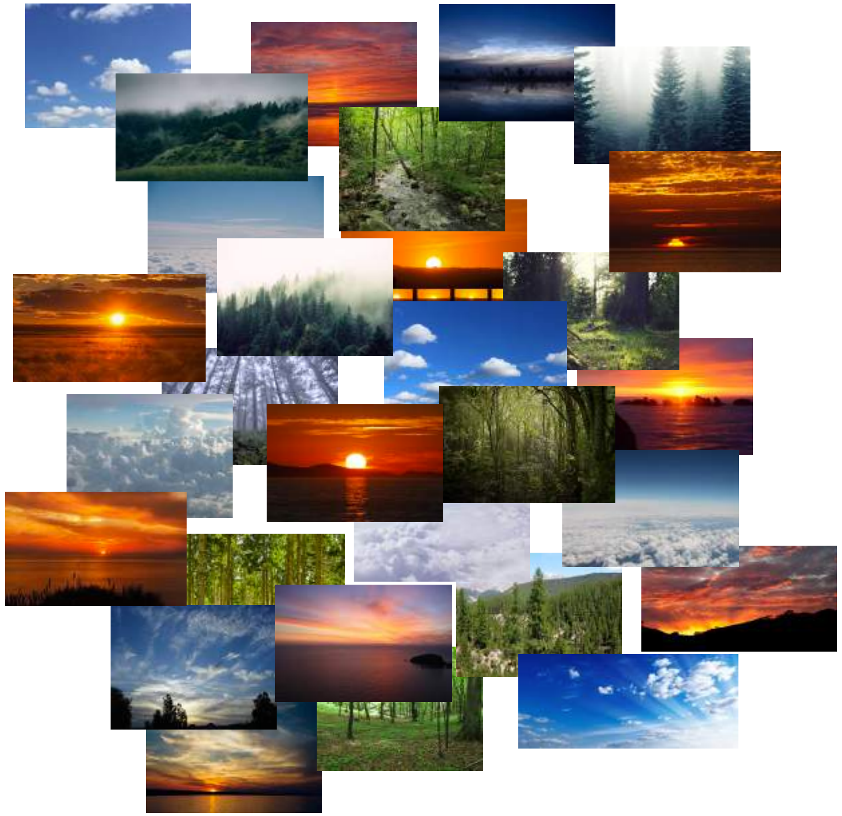
captures **uncertainty** in clustering

Failure modes of k-means

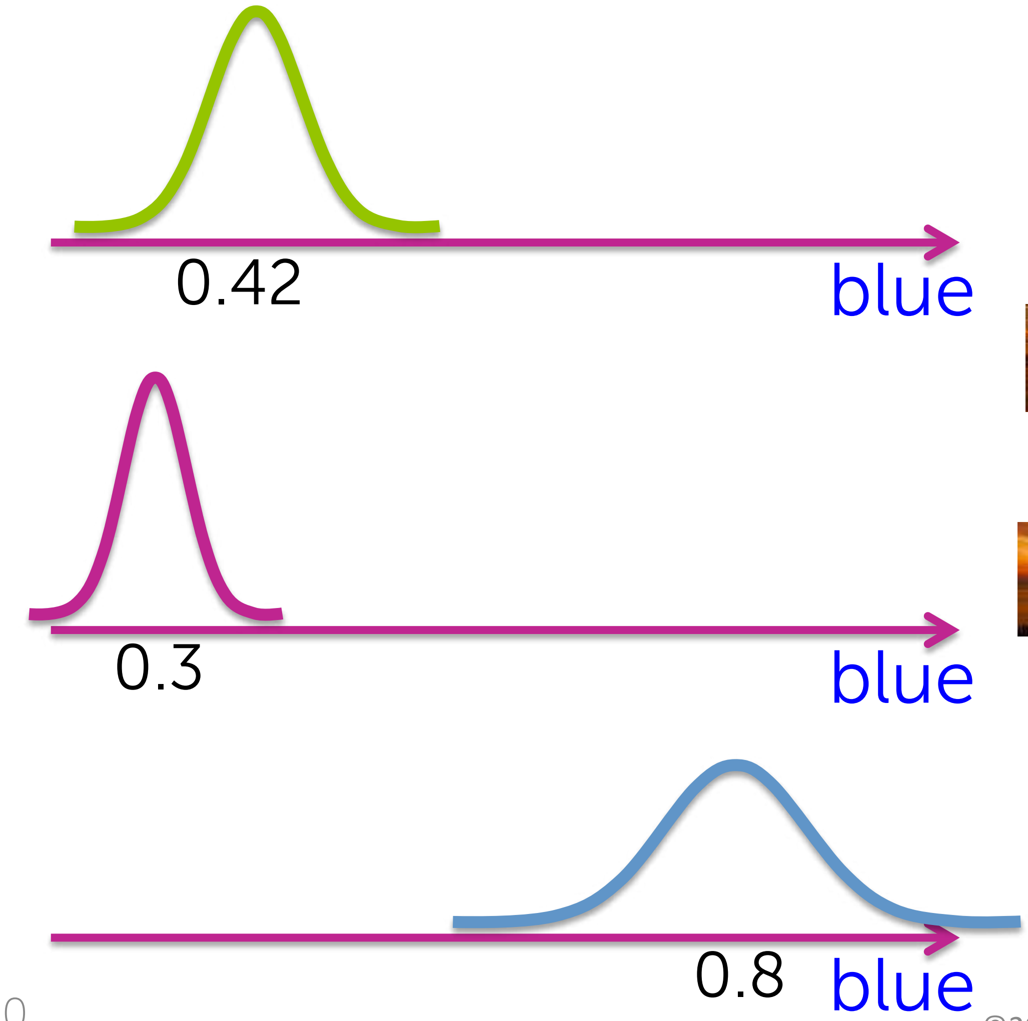


Jumble of unlabeled images





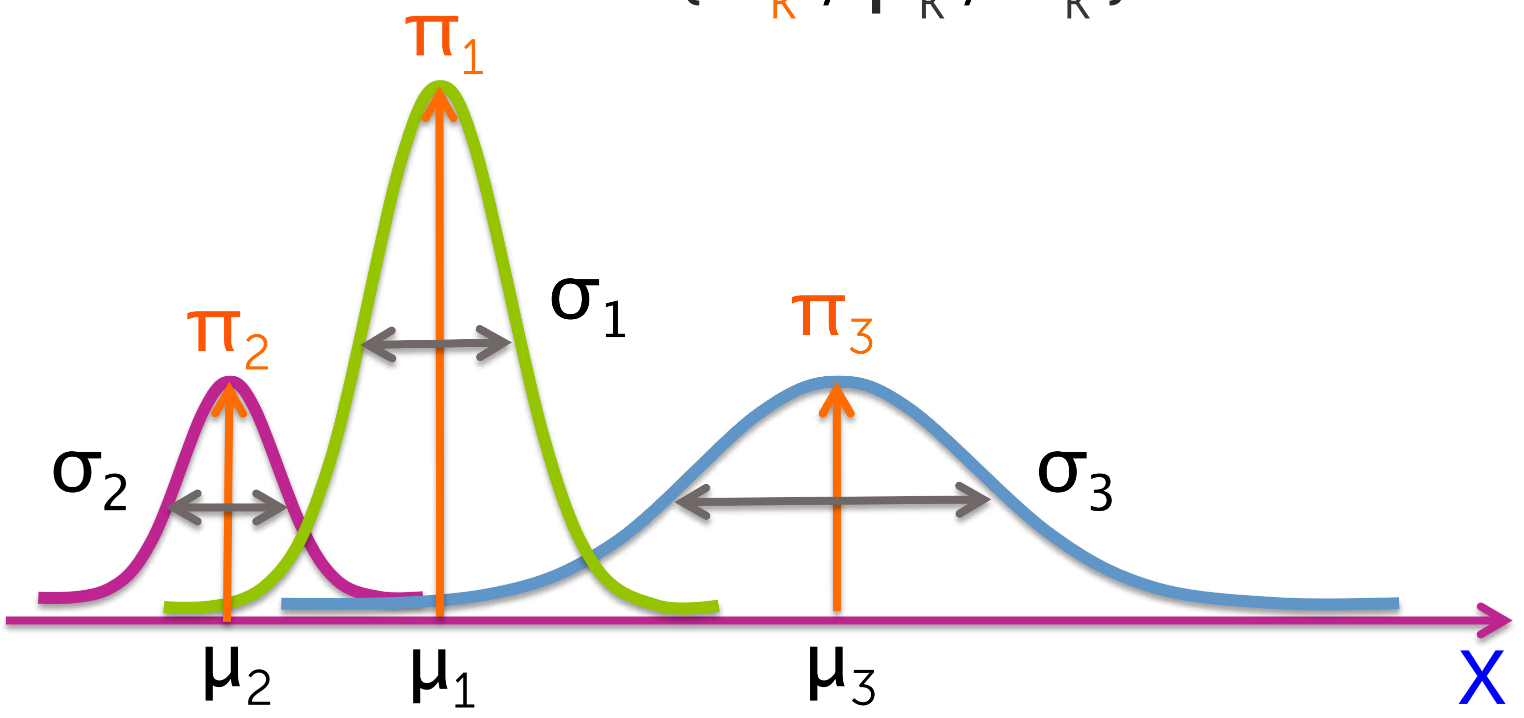
Model of jumble of unlabeled images



Mixture of Gaussians (1D)

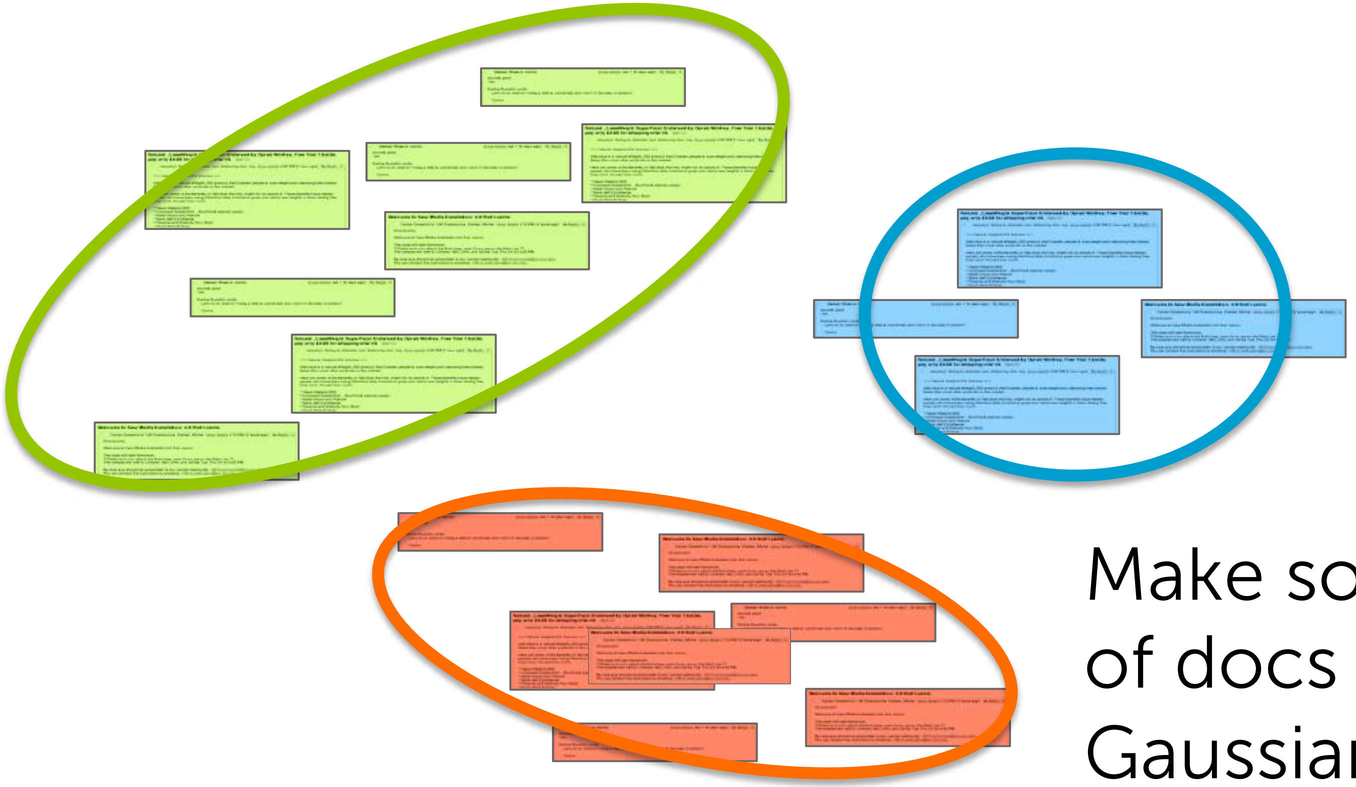
Each mixture component represents a unique cluster specified by:

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



Mixture of Gaussians for clustering documents

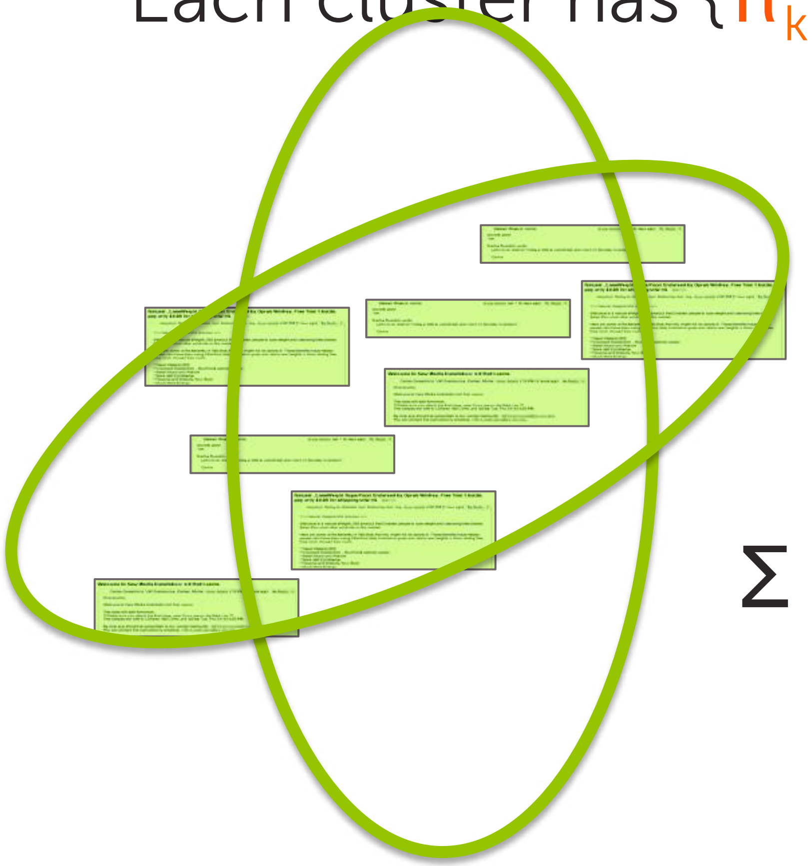
Space of all documents
(really lives in $\mathbf{R}^V$ for vocab size V)



