DATA SCIENCE WITH MACHINE LEARNING: CLUSTERING

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

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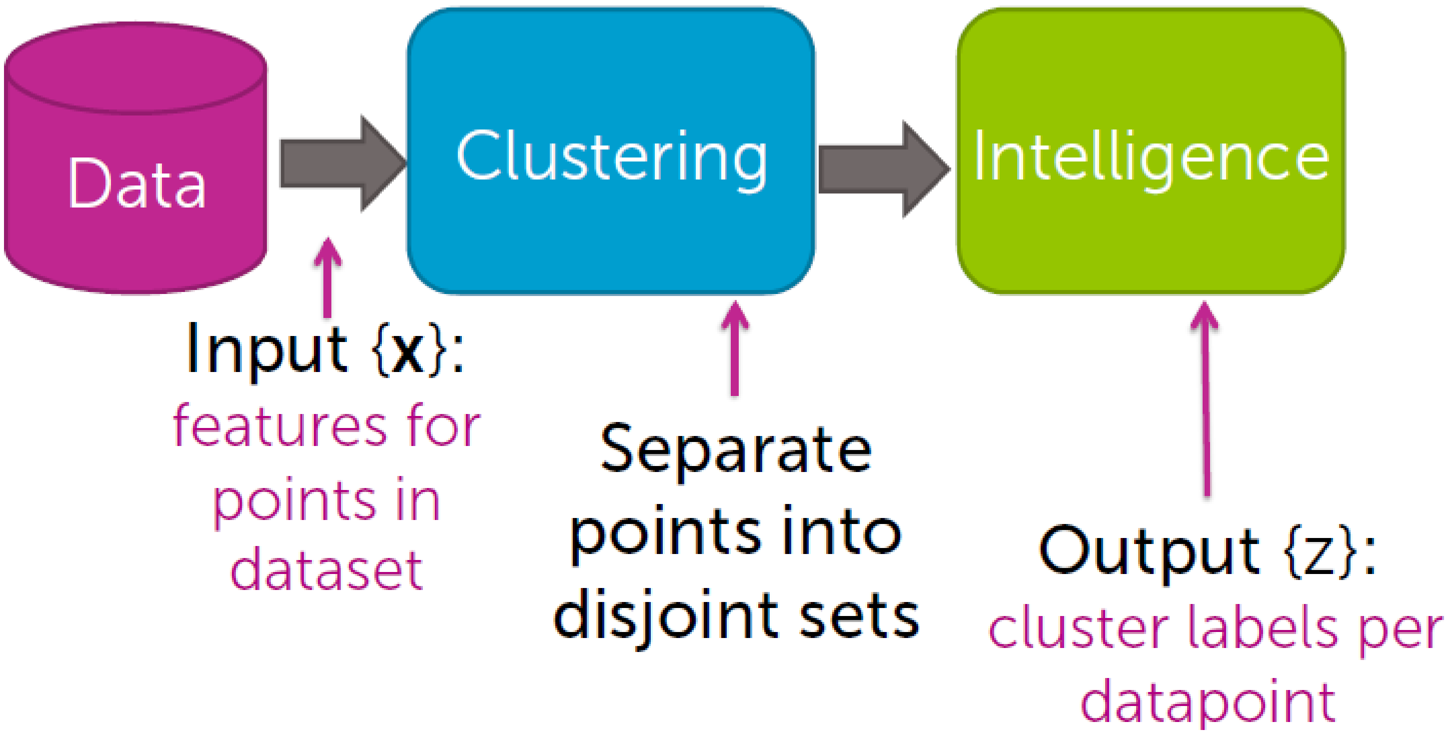
WFAiS UJ, Informatyka Stosowana
I stopień studiów

What is clustering?

Discover groups of similar inputs



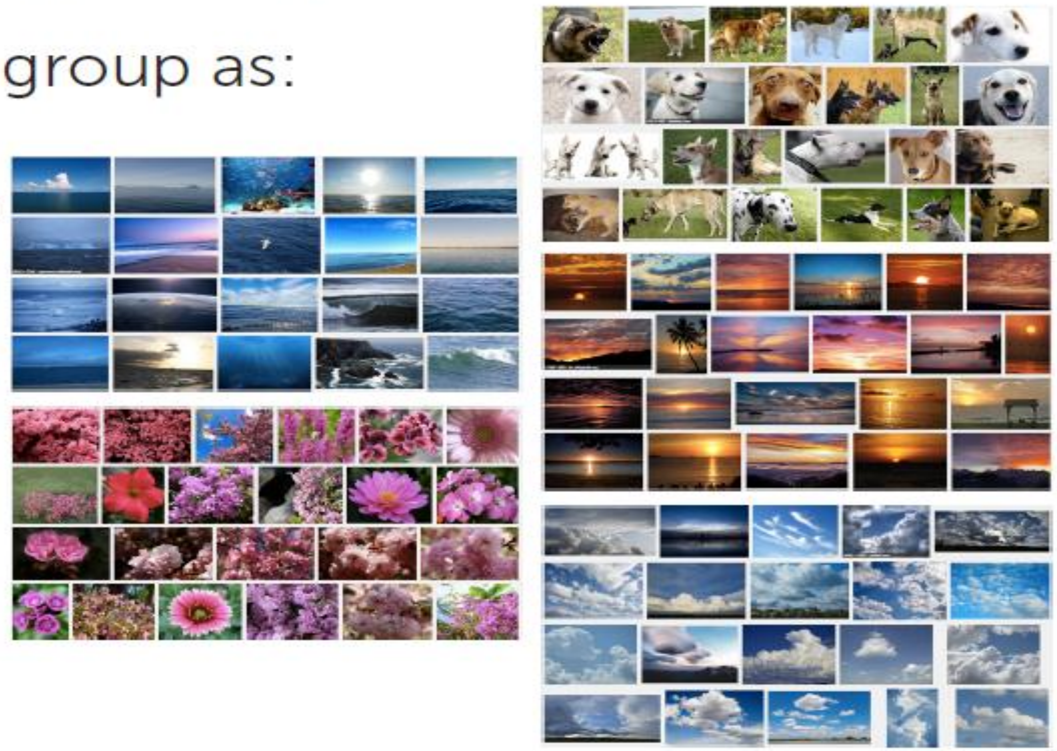
Clustring applications

Clustering applications

Clustering images

For search, group as:

– Ocean
– Pink flower
– Dog
– Sunset
– Clouds
– ...



Overwiew of content

Models
- Nearest neighbors
- Clustering
- Mixture of Gaussians
- Latent Dirichlet allocation

Algorithms
- KD-trees
- Locality sensitive hashing
- k-means
- MapReduce
- Expectation Maximization
- Gibbs sampling

Core ML
- Distance metrics
- Approximation algorithms
- Unsupervised learning
- Probabilistic modeling
- Data parallel problems
- Bayesian inference

Clustering:

An unsupervised learning task

Motivation

Goal: Structure documents by topic

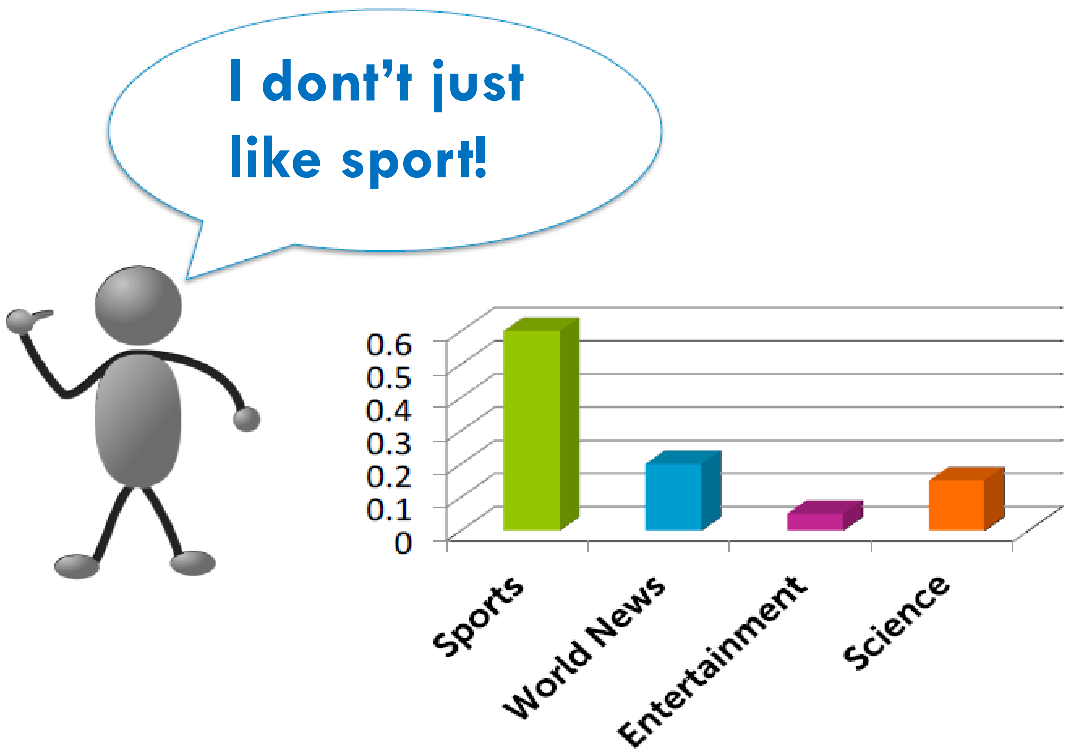
Discover groups (*clusters*) of related articles

SPORTS

WORLD NEWS

Motivation

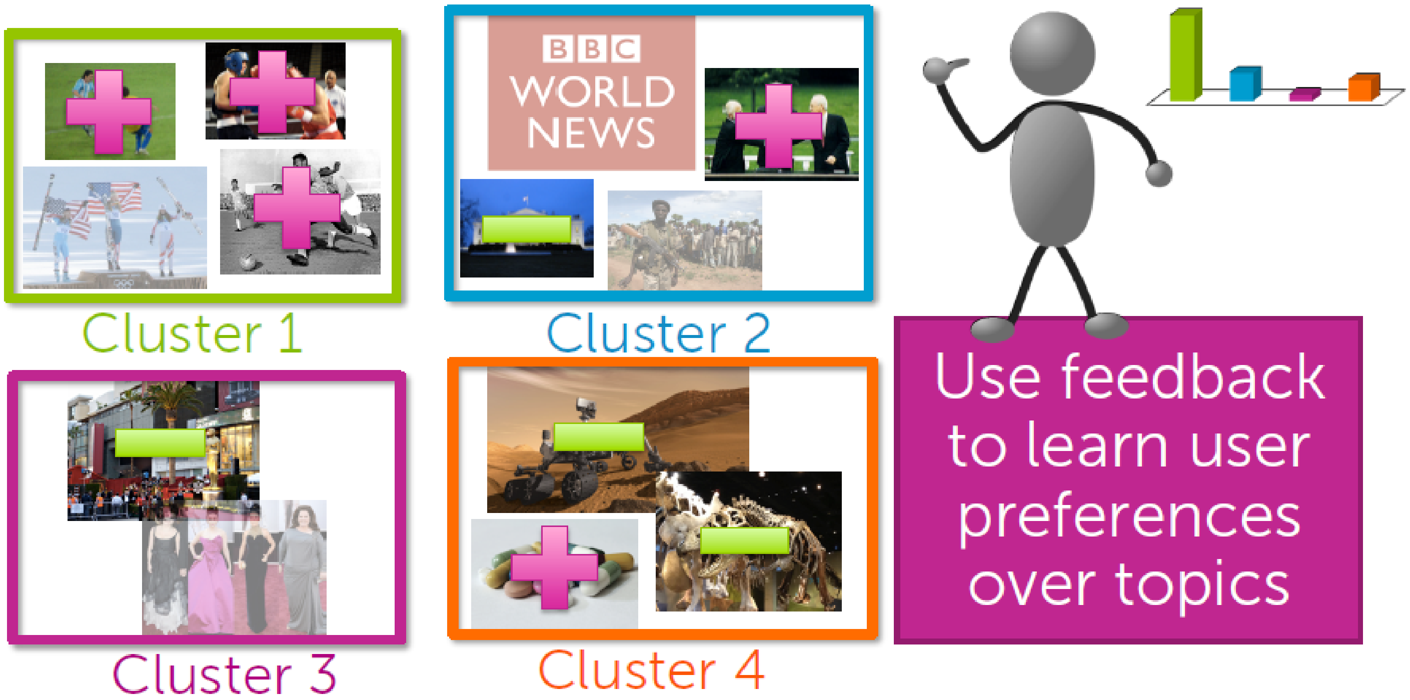
Why might clustering be useful?



Motivation

Learn user preferences

Set of clustered documents read by user



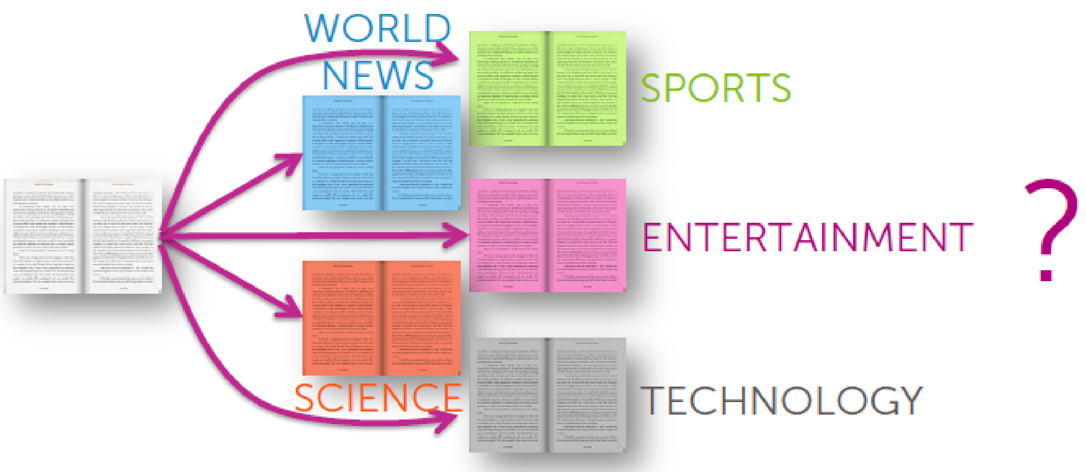
Clustering: a supervised learning

What if some of the labels are known?

Training set of labeled docs

Custering: a supervised learning

Multiclass classification problem



Example of supervised learning

Clustering: an unsupervised learning

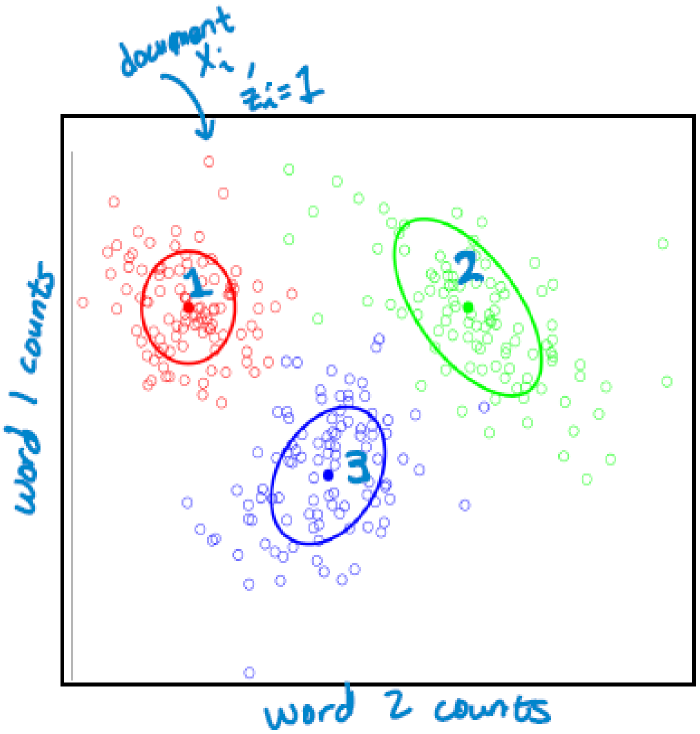
No labels provided

...uncover cluster structure from input alone

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

Output: cluster labels z_i

An unsupervised learning task



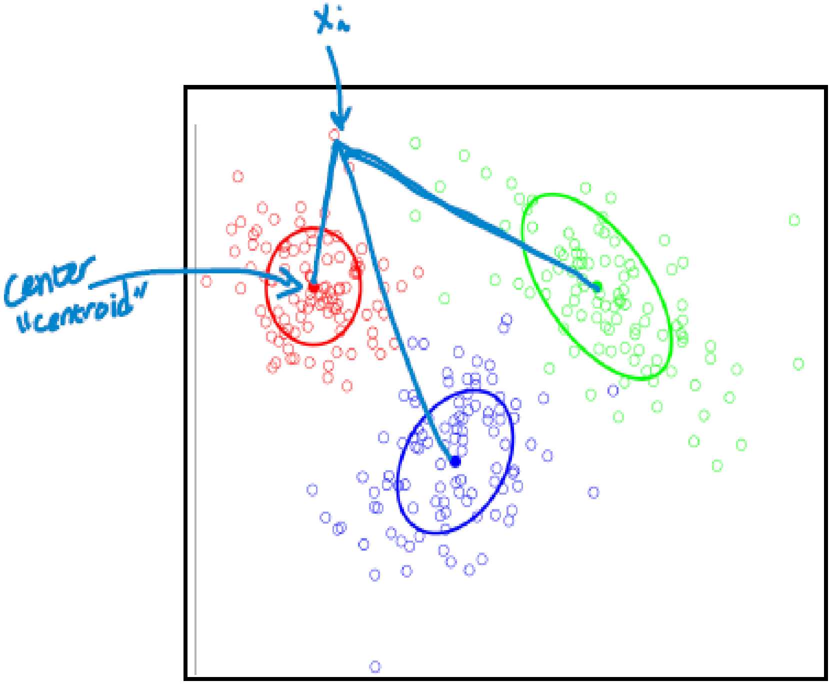
What defines a cluster ?

Cluster defined by
center & shape/spread

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

– Score under cluster k is higher than under others

– For simplicity, often define score as distance to cluster center (ignoring shape)