Make soft assignments of docs to each Gaussian

Restricting to diagonal covariance

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



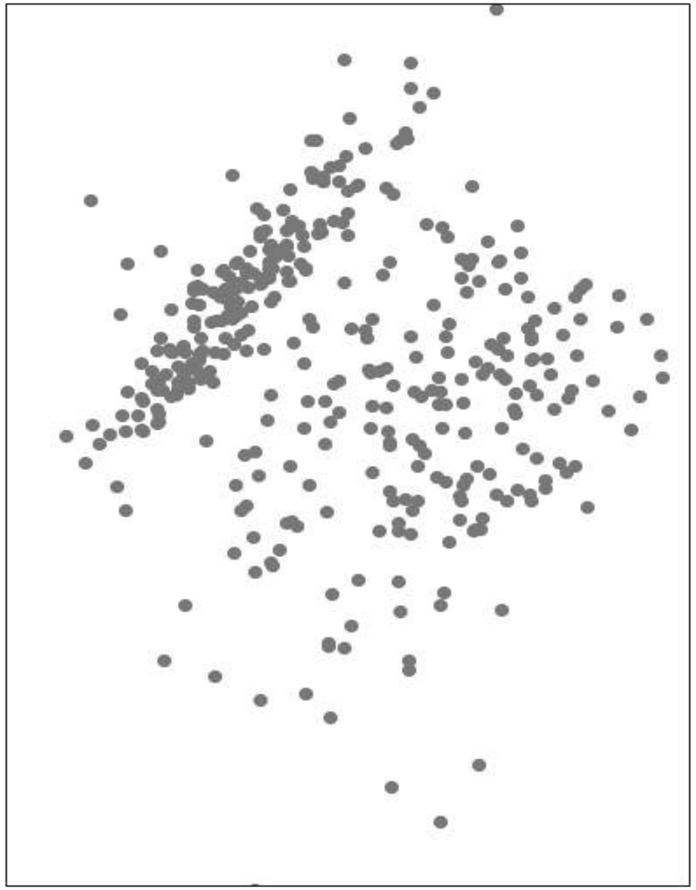
V params

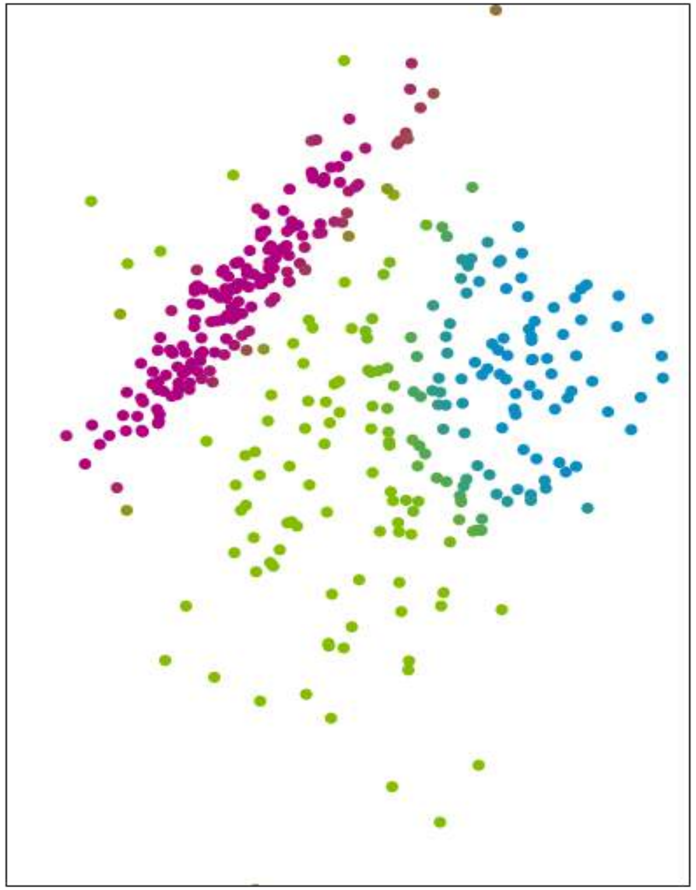
$$\Sigma = \begin{pmatrix} \sigma_1^2 & & & & 0 \\ & \sigma_2^2 & & & \\ & & \sigma_3^2 & & \\ & 0 & & \ddots & \\ & & & & \sigma_V^2 \end{pmatrix}$$

Inferring cluster labels

EM algorithm →
soft assignments

Data





Expectation maximization (EM):
An iterative algorithm

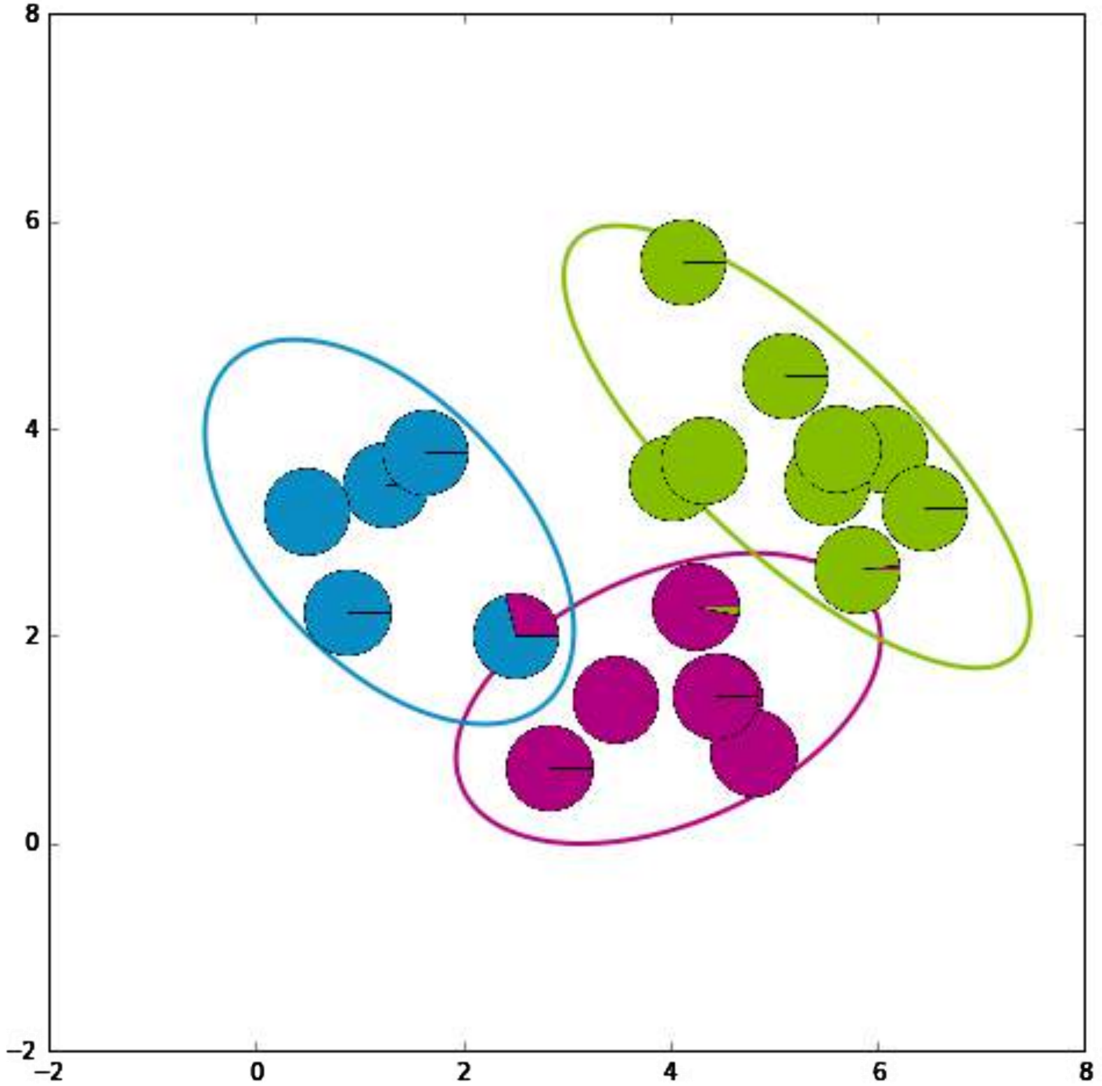
1. **E-step:** estimate cluster responsibilities given current parameter estimates

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

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

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

EM for mixtures of Gaussians in pictures - replay

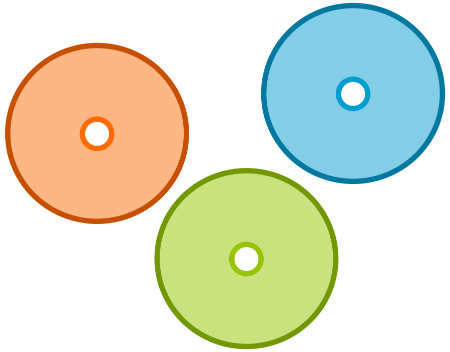


Relationship to k-means

Consider Gaussian mixture model with

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

Spherically
symmetric clusters



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

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

Module 4: Latent Dirichlet allocation

Topic vocab distributions:

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

TECH	
develop	0.18
computer	0.09
processor	0.032
user	0.027
internet	0.02
…	…

SPORTS	
player	0.15
score	0.07
team	0.06
goal	0.03
injury	0.01
…	…

⋮

Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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

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

Abstract

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

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

1. Introduction

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

Clustering:

One topic indicator z_i per **document** i

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

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

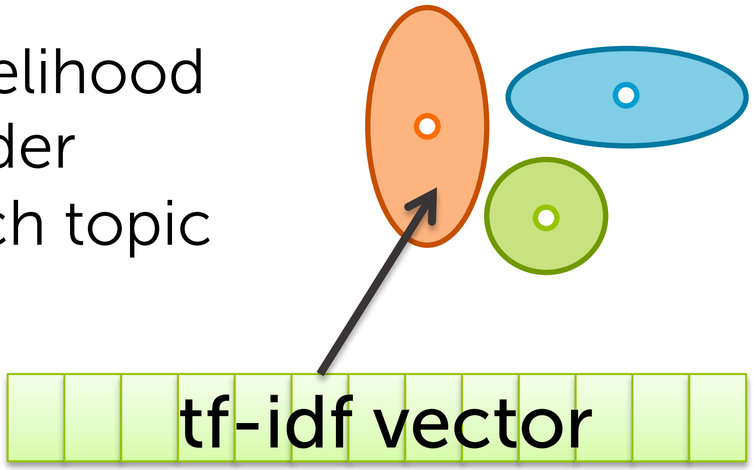
Comparing and contrasting

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**

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
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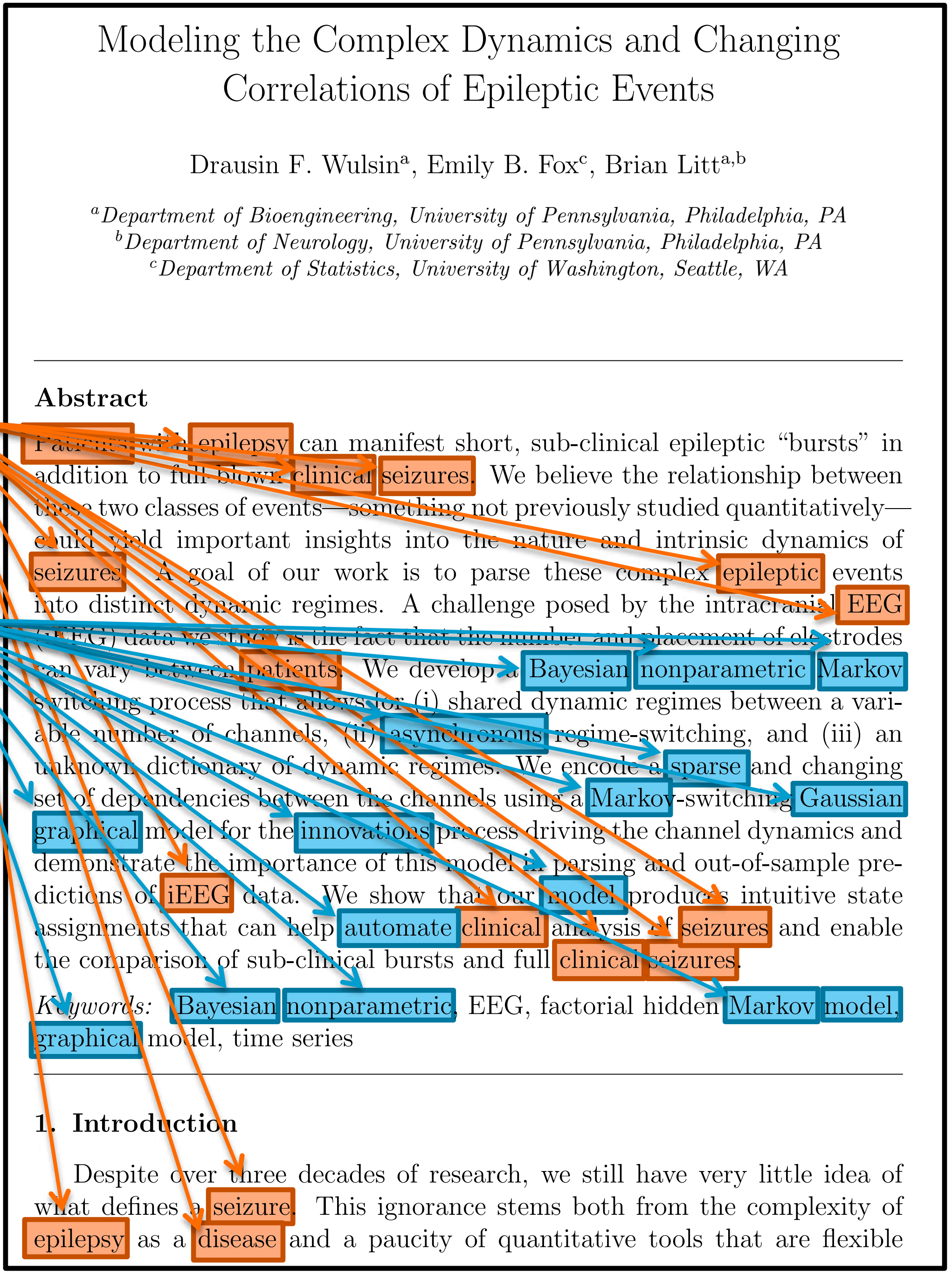
⋮



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In LDA:

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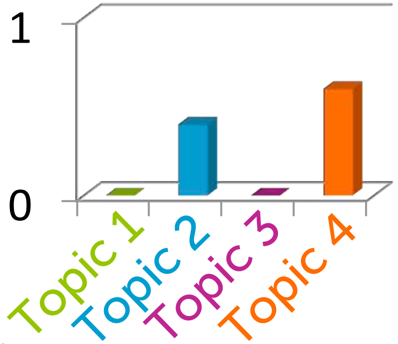
Each word scored under topic z_{iw}

Distribution on topics in **document**

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



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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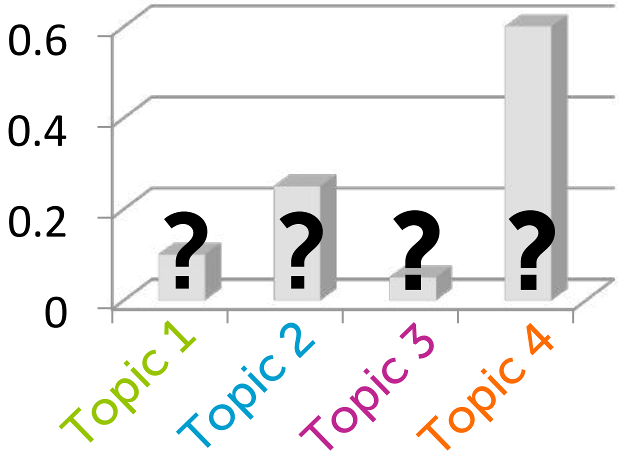
Document topic proportions:

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



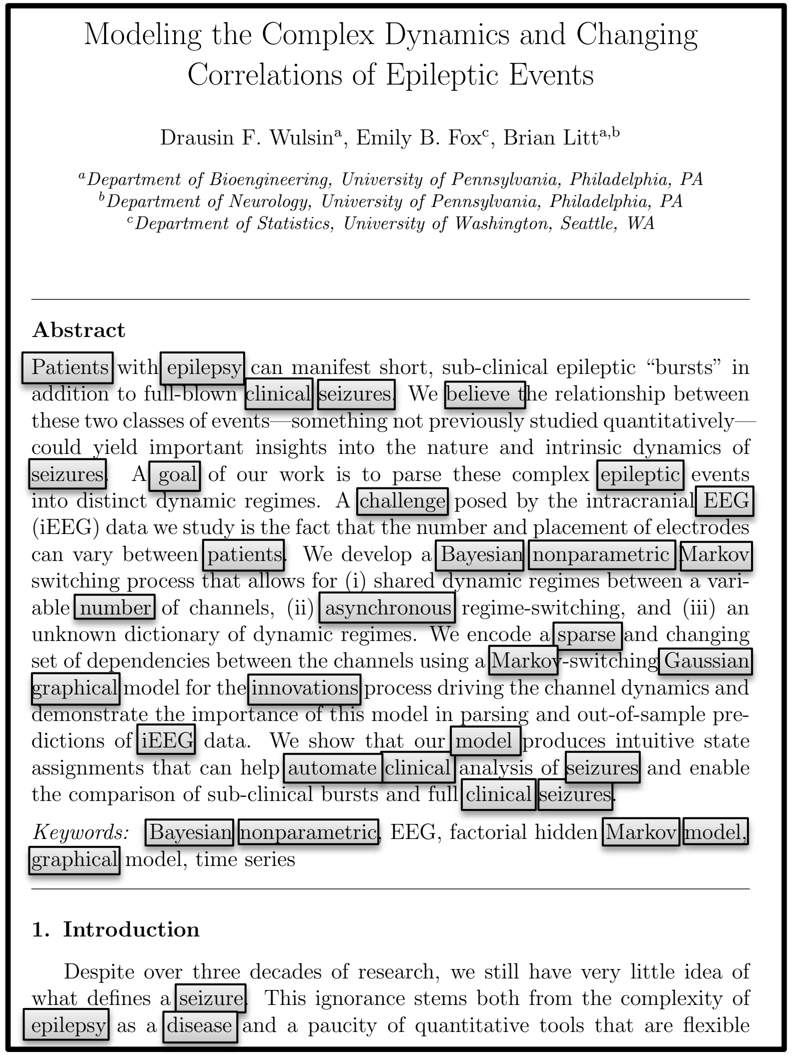
Gibbs sampling for LDA

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

1. Introduction

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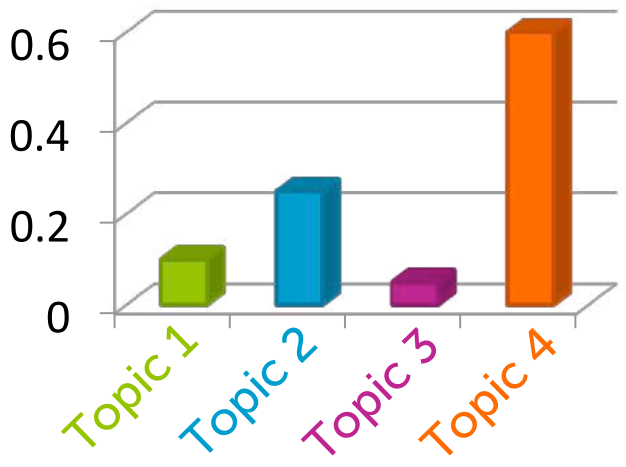


Step 1: Randomly reassign all z_{iw} based on

- doc topic proportions
- topic vocab distributions

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

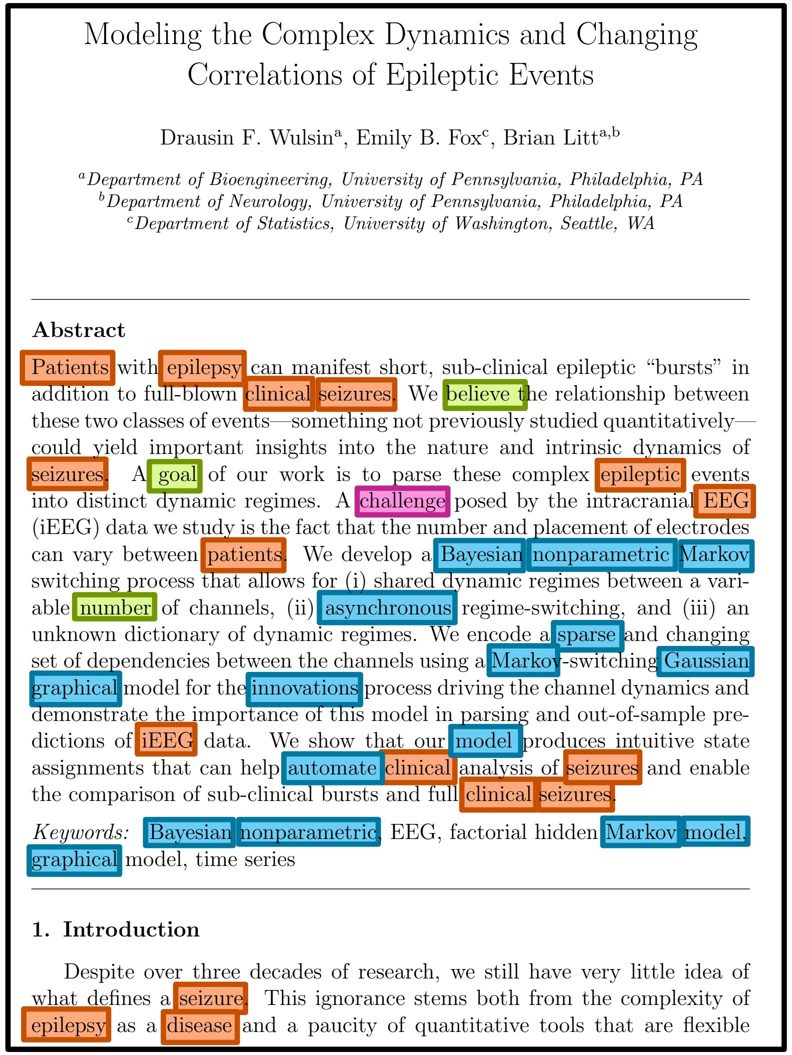
Gibbs sampling for LDA

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

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

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

⋮


Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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

[a]Department of Bioengineering, University of Pennsylvania, Philadelphia, PA
[b]Department of Neurology, University of Pennsylvania, Philadelphia, PA
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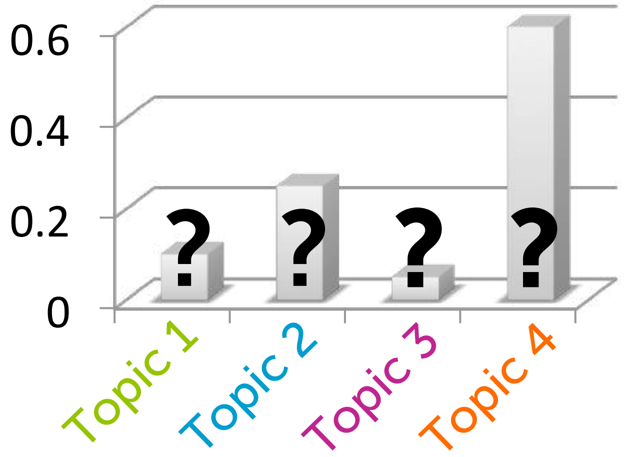


Step 2: Randomly reassign doc topic proportions based on assignments z_{iw} in **current doc**

Step 3: Repeat for all docs

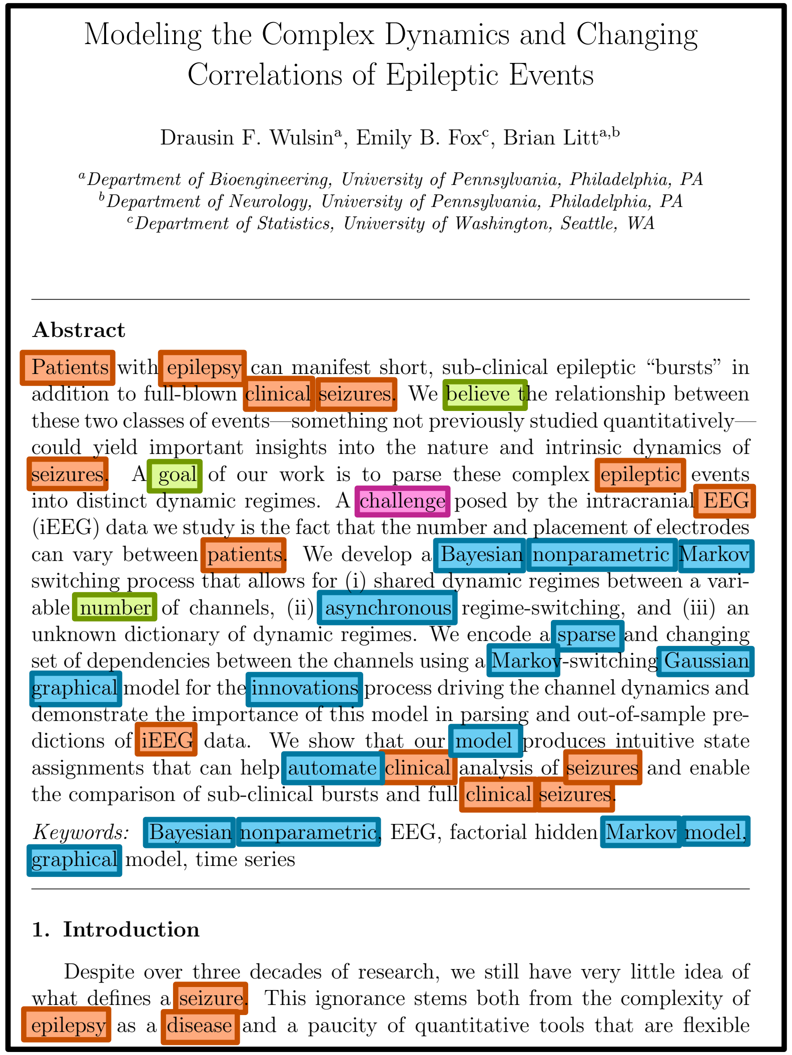
Gibbs sampling for LDA

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

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

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

⋮



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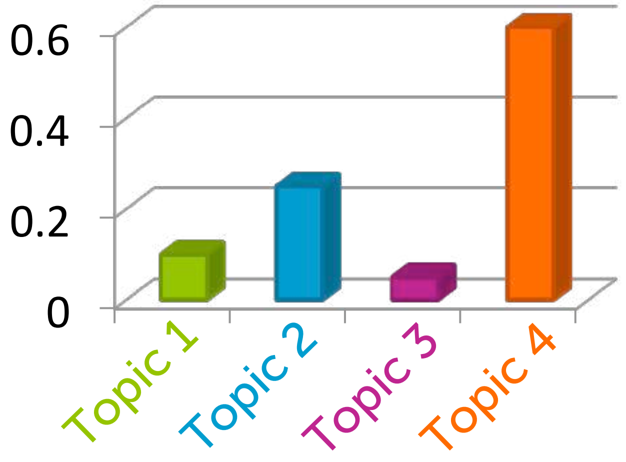

Step 4: Randomly reassign topic vocab distributions based on assignments z_{iw} in **entire corpus**

Collapsed Gibbs sampling for LDA

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

TOPIC 2	
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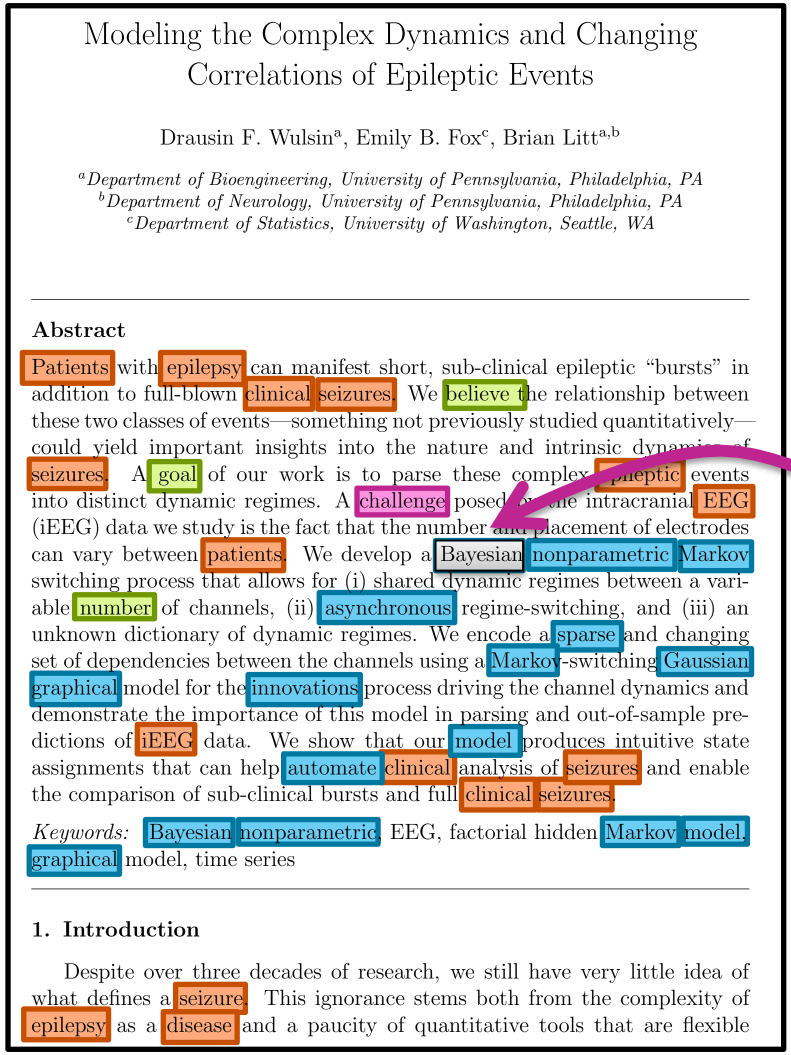

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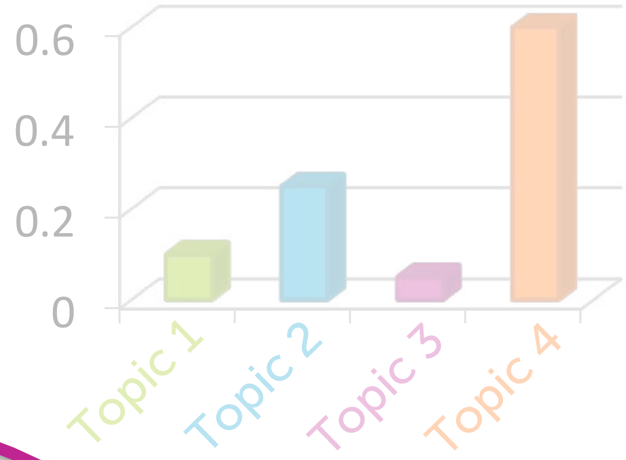


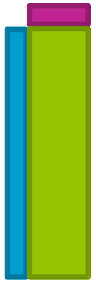
Randomly reassign z_{iw} based on current assignments z_{jv} of all other words **in doc and corpus**

Collapsed conditional distribution

3	?	1	3	1
epilepsy	dynamic	Bayesian	EEG	model

Topic 1

Topic 2



Topic 3

Probability of assignment of word in doc i to topic k proportional to:

How much doc likes topic

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

How much topic likes word

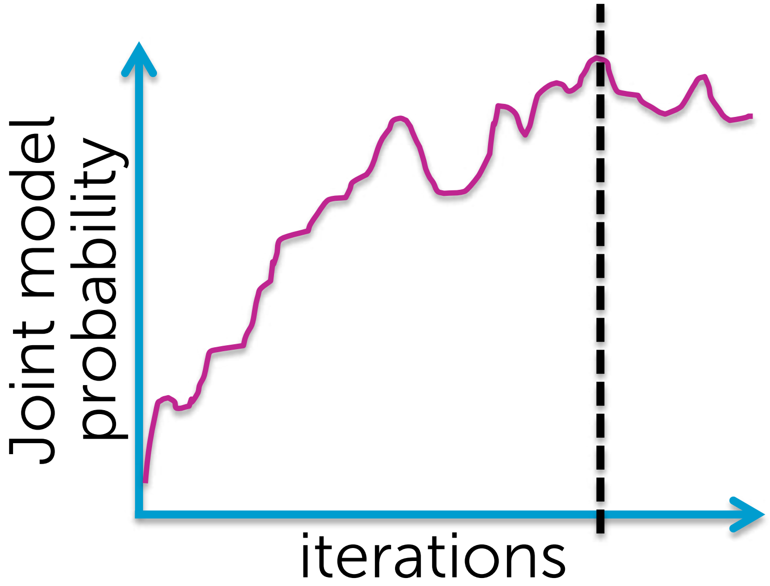
What to do with sampling output?