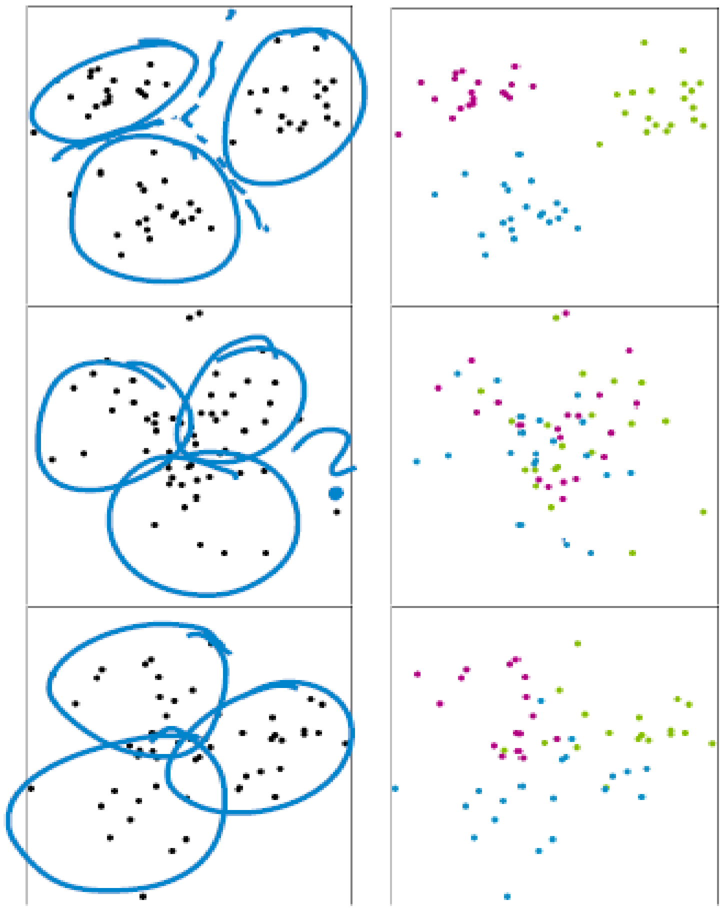


Hope for unsupervised learning

Easy

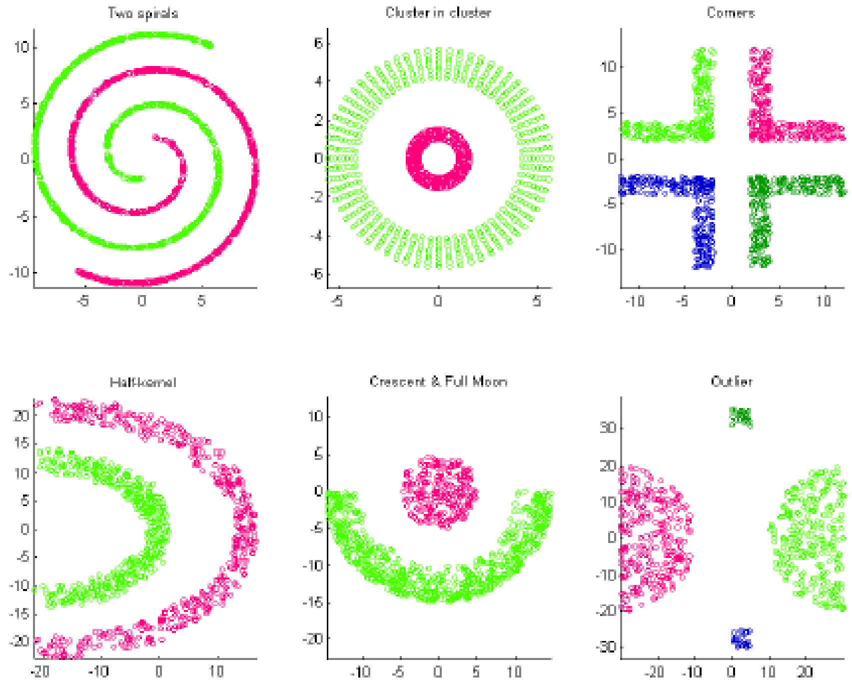
Impossible

In between



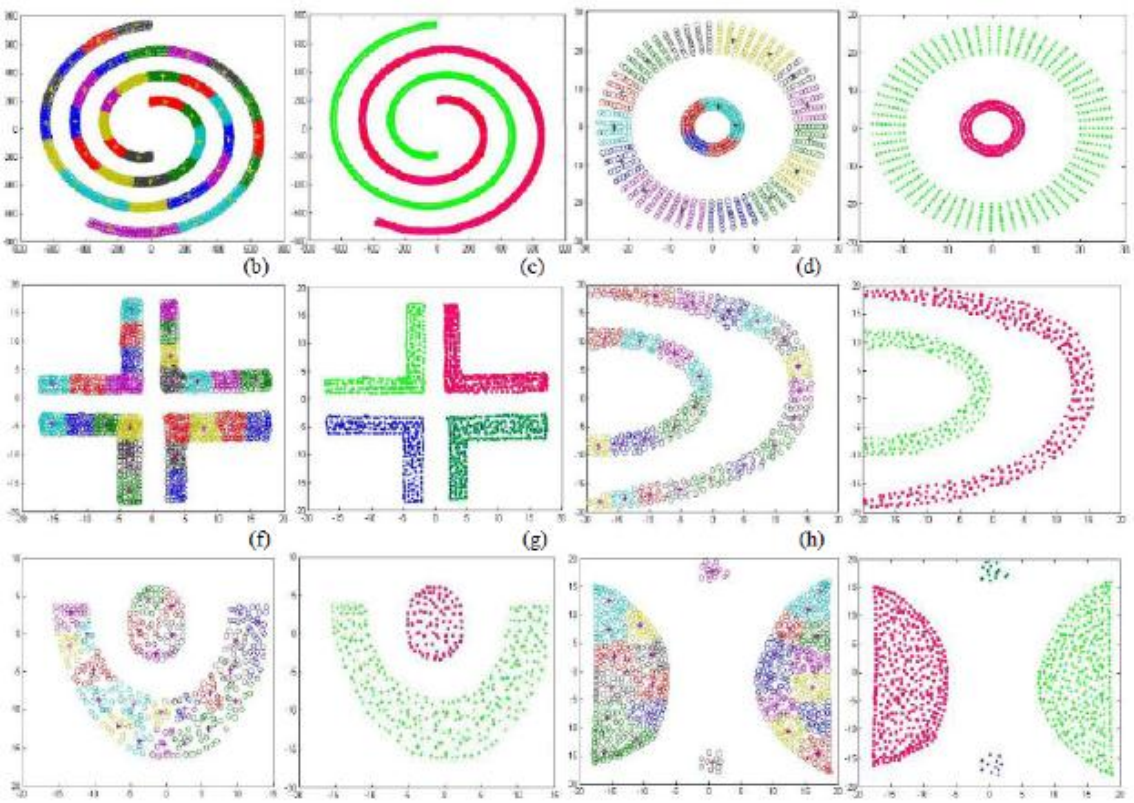
Other (challenging!) clusters to discover

Analysed by your eyes



Other (challenging!) clusters to discover

Analysed by clustering algorithms

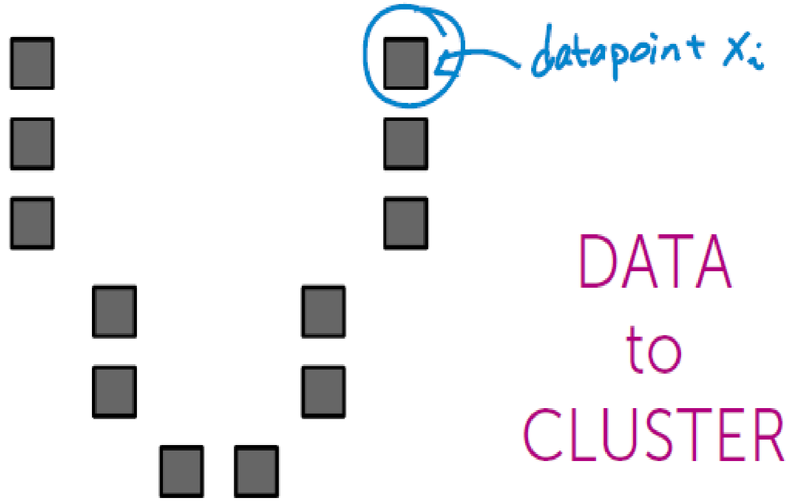


k-means clustering algorithm

k-means clustering algorithm

Assume

- Score= distance to cluster center (smaller better)

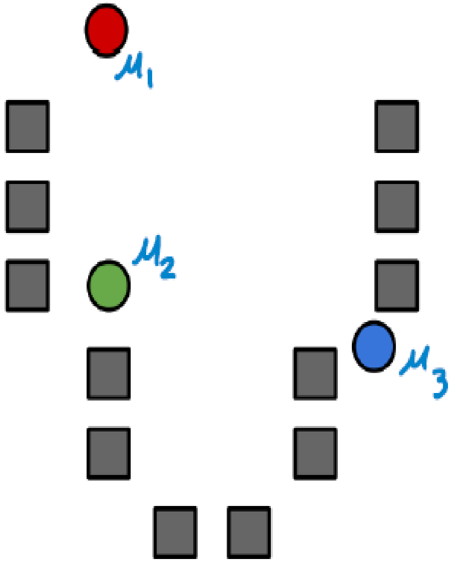


DATA
to
CLUSTER

k-means clustering algorithm

0. Initialize cluster centers

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



(k=3 clusters)

k-means clustering algorithm

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

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

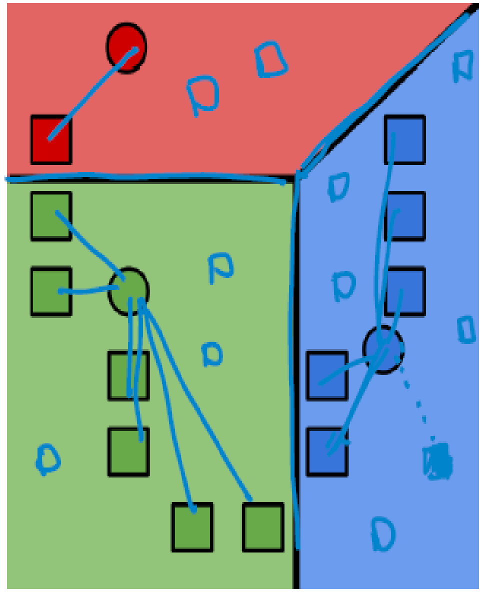
j^{th} cluster center (varying)

i^{th} obs. (fixed)

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

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

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



Voronoi tesselation

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

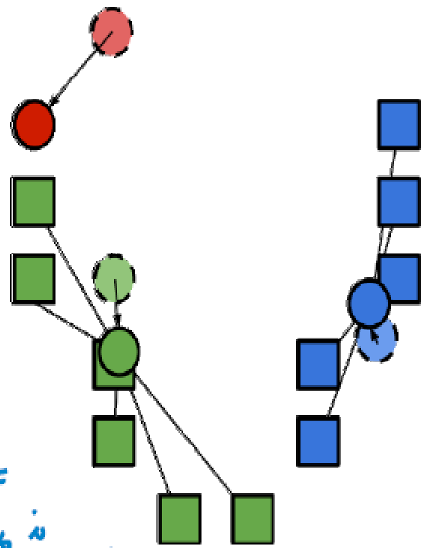
k-means clustering algorithm

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

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

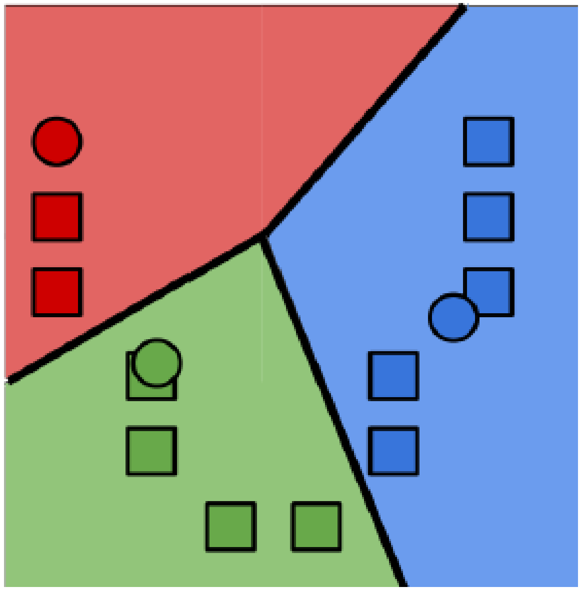
all obs. i such that $z_i = j$ (obs i is in cluster j)

# of obs. in cluster j



k-means clustering algorithm

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



K-means as coordinate descent algorithm

1. Assign observations to closest cluster center

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

2. Revise cluster centers as mean of assigned observations

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

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

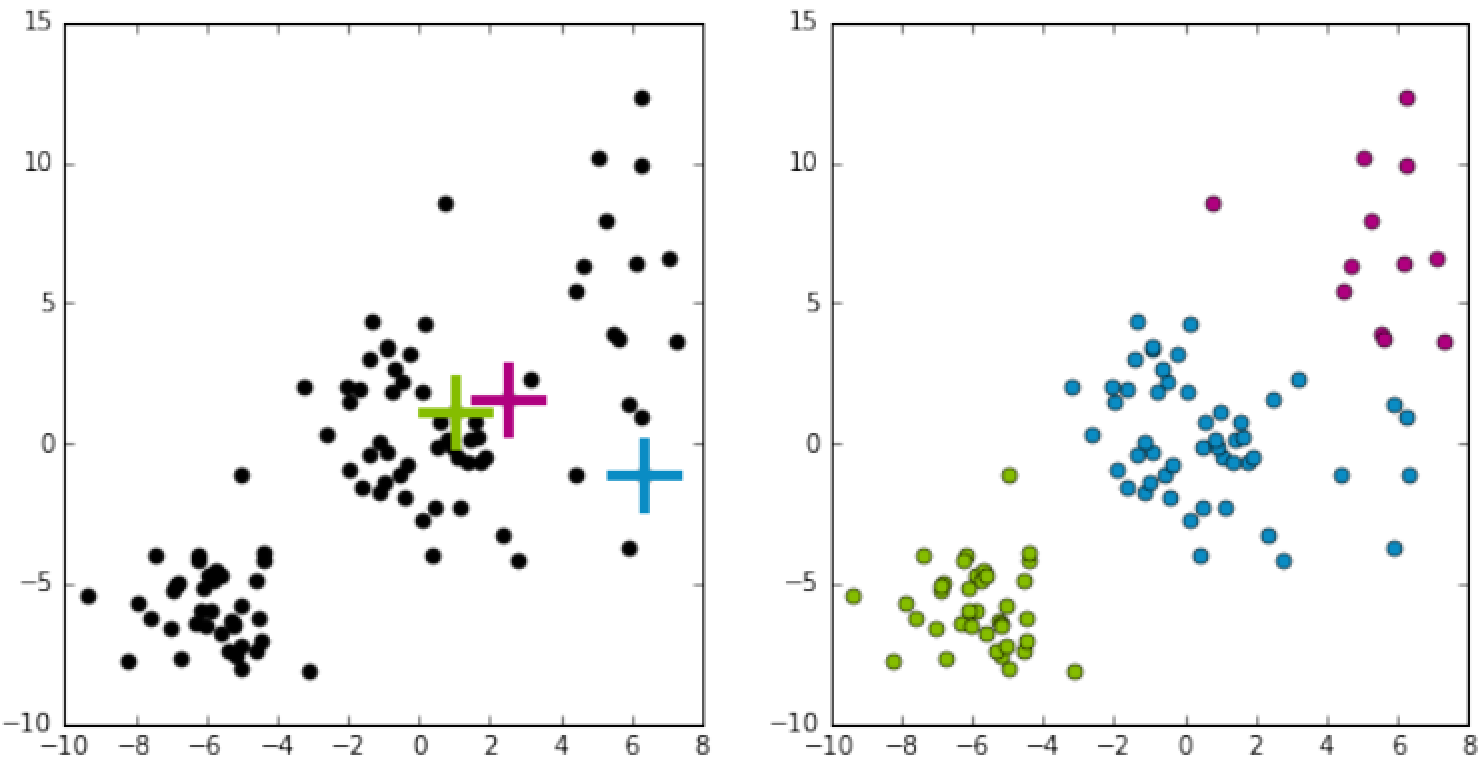
Convergence of k-means

Converges to:

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

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

Convergence of k-mans to local mode



Crosses: initialised centers

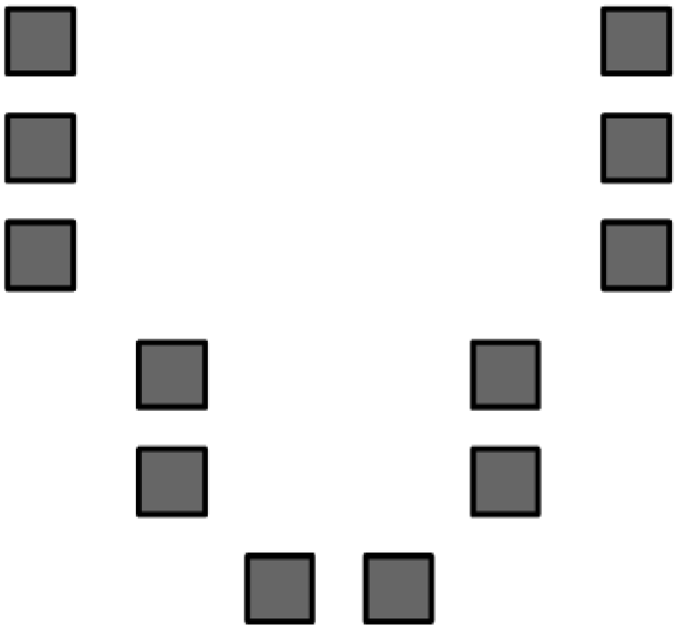
Smart initialisation: k-means++ overwiew

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

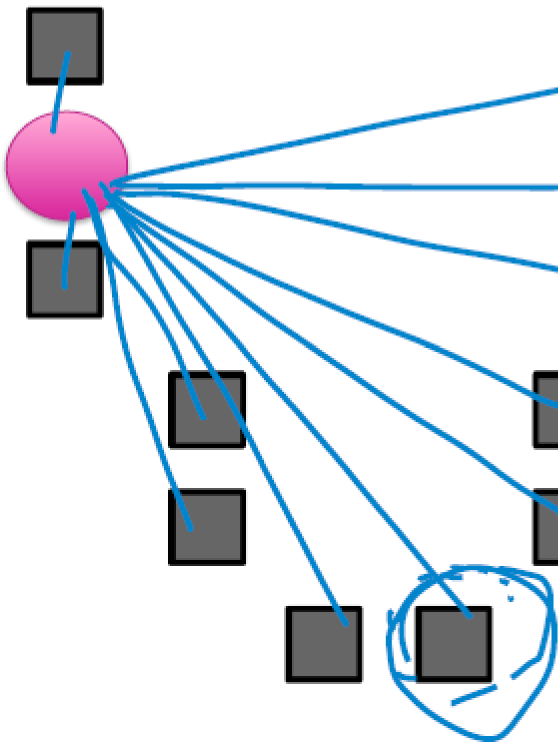
Smart initialization:

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

k-means++ visualised

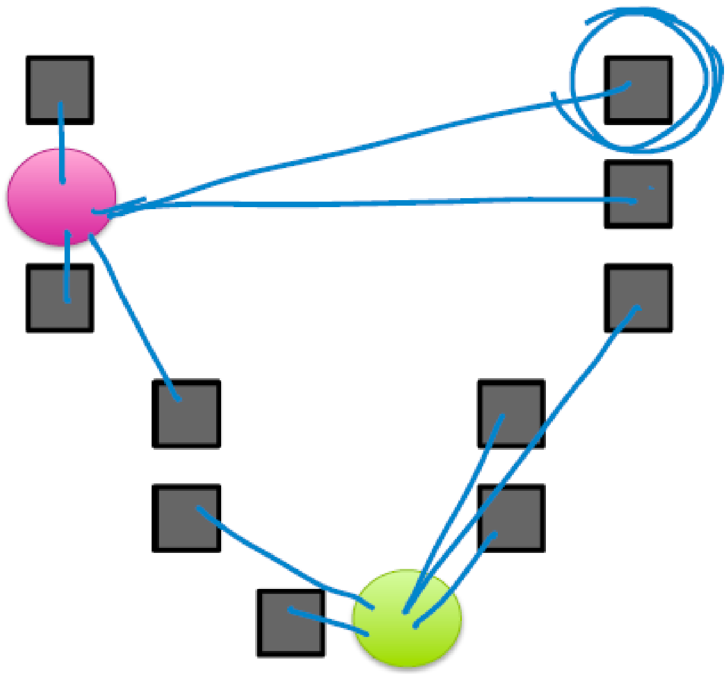


k-means++ visualised

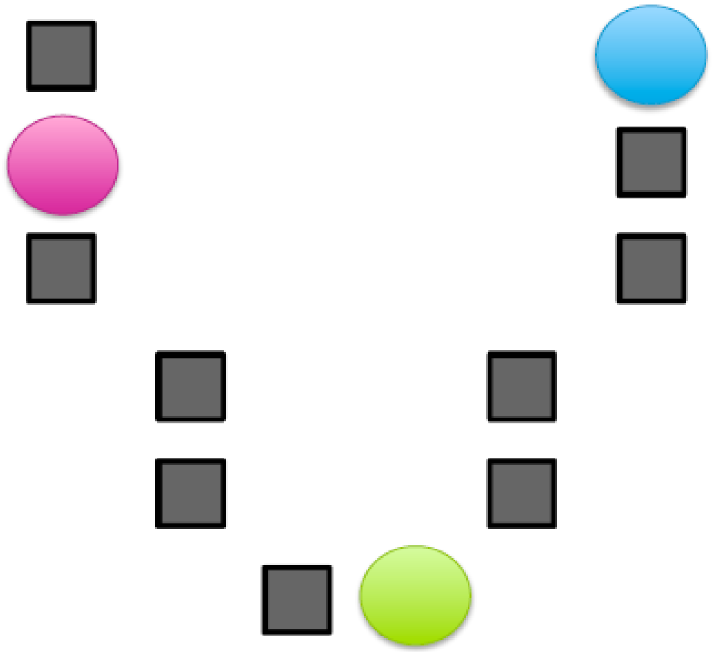


more likely to select a datapoint as a cluster center if that datapoint is far away (dist^2 increases this effect)

k-means++ visualised



k-means++ visualised



Smart initialisation: k-means++ overwiew

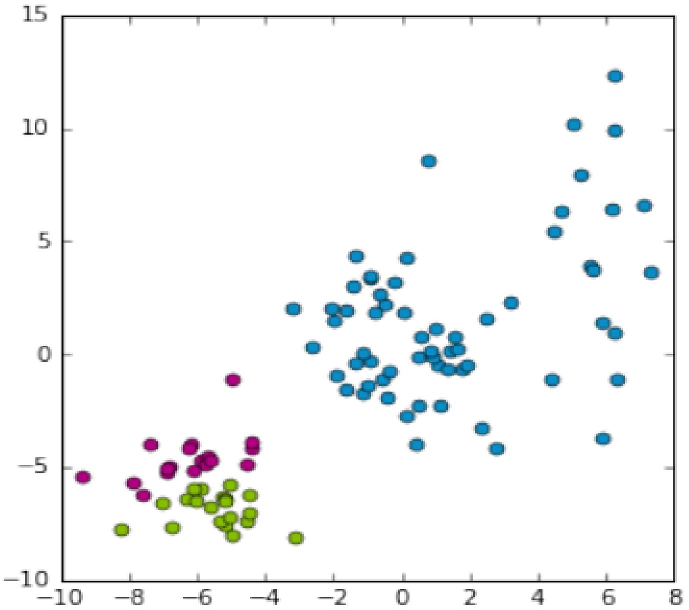
k-means++ pros/cons

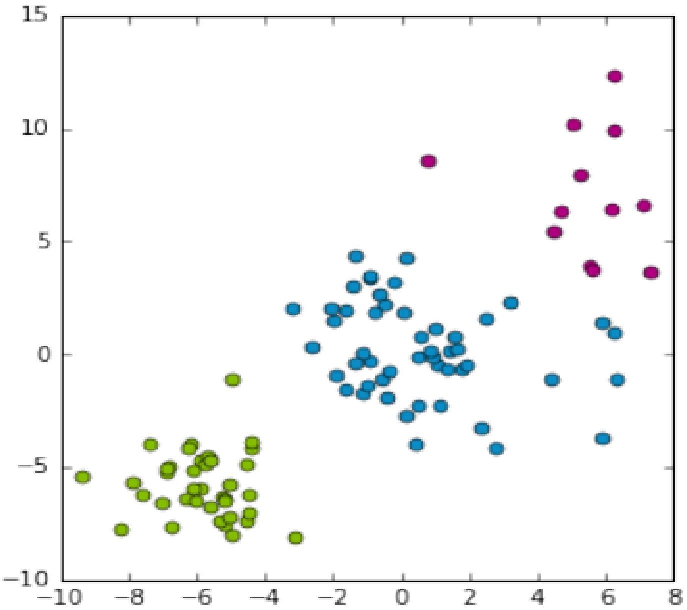
Computationally costly relative to random initialization, but the subsequent k-means often converges more rapidly