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"



Summary of what we learned

Models

- Nearest neighbors — Module 1
- Clustering — Module 2, 3
- Mixture of Gaussians — Module 3
- Latent Dirichlet allocation — Module 4

Algorithms

- KD-trees — Module 1
- Locality sensitive hashing — Module 1
- k-means — Module 2
- MapReduce — Module 2
- Expectation Maximization — Module 3
- Gibbs sampling — Module 4

Core ML

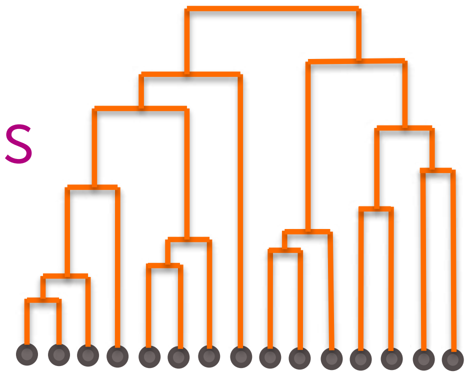
- Distance metrics — Module 1
- Approximation algorithms — Module 1
- Unsupervised learning — Module 2
- Probabilistic modeling — Module 2, 3, 4
- Data parallel problems — Module 2
- Bayesian inference — Module 4

Bonus content:
Hierarchical clustering

Why hierarchical clustering?

- Avoid choosing # clusters beforehand

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

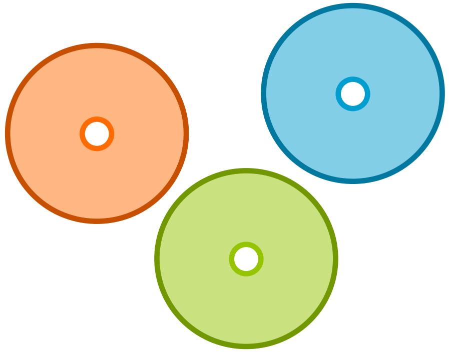


- Most algorithms allow user to choose any distance metric
  - k-means restricted us to Euclidean distance

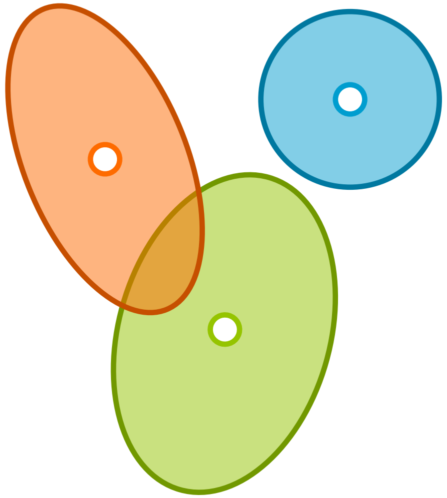
Why hierarchical clustering?

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

k-means: spherical clusters



Gaussian mixtures: ellipsoids



Why hierarchical clustering?

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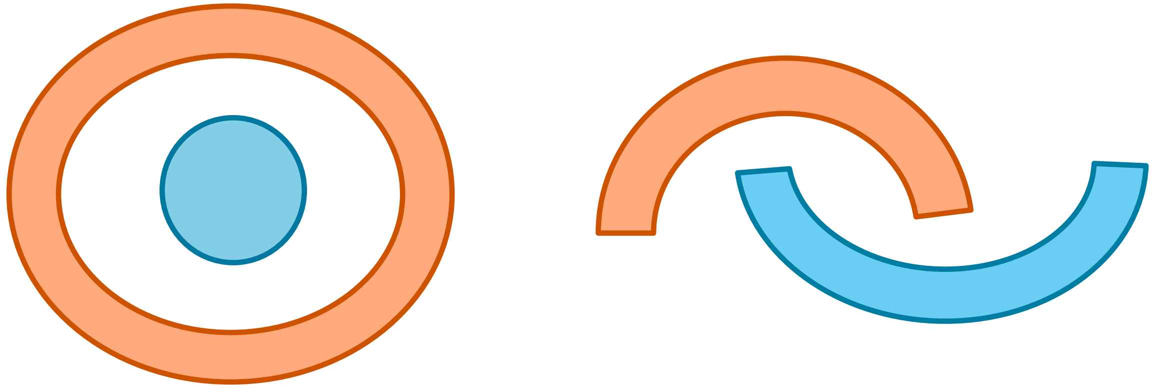
What about these?