Tends to improve quality of local optimum and lower runtime

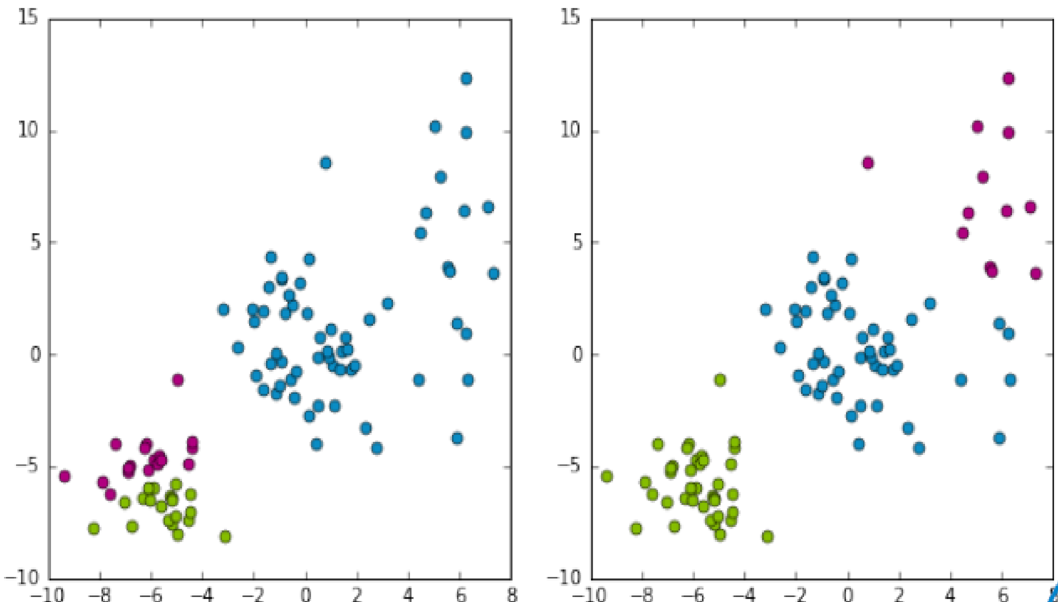
Assessing quality of the clustering

Which clustering do I prefer?





K-means objective



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

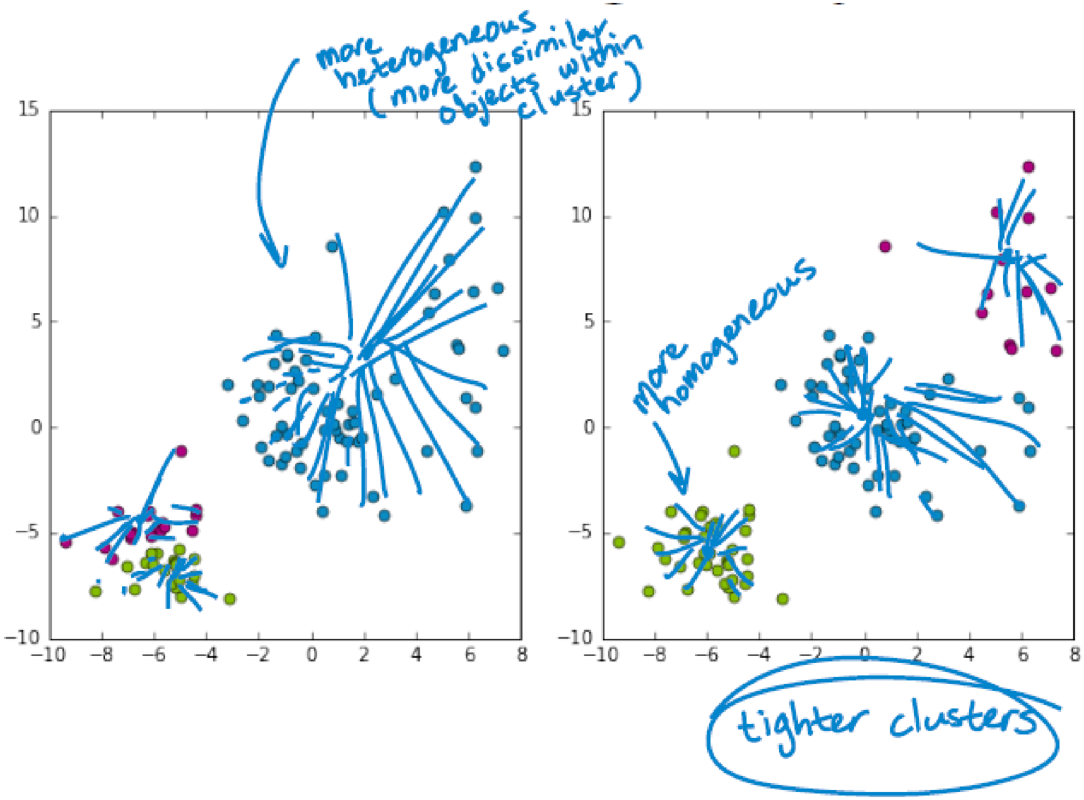
sum over all clusters

sum of squared distances in cluster j

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

$\min_{\{z_i\},\{\mu_j\}}$

Cluster heterogeneity



Measure of quality of given clustering:

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

Lower is better!

What happens to heterogeneity as k increases?

Can refine clusters more and more to the data

→ overfitting!

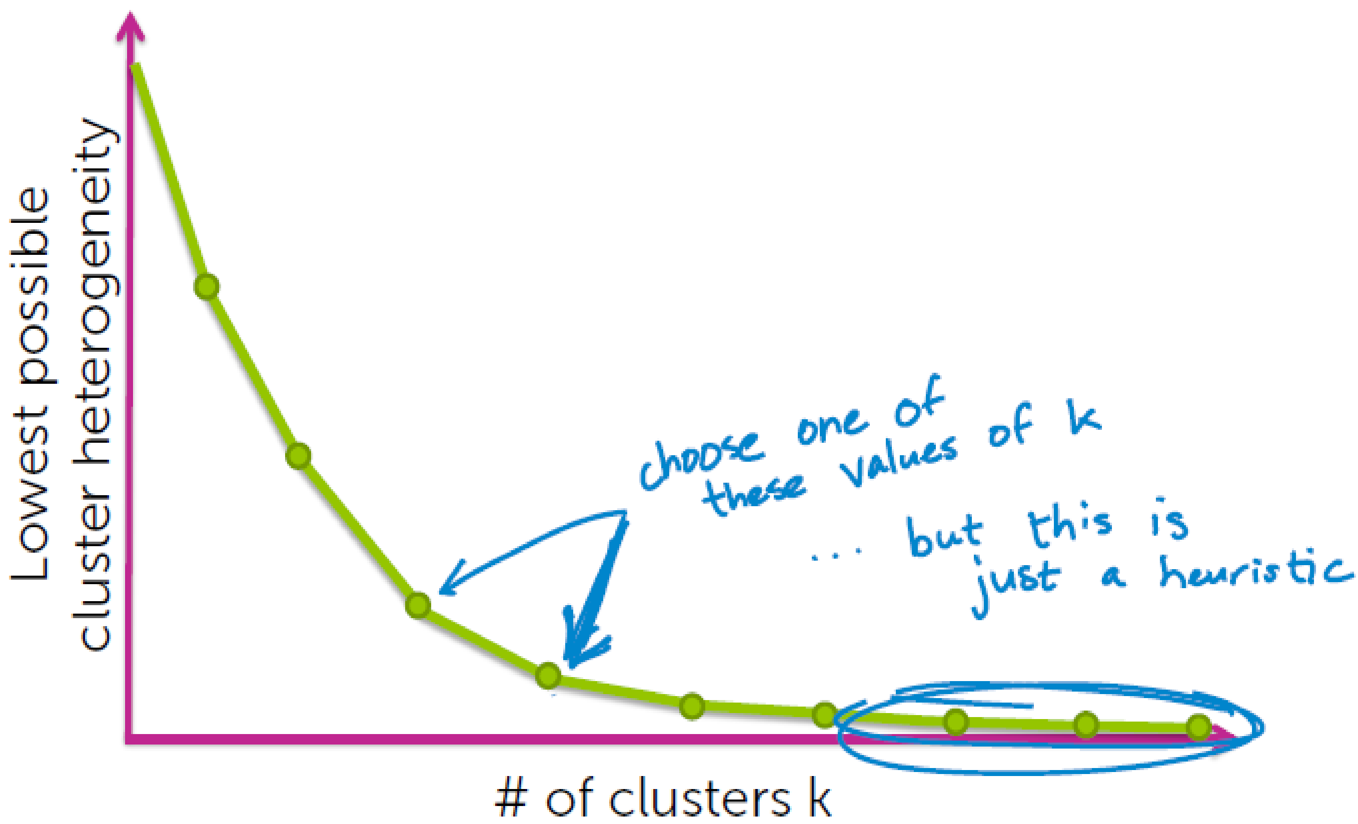
Extreme case of k=N: # of observations

– can set each cluster center equal to datapoint

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

Lowest possible cluster heterogeneity decreases with increasing k

How to choose k?