Two main types of algorithms

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

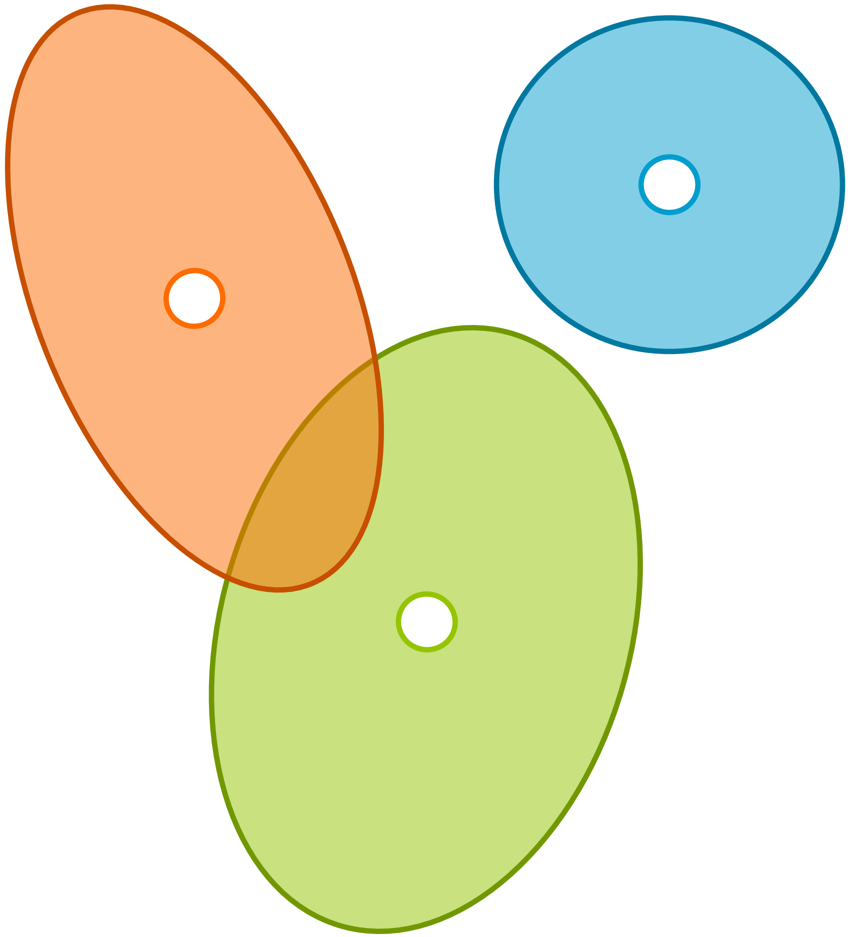
- Example: recursive k-means

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

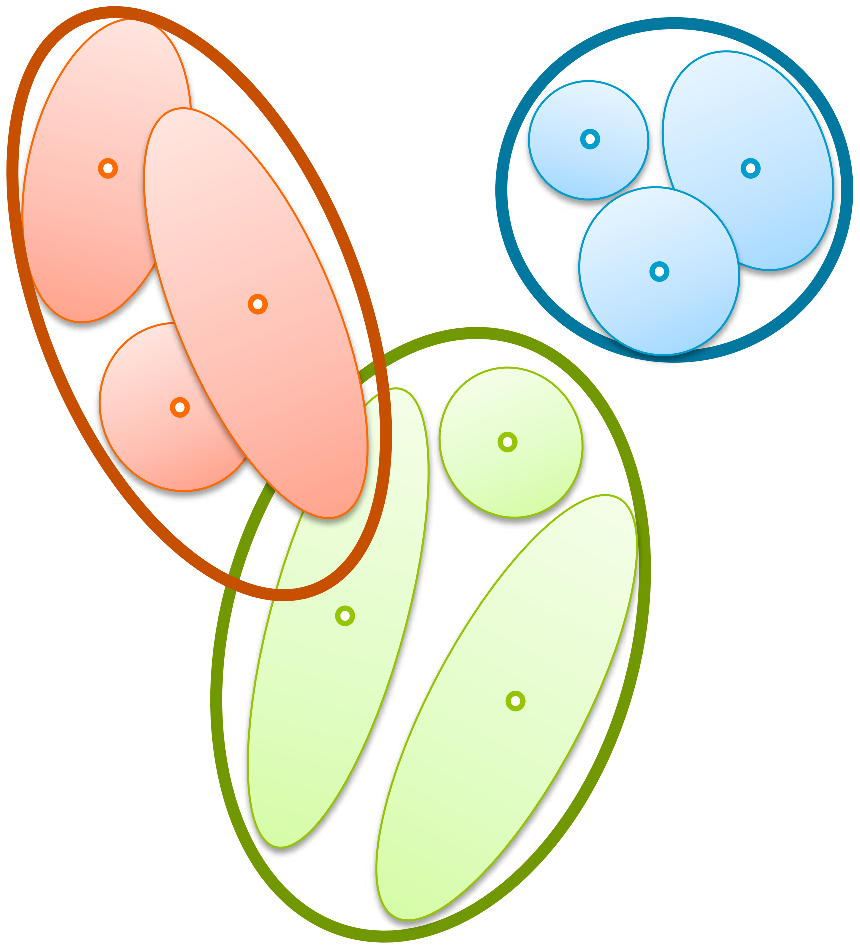
- Example: single linkage

Divisive clustering

Divisive in pictures – level 1

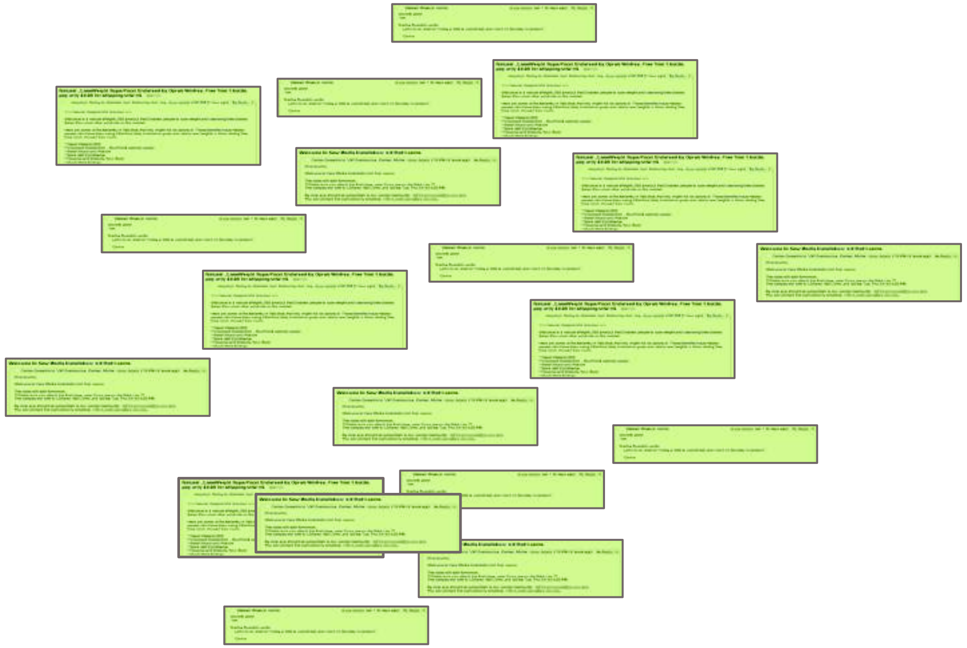


Divisive in pictures – level 2



Divisive: Recursive k-means

Wikipedia

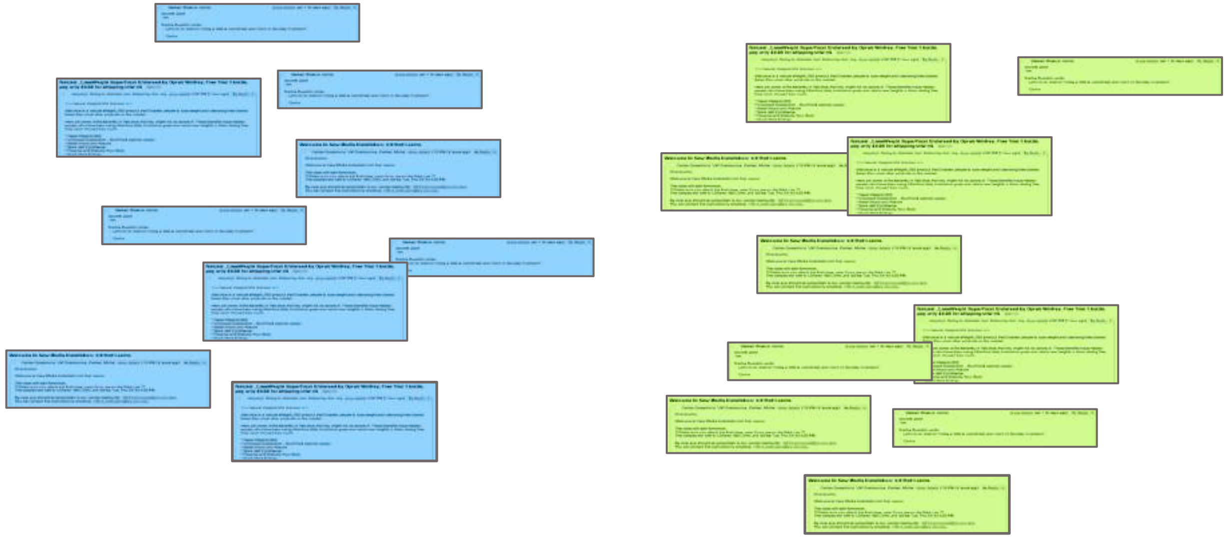


Divisive: Recursive k-means

Wikipedia

Athletes

Non-athletes



Divisive: Recursive k-means

Wikipedia

Athletes

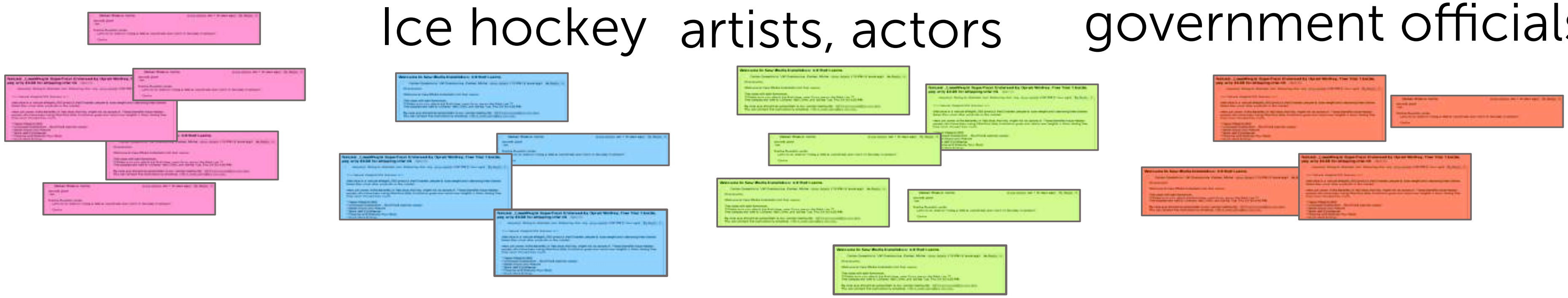
Non-athletes

Baseball

Soccer/ Ice hockey

Musicians, artists, actors

Scholars, politicians, government officials



⋮

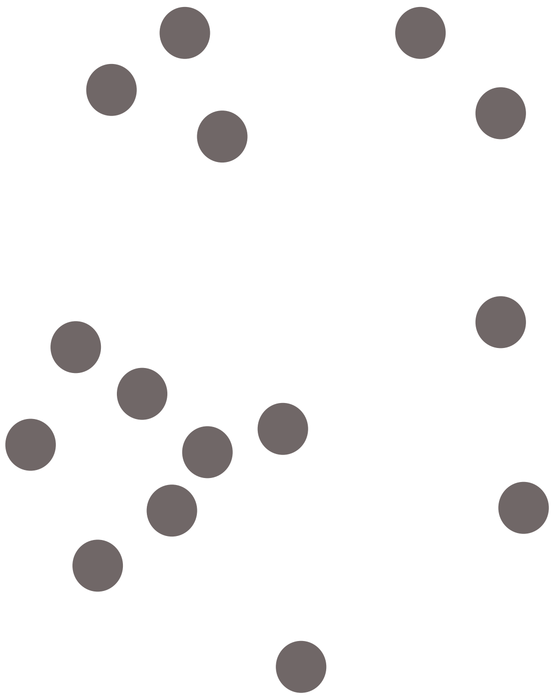
Divisive choices to be made

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

Agglomerative clustering

Agglomerative: Single linkage

1. Initialize each point to be its own cluster



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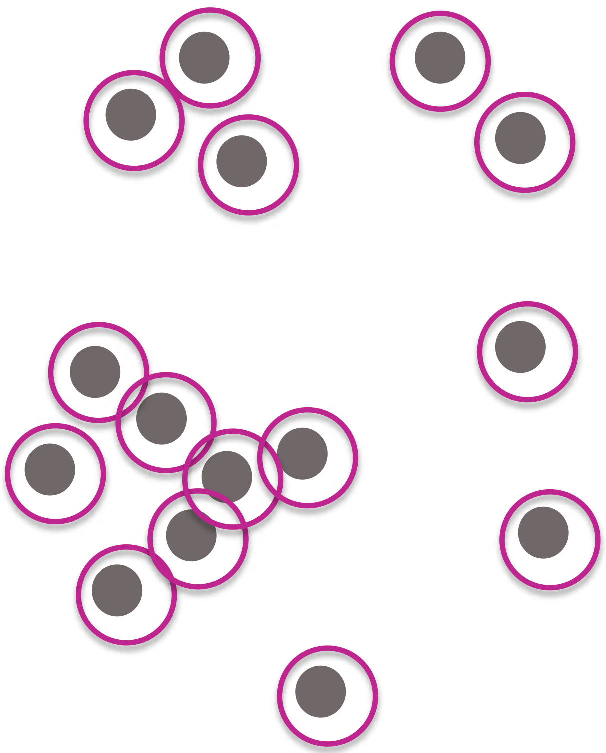
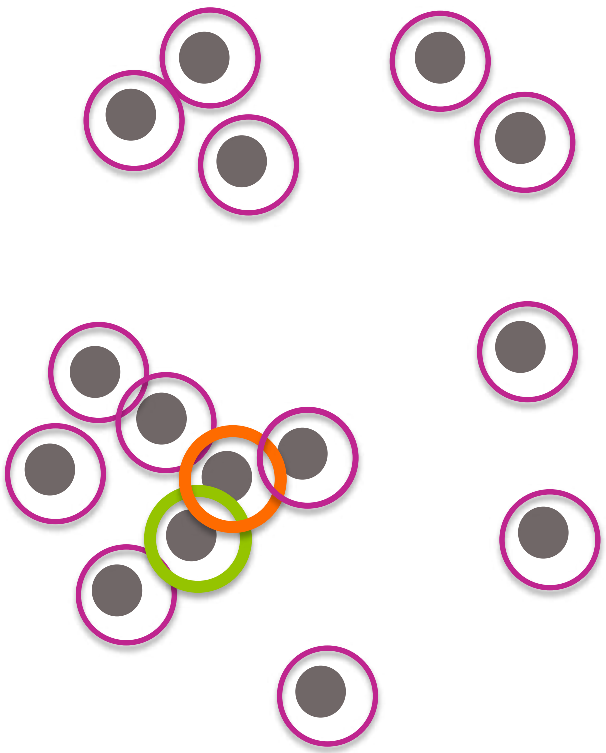


Agglomerative: Single linkage

2. Define distance between clusters to be:



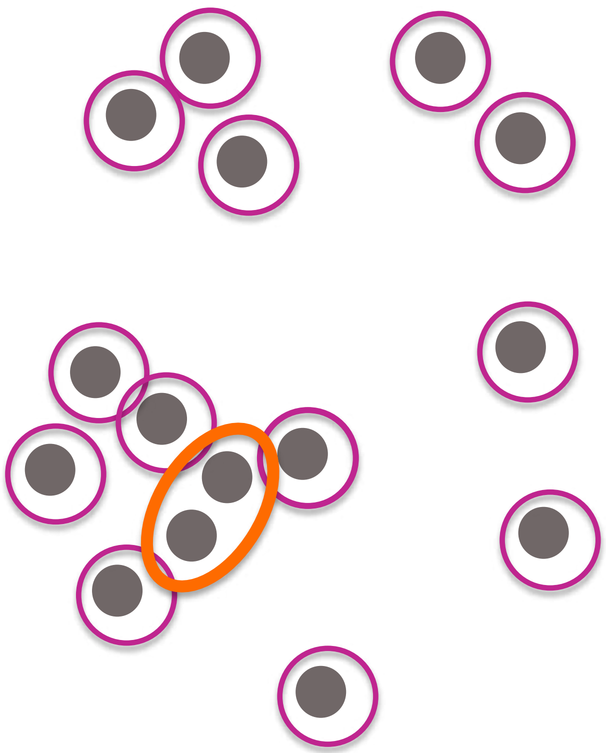
$$\text{distance}(C_1,C_2) = \boxed{\min_{\mathbf{x}_i \text{ in } C_1,\ \mathbf{x}_j \text{ in } C_2} d(\mathbf{x}_i, \mathbf{x}_j)}$$

specified pairwise distance function

Linkage criteria

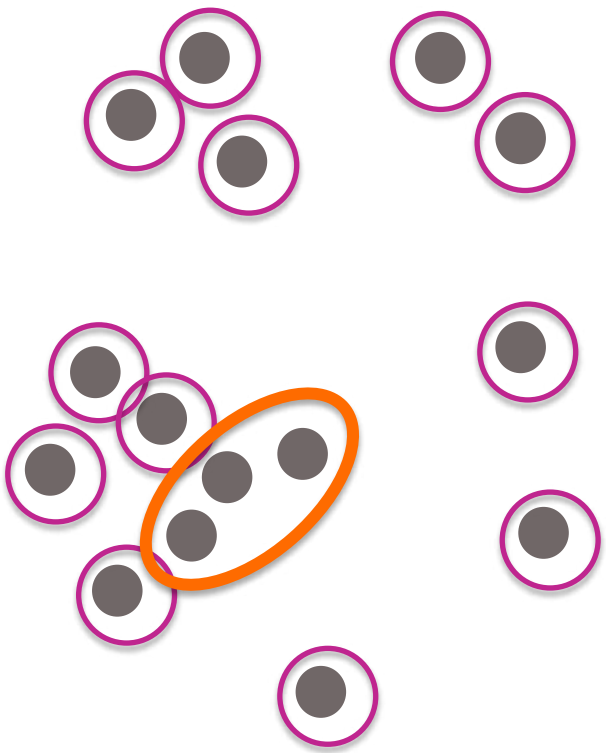
Agglomerative: Single linkage

3. Merge the two closest clusters



Agglomerative: Single linkage

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



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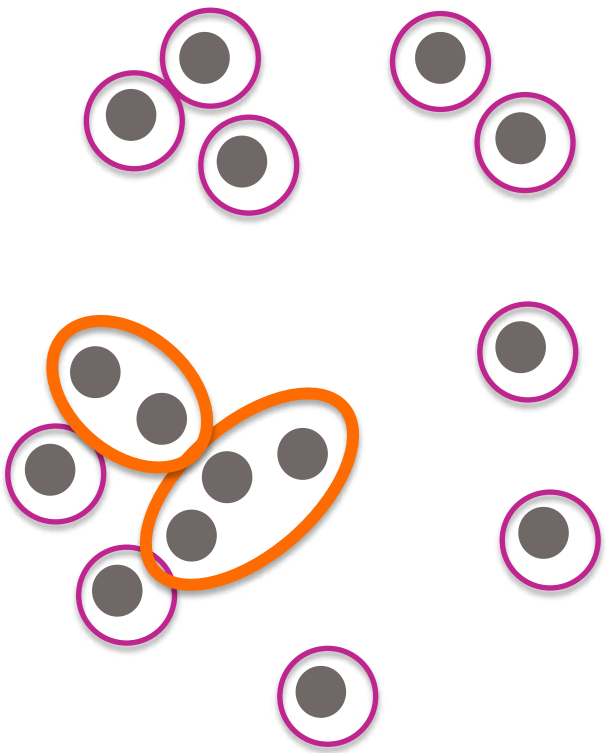

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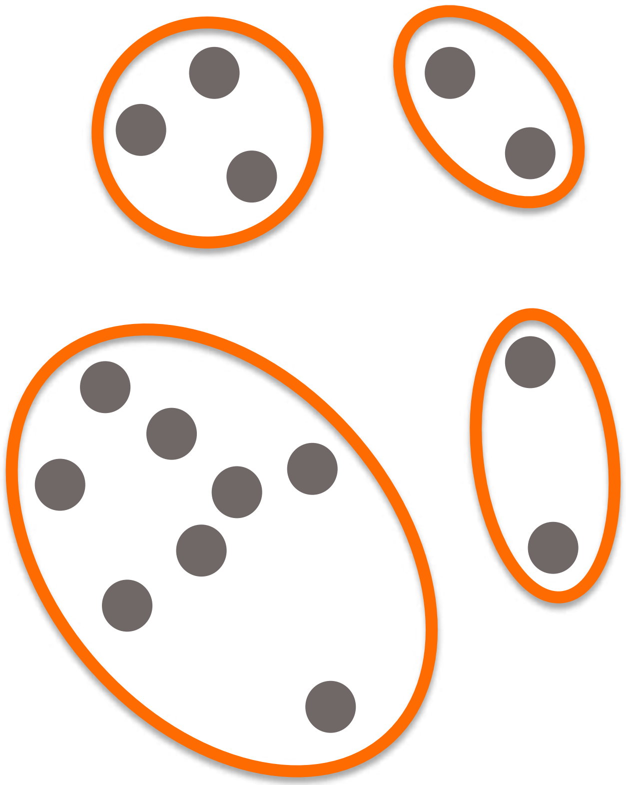

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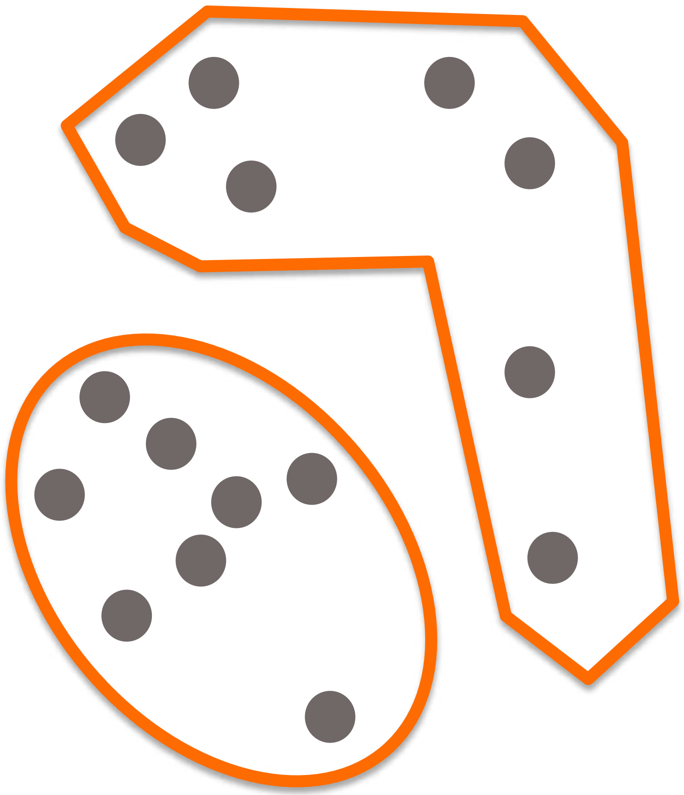

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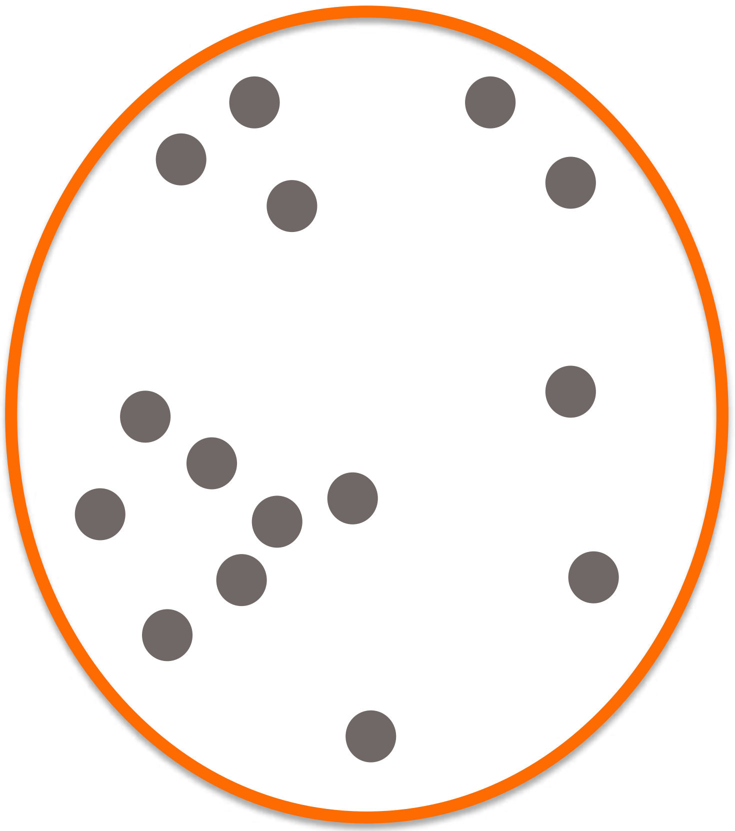
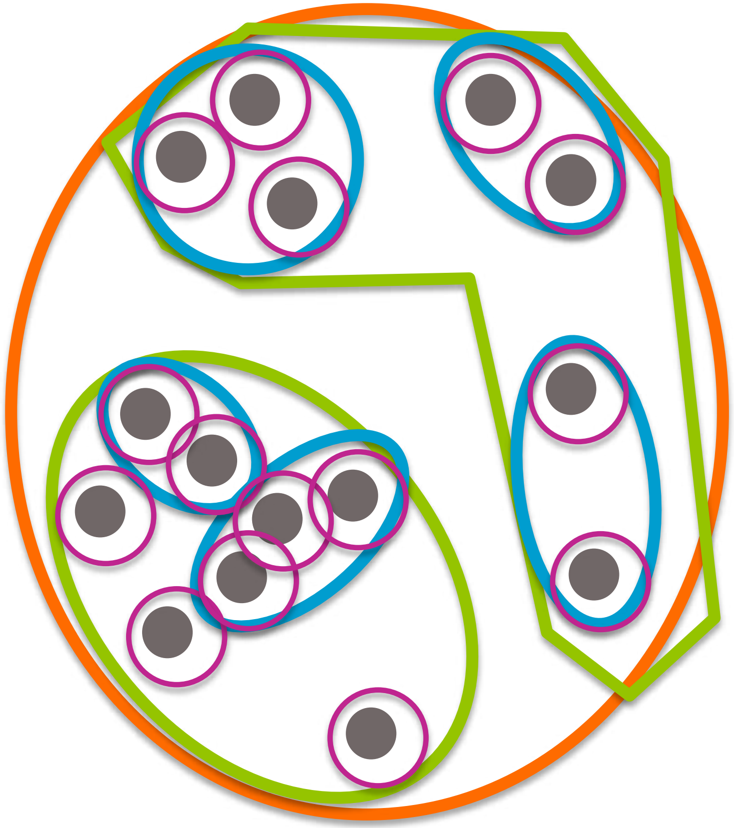