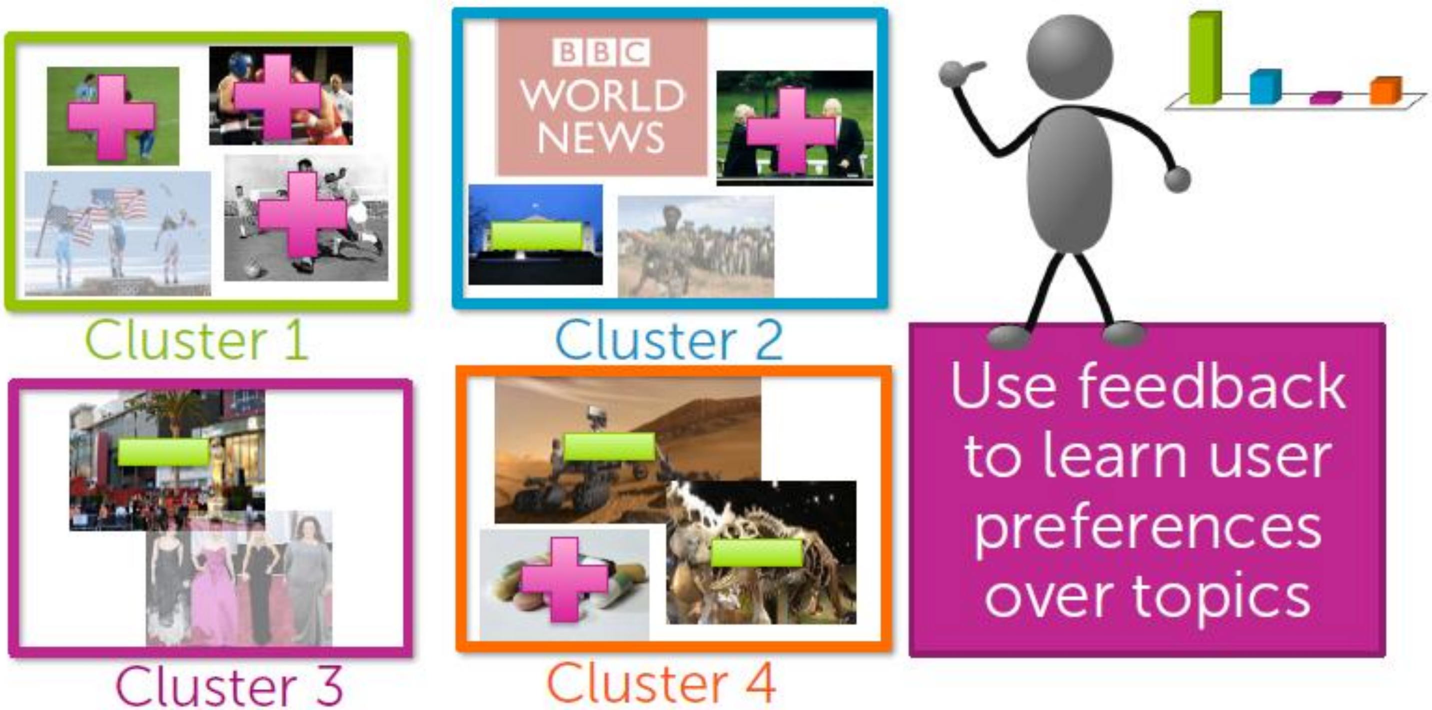


Probabilistic approach: mixture model

Why probabilistic approach?

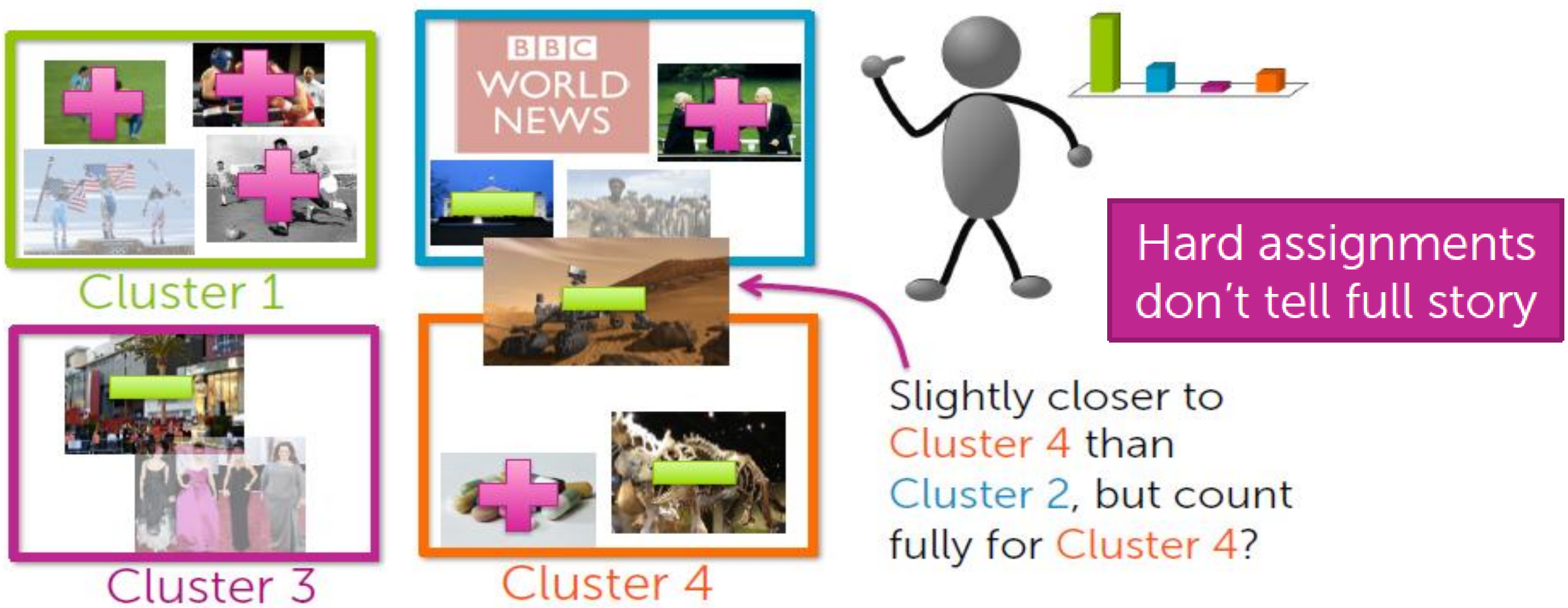
Learn user preferences

Set of clustered documents read by user



Why probabilistic approach?

Uncertainty in cluster assignments



Why probabilistic approach?

Other limitations of k-means

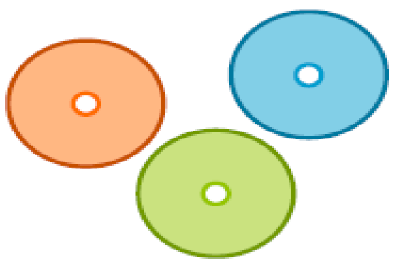
Assign observations to closest cluster center

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

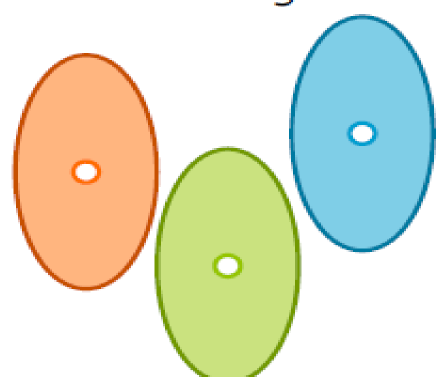
Can use weighted Euclidean, but requires *known* weights

Only center matters

Equivalent to assuming spherically symmetric clusters

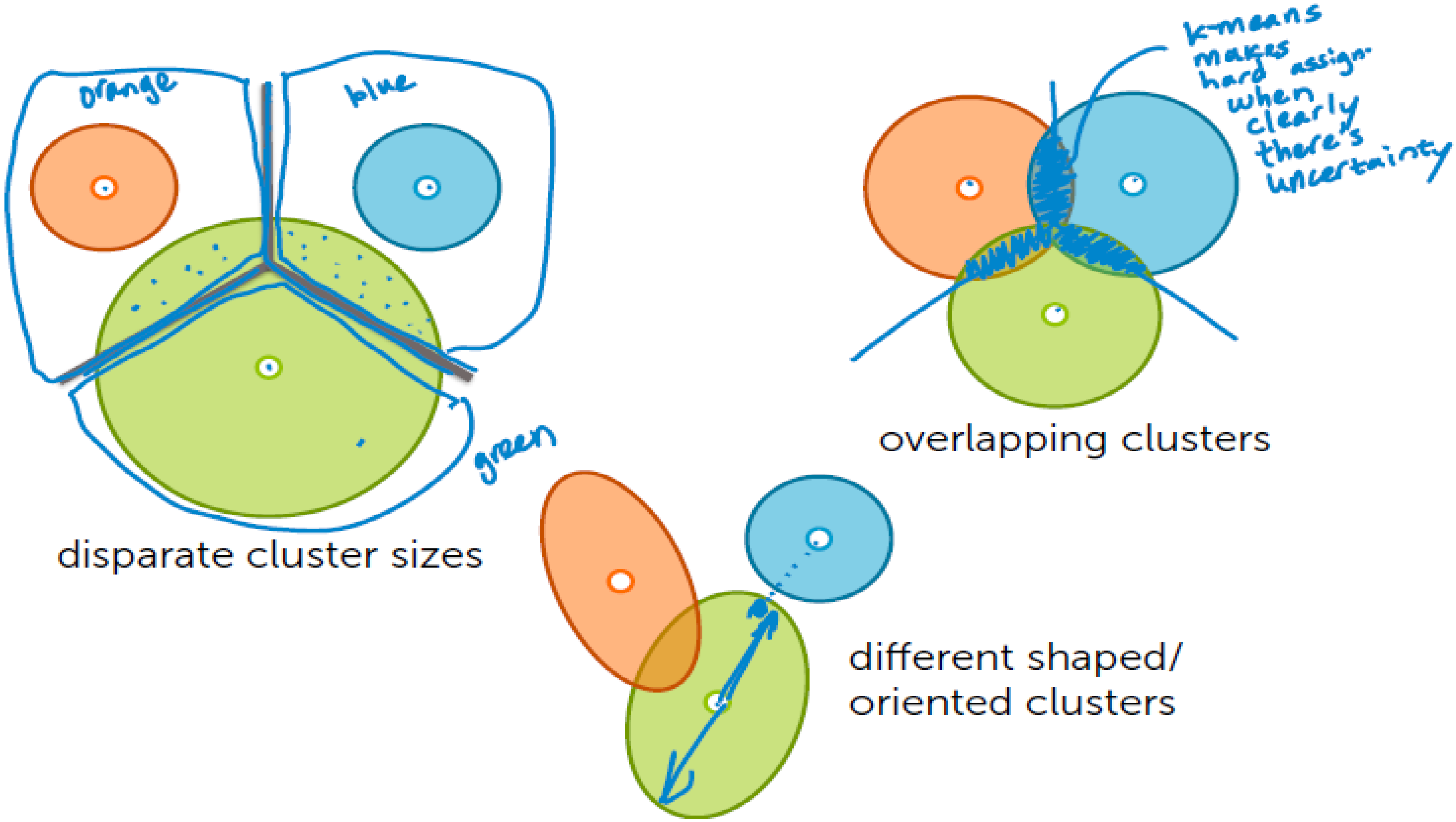


Still assumes all clusters have the same axis-aligned ellipses



Why probabilistic approach?