Clusters of clusters

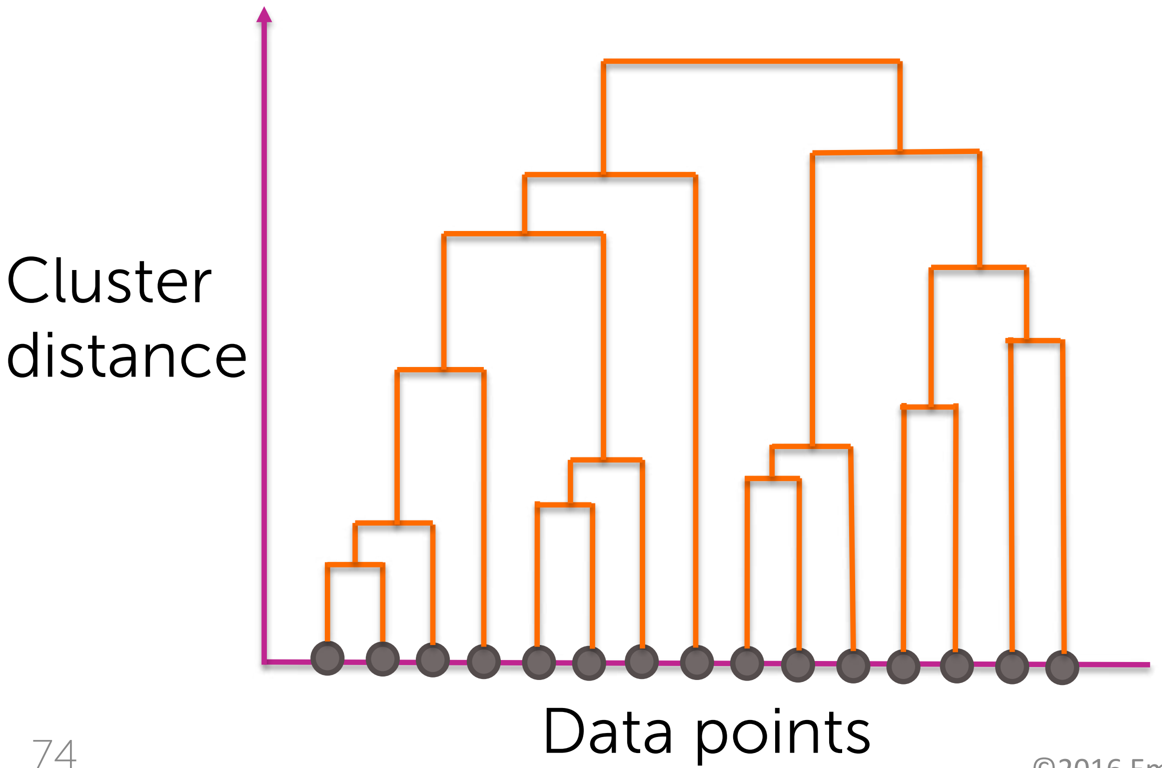
Just like our picture for divisive clustering…



The dendrogram for agglomerative clustering

The dendrogram

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



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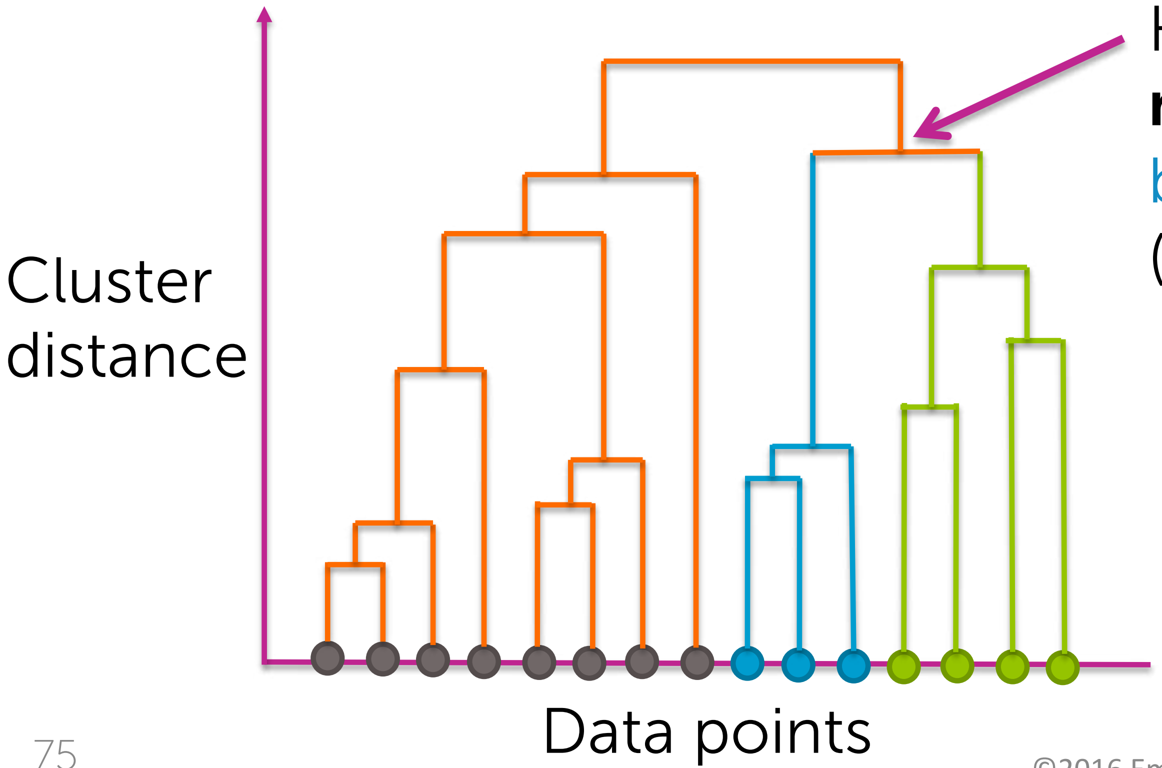
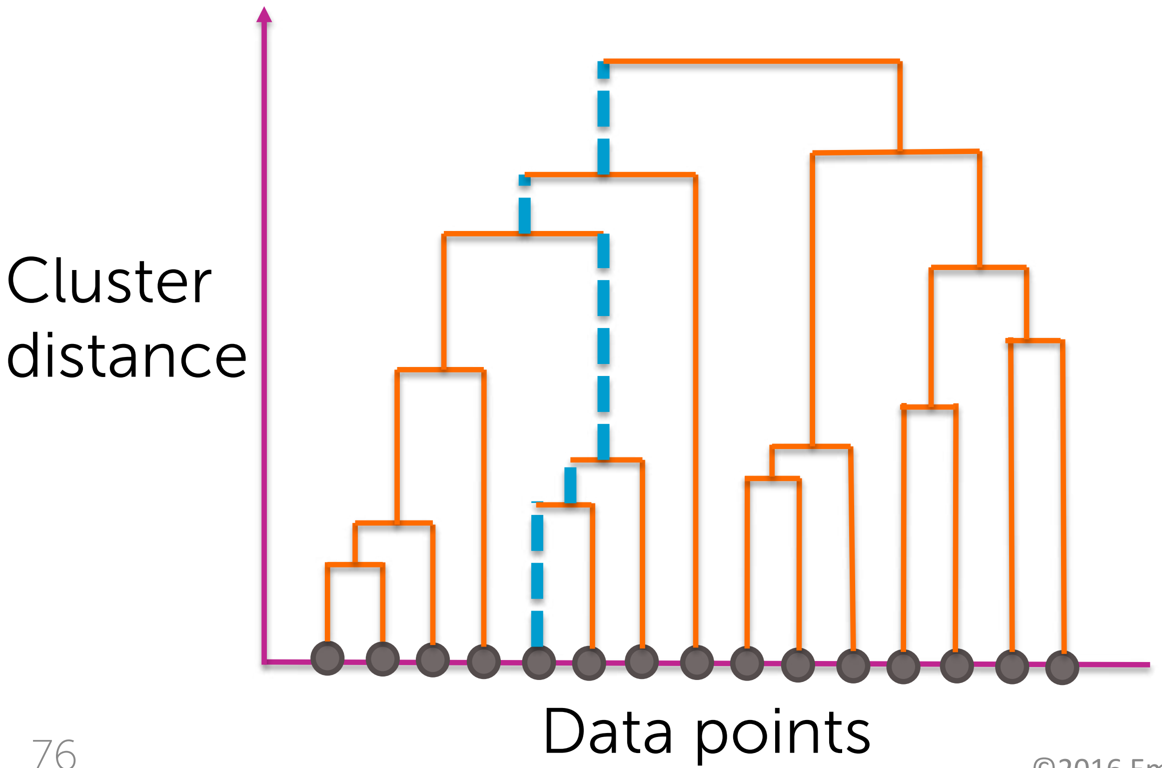


Height here indicates **min distance** between blue pts and green pts (2 clusters)

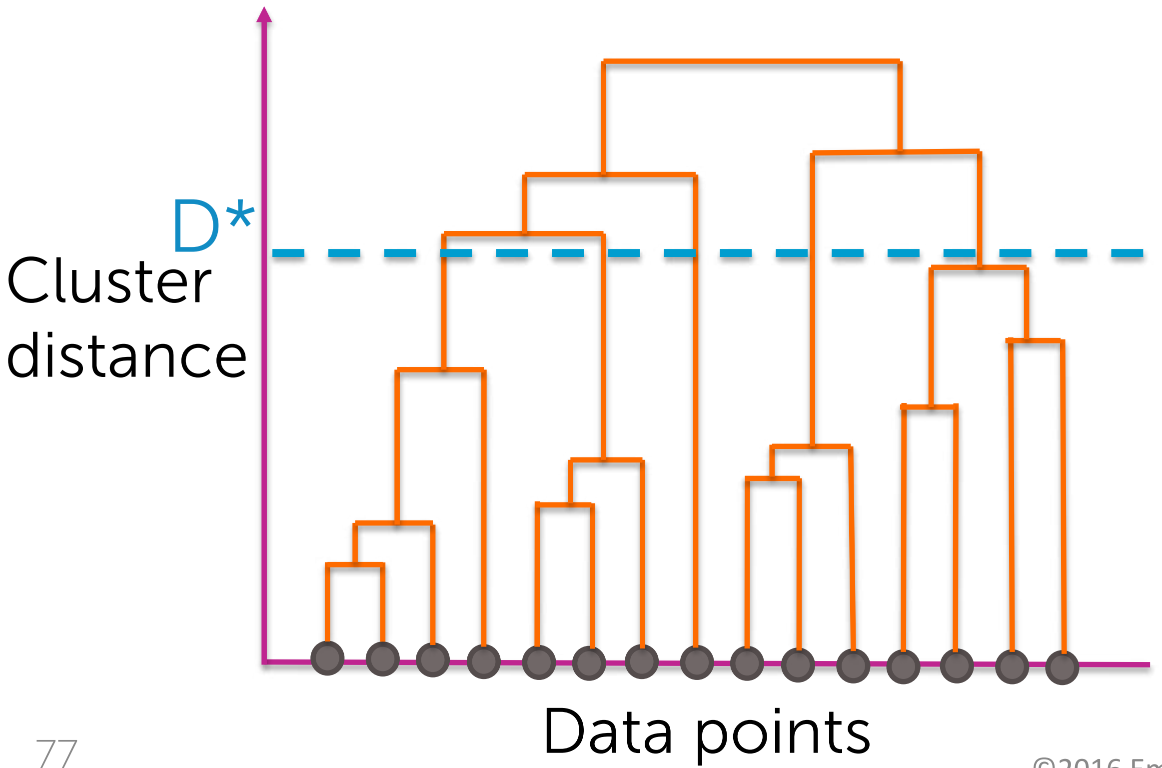
The dendrogram

Path shows all clusters to which a point belongs and the order in which clusters merge



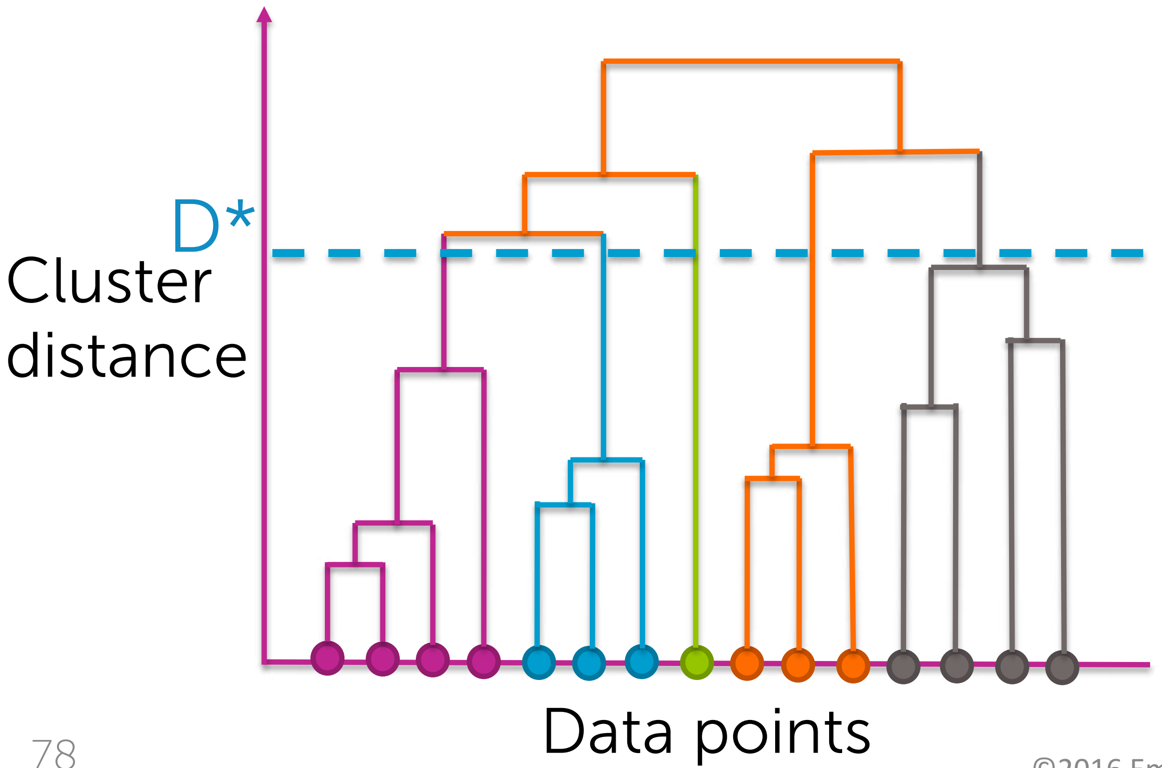
Extracting a partition

Choose a distance D* at which to cut dendogram



Extracting a partition

Every branch that crosses D*
becomes a separate cluster



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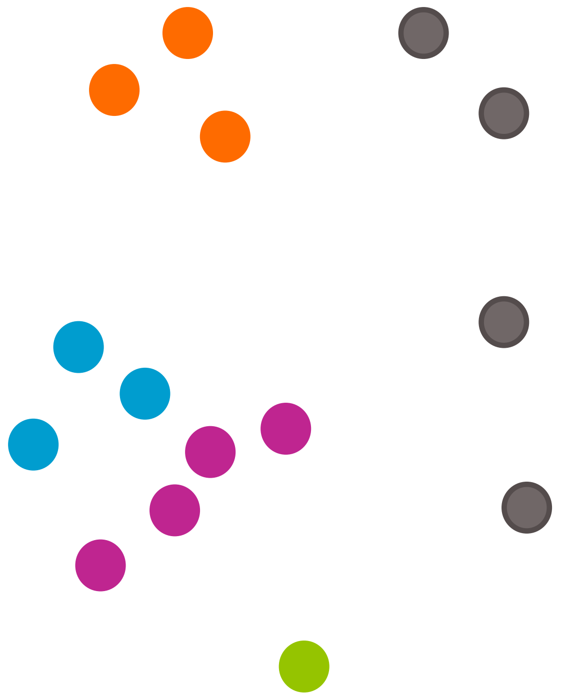
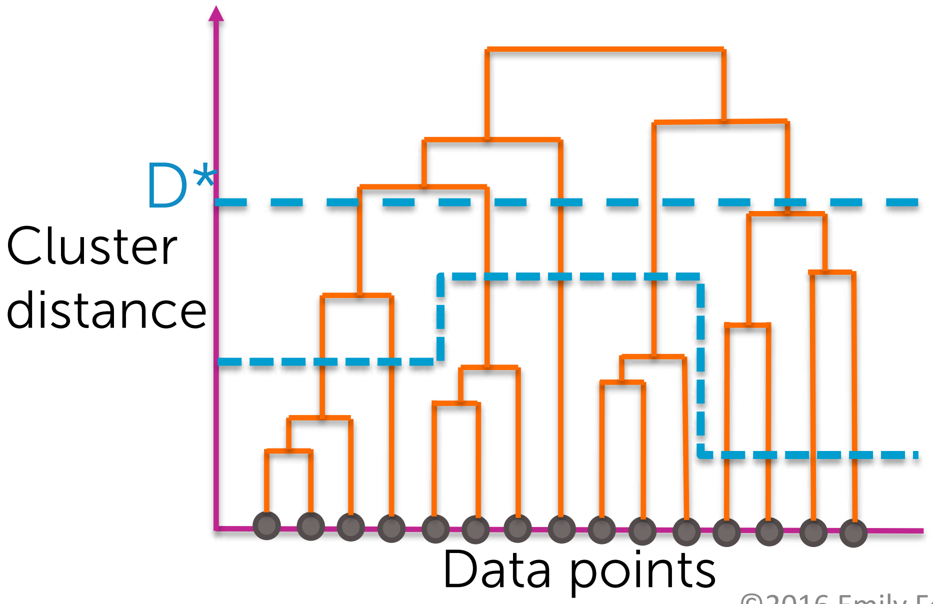