Failure modes of k-means



Mixture models

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

Application: clustering images

Discover groups of similar images

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

Application: clustering images

Simple image representation

Consider average red, green, blue pixel intensities

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

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

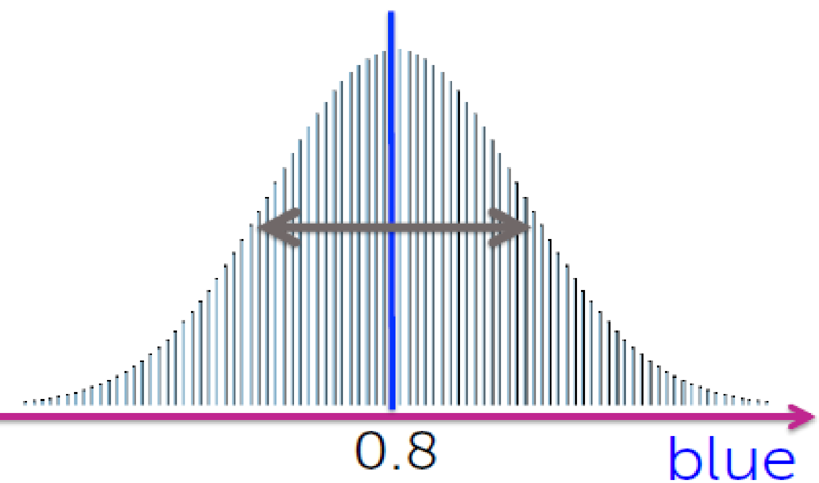
[R = 0.02, G = 0.95, B = 0.4]