Agglomerative clustering details

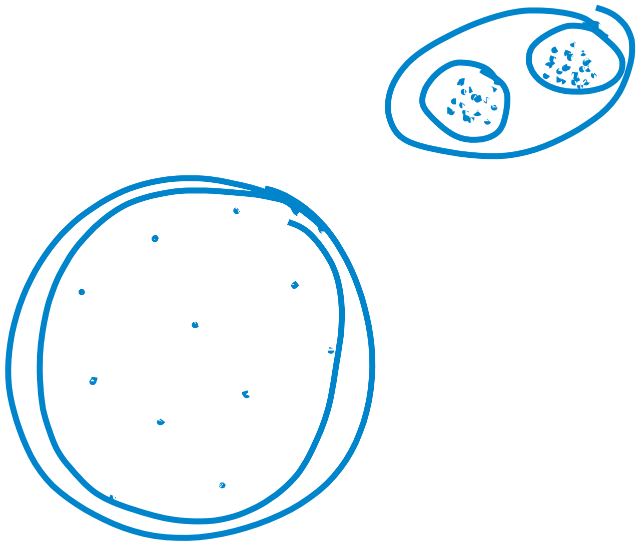
Agglomerative choices to be made

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



More on cutting dendrogram

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



Computational considerations

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

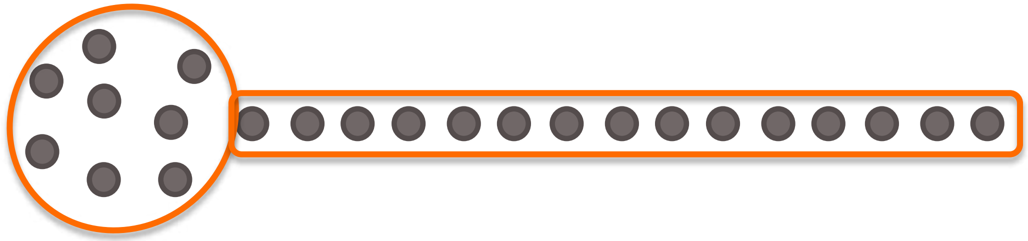
datapoints

- Smart implementations use triangle inequality to rule out candidate pairs

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

Statistical issues

Chaining: Distant points clustered together if there is a chain of pairwise close points between

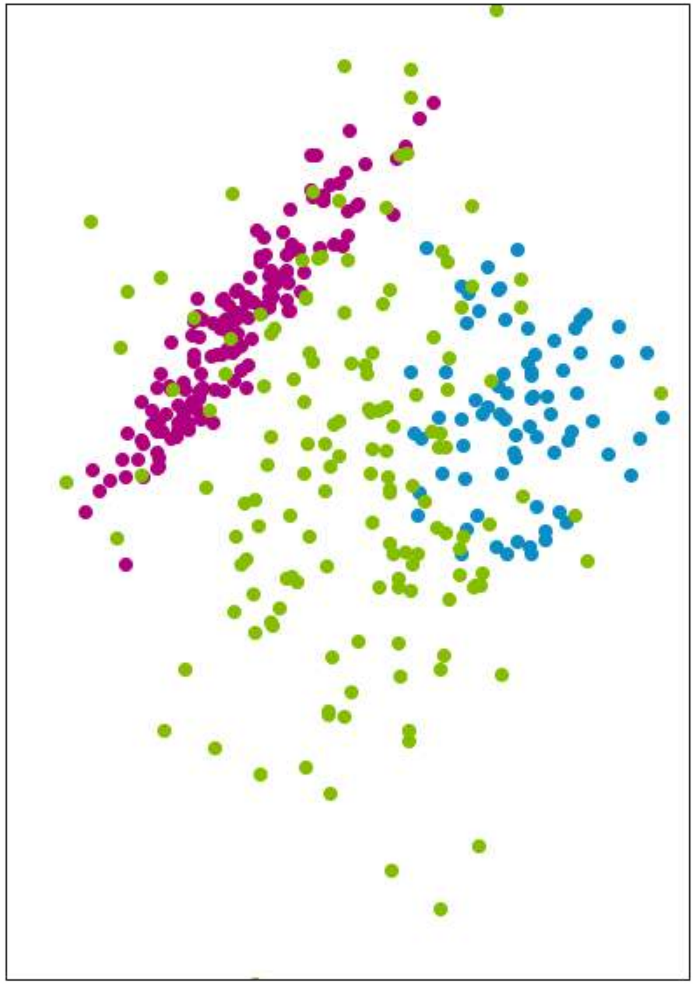


Other linkage functions can be more robust, but restrict the shapes of clusters that can be found

- **Complete linkage**:
  max pairwise distance between clusters
- **Ward criterion**:
  min within-cluster variance at each merge

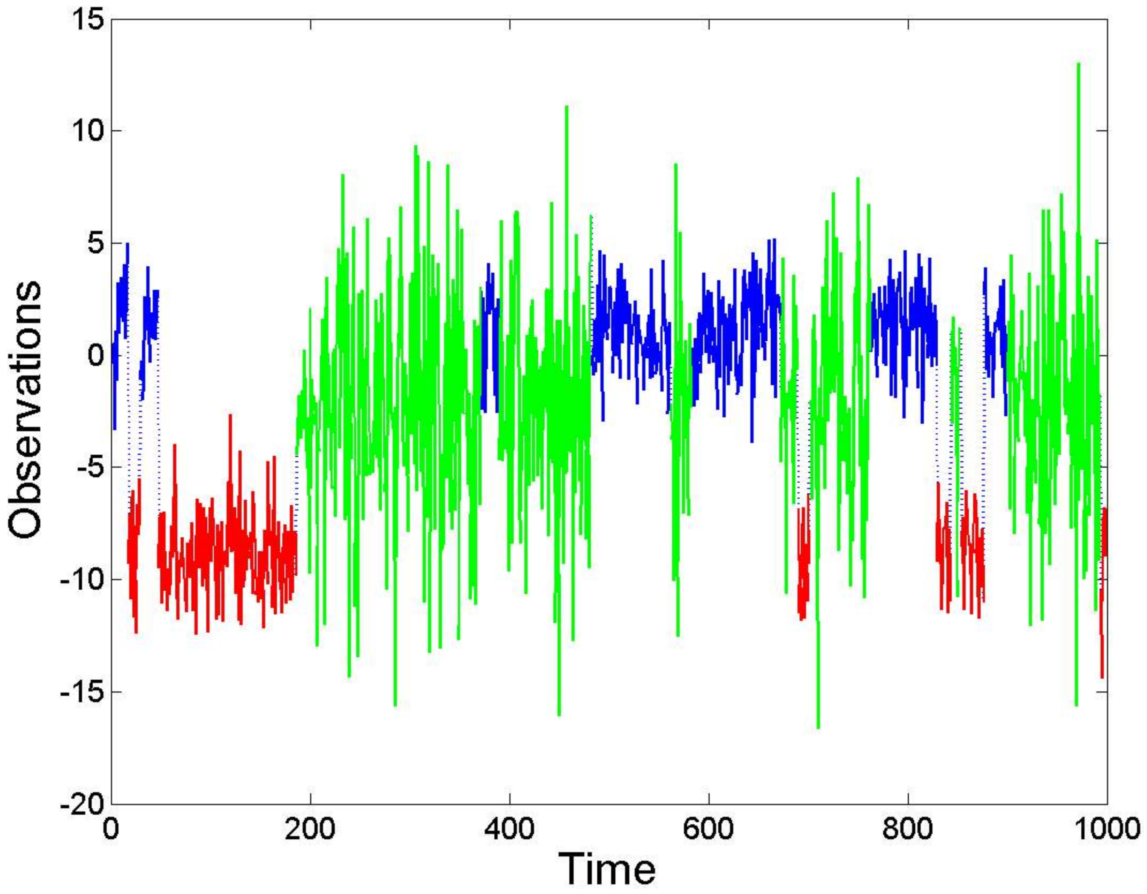
Hidden Markov models (HMMs): Another notion of "clustering"

So far, looked at clustering unordered data



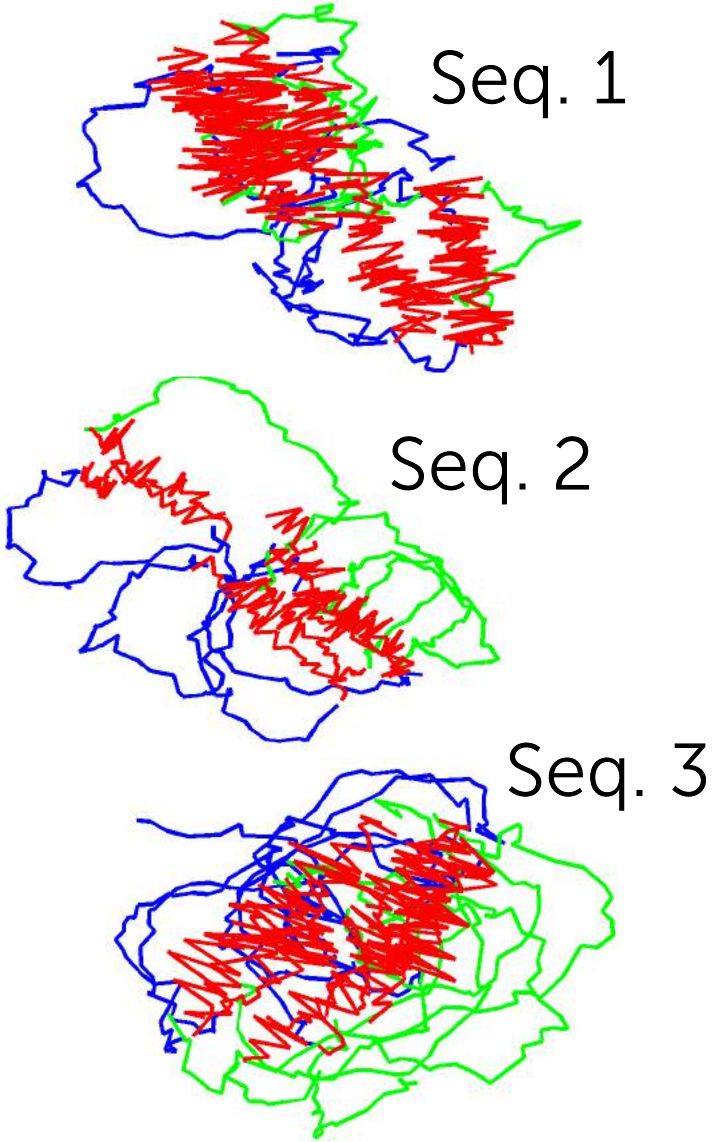
Data index (i.e., when observation was recorded) does not influence clustering

What if we have time series data?



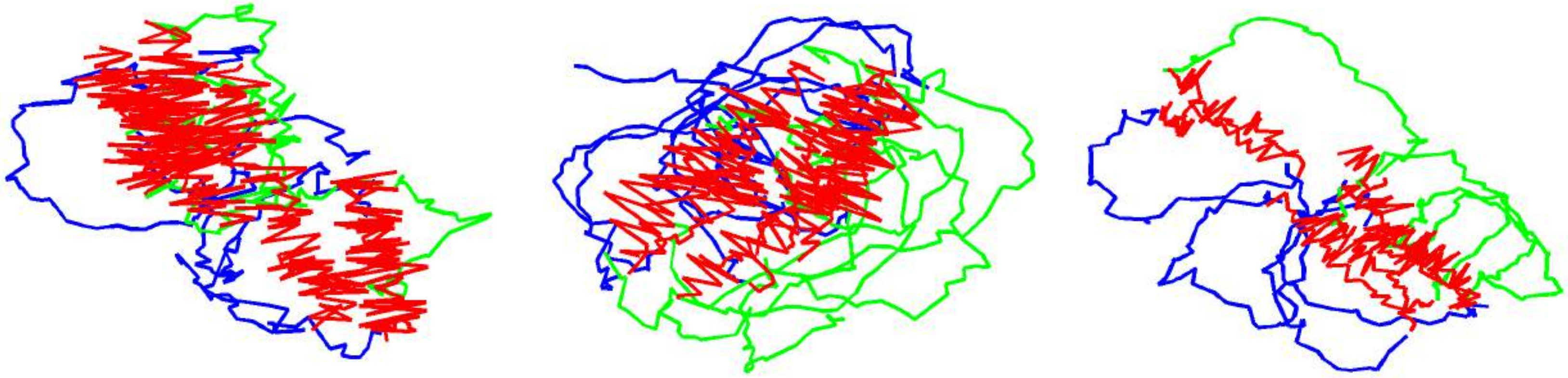
Would be hard to distinguish red, blue, and green clusters if we ignored order of data

Example: Honey bee dances

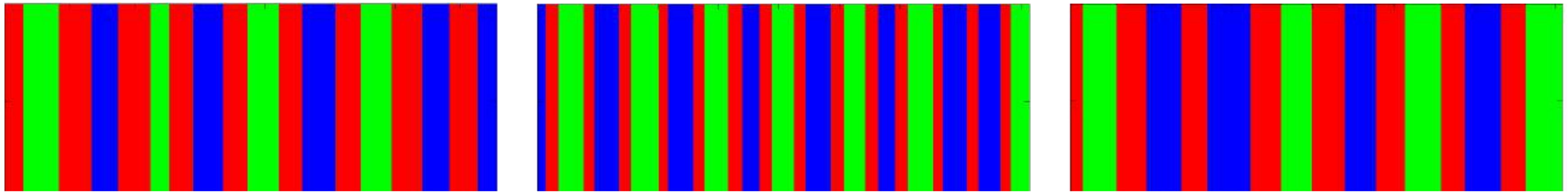


Repeated patterns of dance transitions

Sequence 1 Sequence 2 Sequence 3



Cluster labels over time

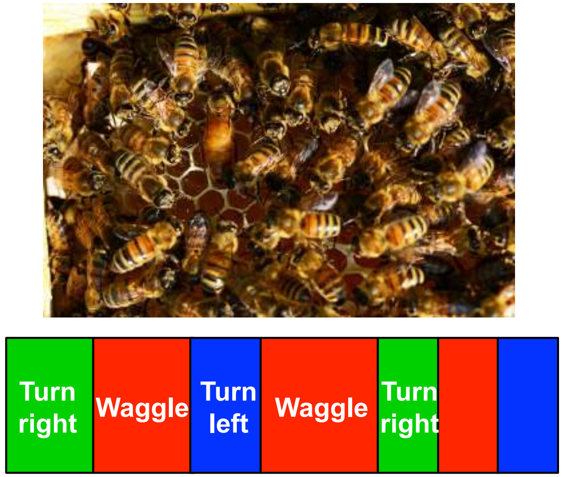


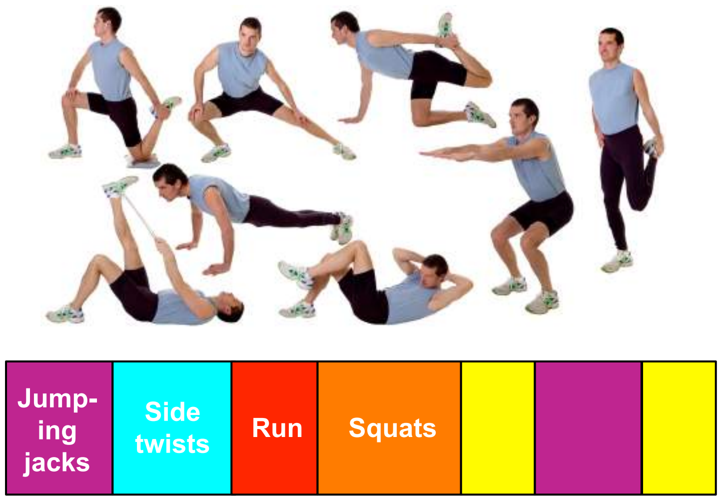
waggle dance

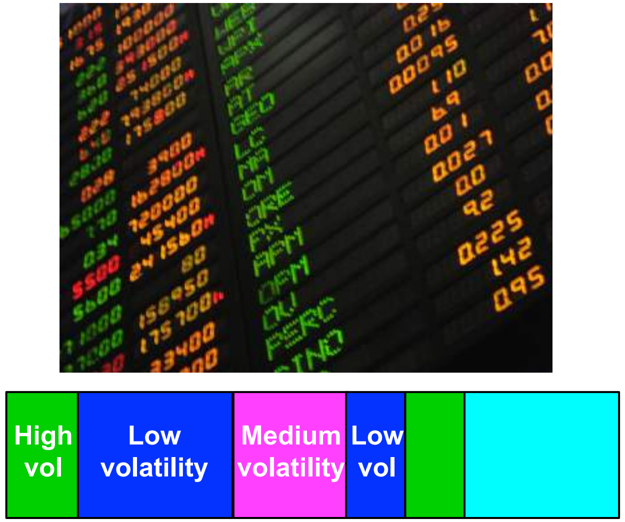
turn right

turn left

Similar ideas appear in many applications





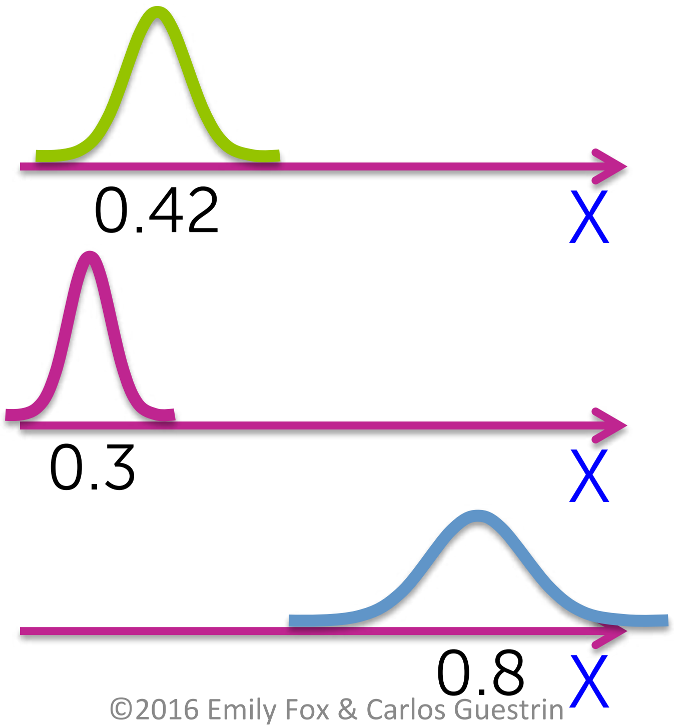


Hidden Markov model (HMM)

As in mixture model…

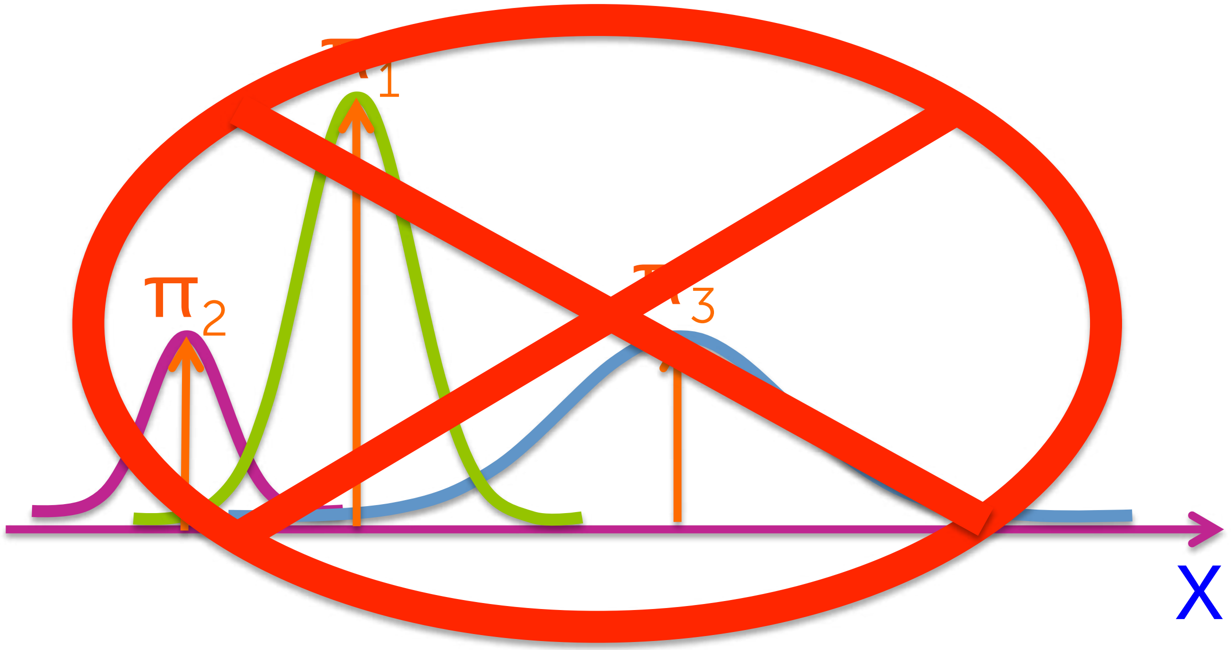
Every observation x_t is associated with cluster assignment variable z_t

Each cluster has a distribution over observed values



Hidden Markov model (HMM)

Difference from mixture model:
Probability of (z_t = k) depends on previous cluster assignment z_{t-1}



Inference in HMMs

- Learn MLE of HMM parameters using EM algorithm = Baum Welch
- Infer MLE of state sequence given fixed model parameters using dynamic programming = Viterbi algorithm
- Infer soft assignments of state sequence using dynamic programming = forward-backward algorithm

What we didn't cover

Other clustering + retrieval topics

Retrieval:

- Other distance metrics
- Distance metric learning

Clustering:

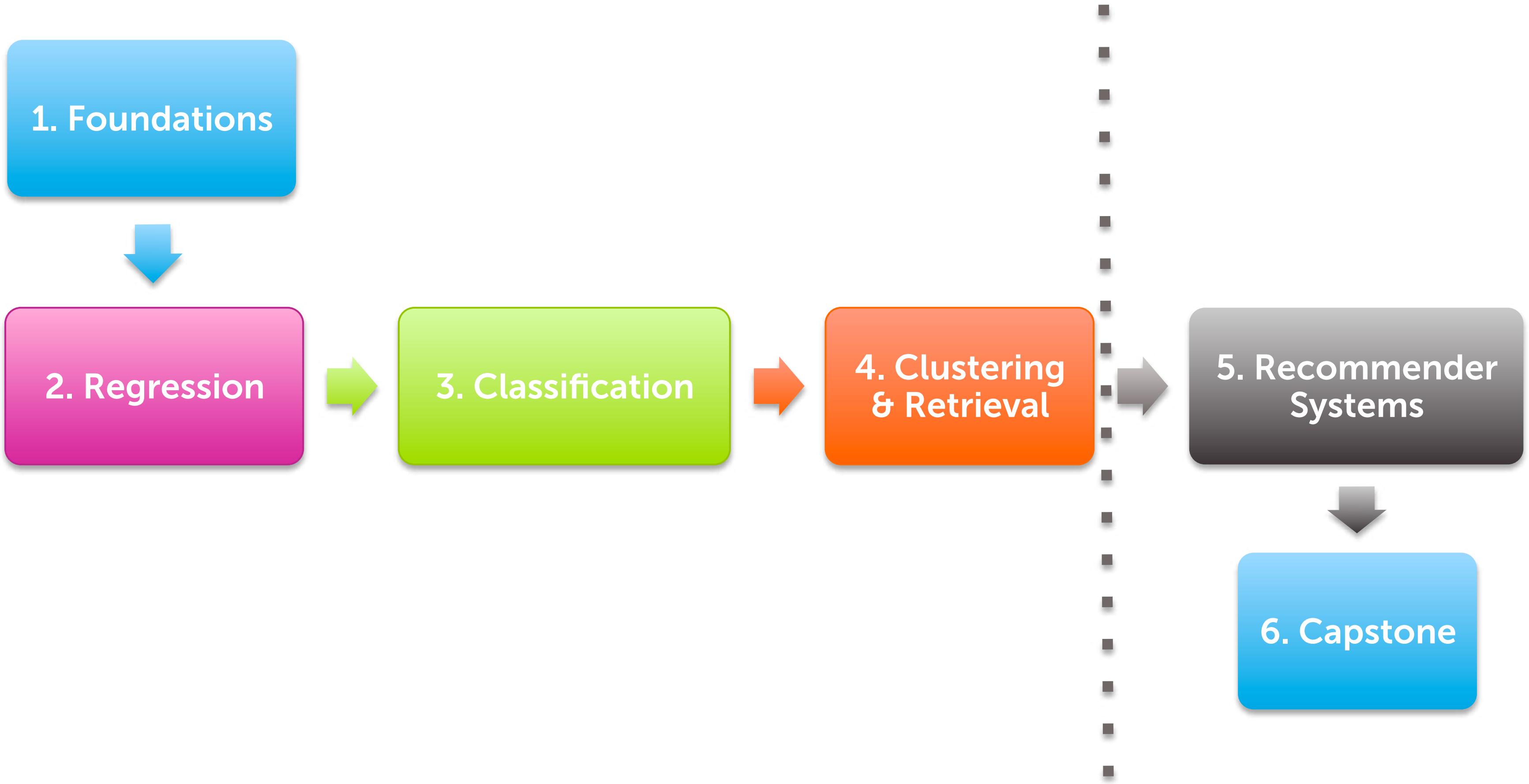
- Nonparametric clustering
- Spectral clustering

Related ideas:

- Density estimation
- Anomaly detection

What's ahead in this specialization

This course is a part of the Machine Learning Specialization



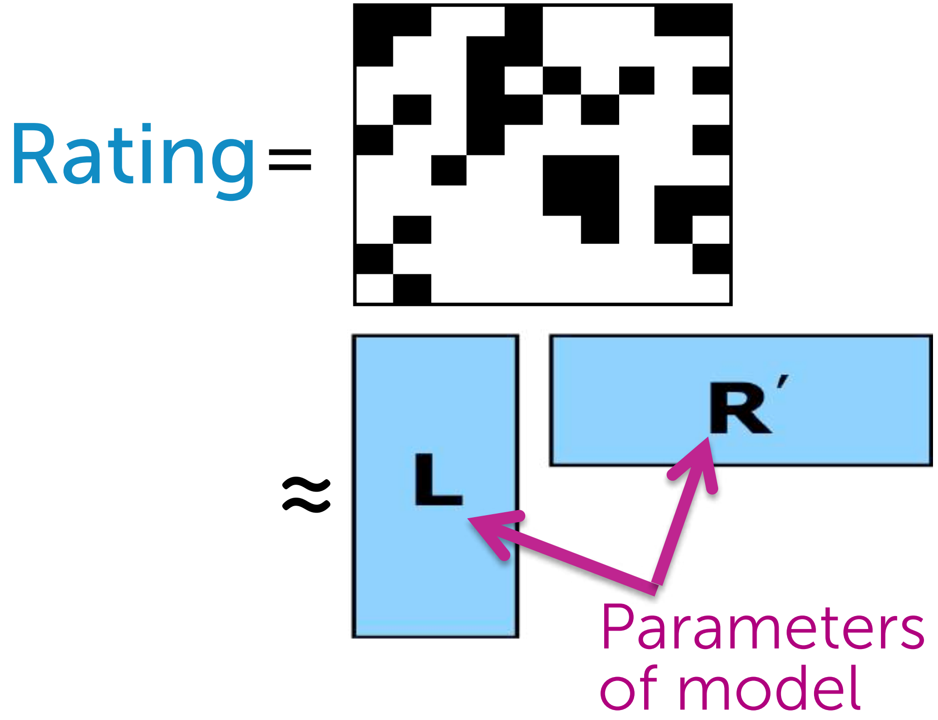
5. Recommender Systems & Dimensionality Reduction

Case study: Recommending Products

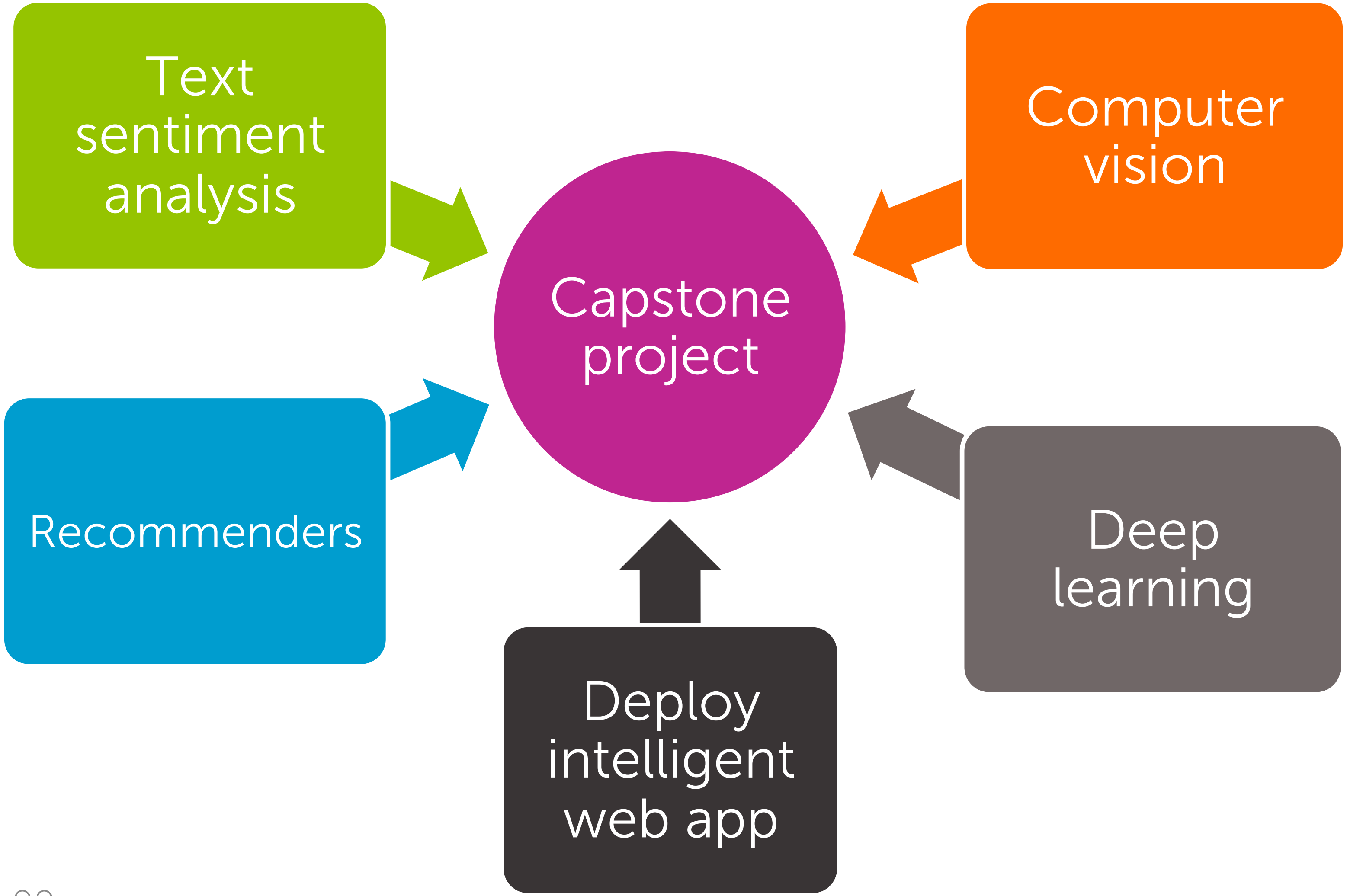
Models
- Collaborative filtering
- Matrix factorization
- PCA

Algorithms
- Coordinate descent
- Eigen decomposition
- SVD

Concepts
- Matrix completion, eigenvalues, cold-start problem, diversity, scaling up



6. Capstone: *Build and deploy an intelligent application with deep learning*



Thank you…