Single RGB vector per image

Application: clustering images

Distribution over all cloud images

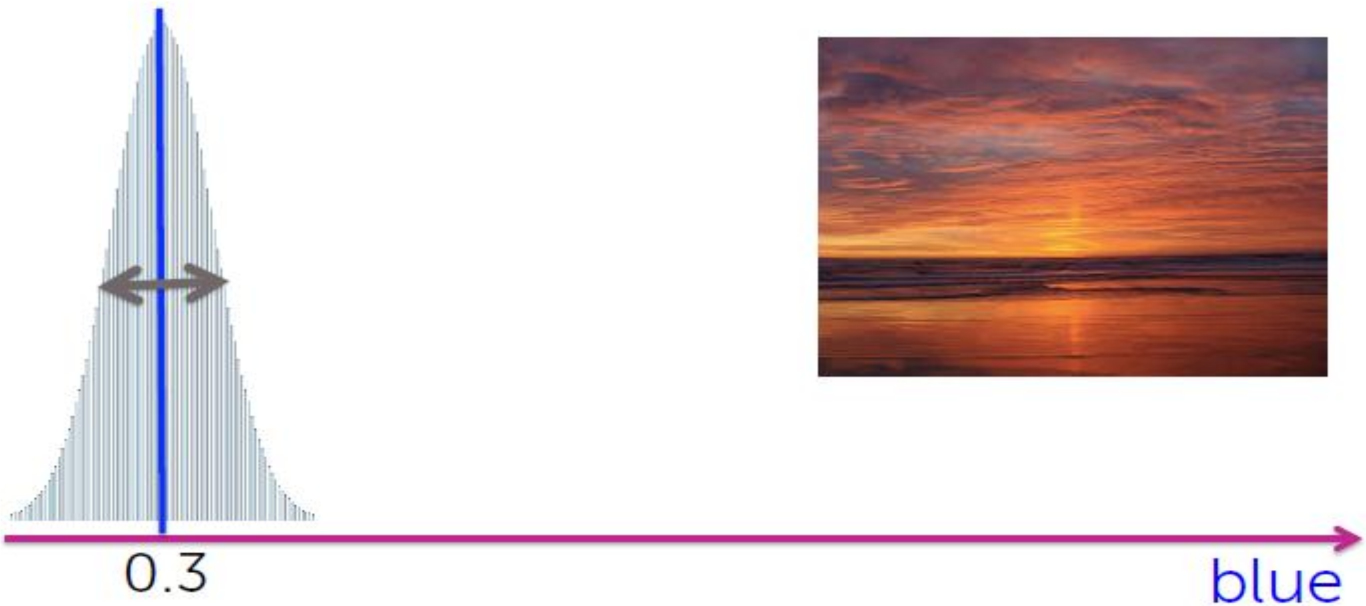
Let's look at just the blue dimension



Application: clustering images

Distribution over all sunset images

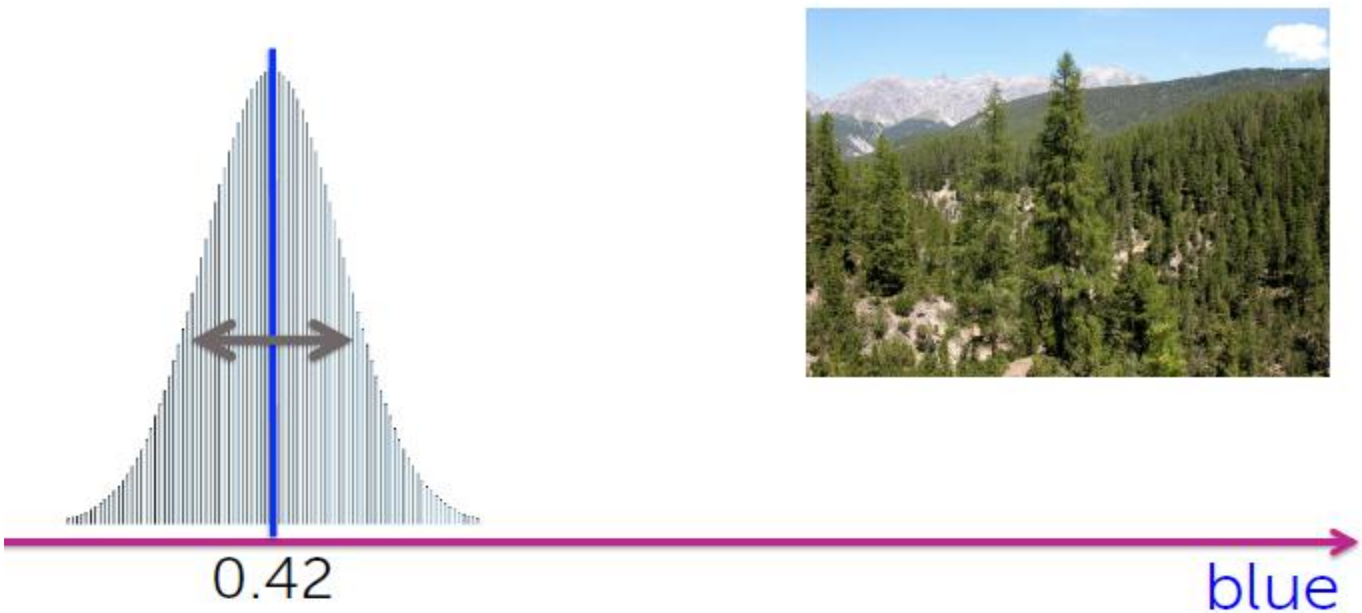
Let's look at just the blue dimension



Application: clustering images

Distribution over all forest images

Let's look at just the blue dimension



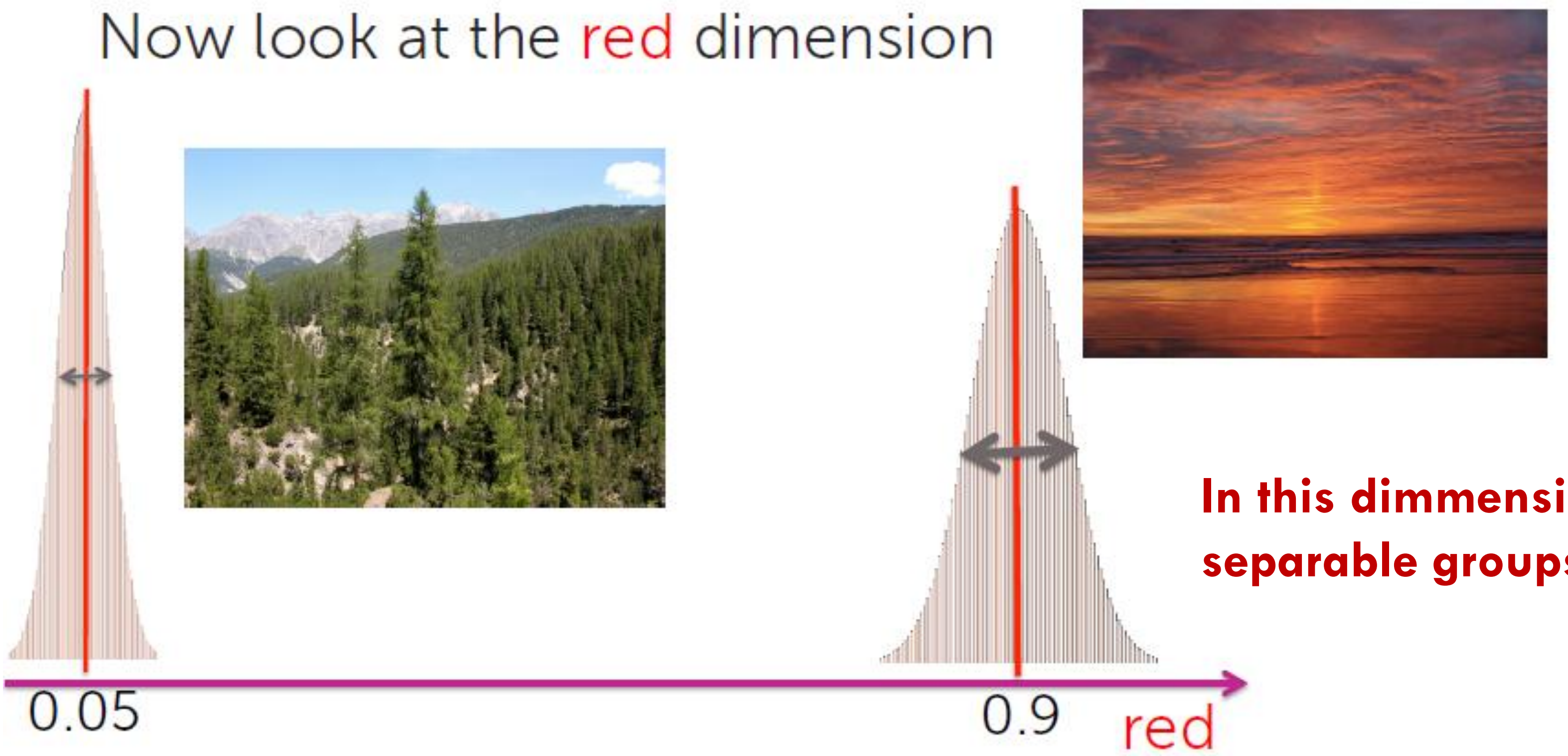
Application: clustering images

Distribution over all images

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

Application: clustering images

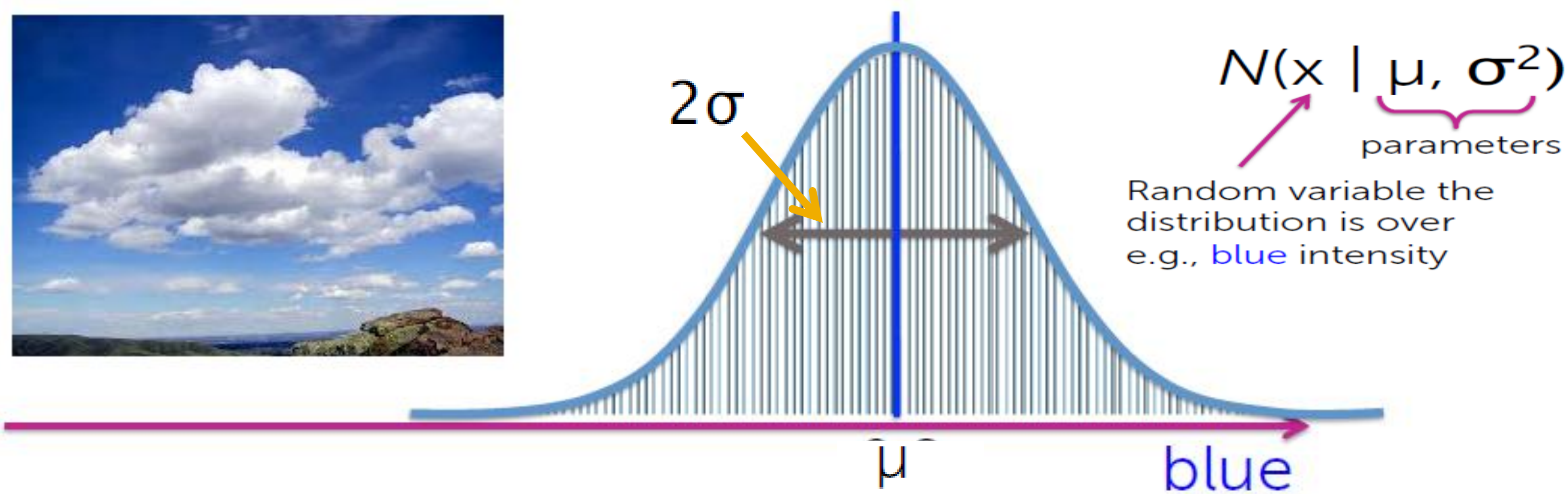
Can be distinguished along other dim



In this dimmension separable groups!

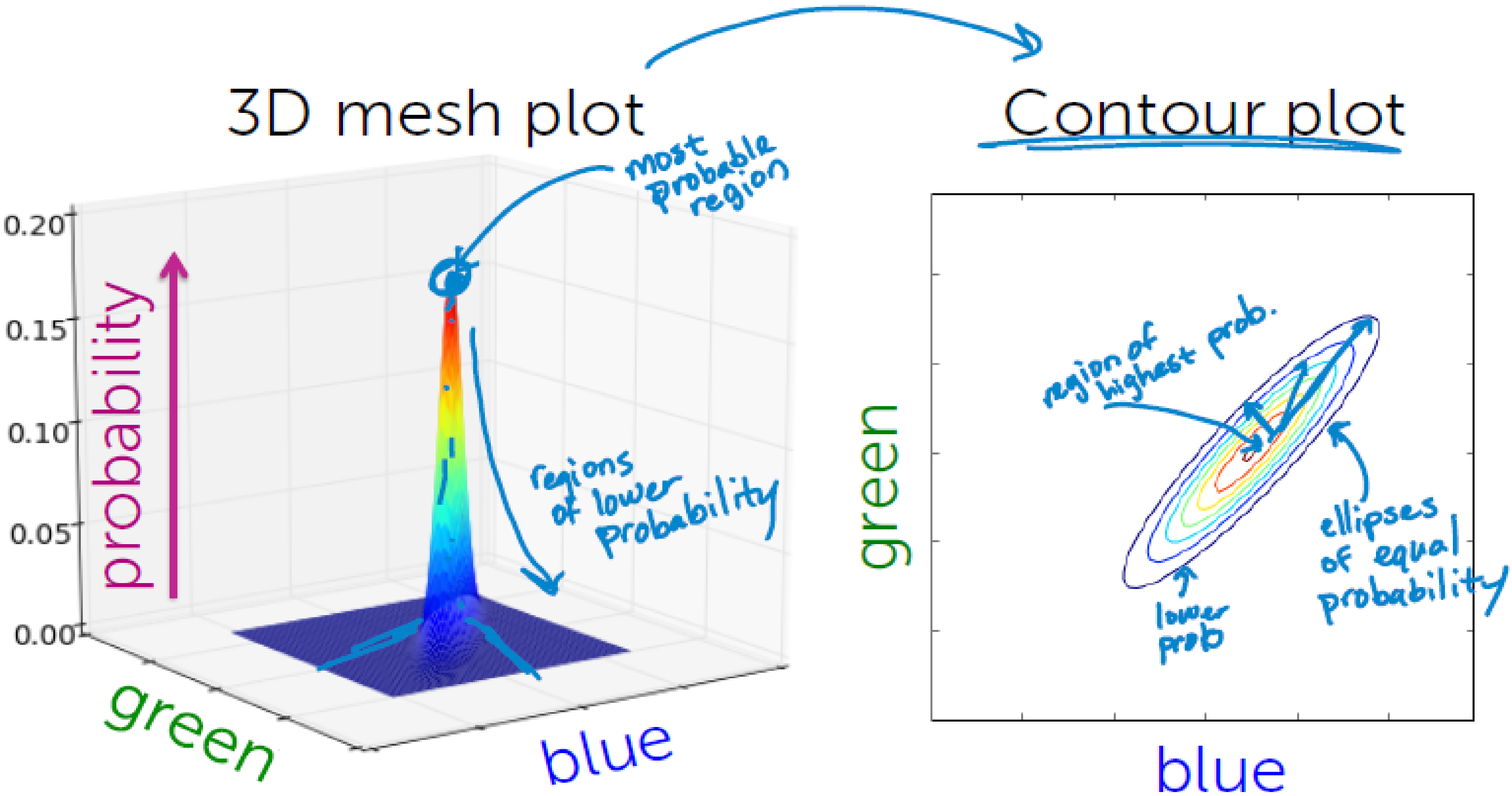
Model for a given image type

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



Model for a given image type

2D Gaussians – Bird's eye view



Application: clustering images

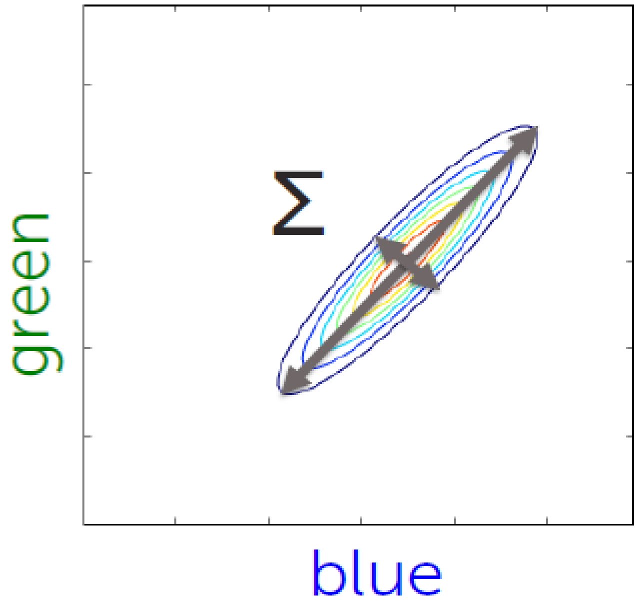
2D Gaussians – Parameters

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

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

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

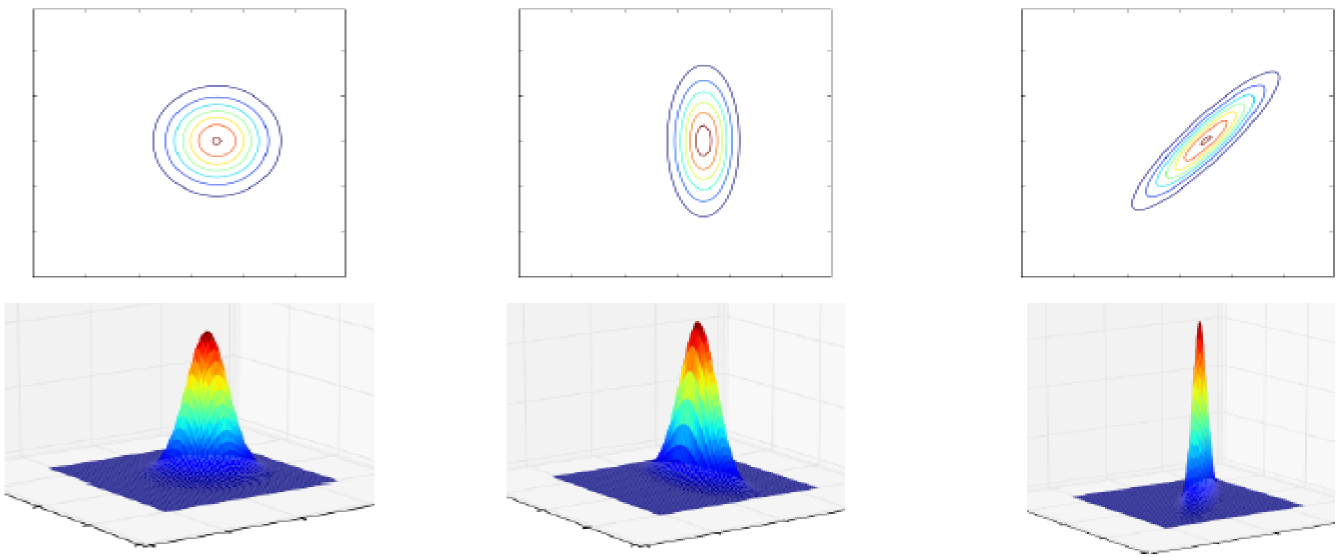
covariance determines
orientation + spread



Application: clustering images

Covariance structures

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

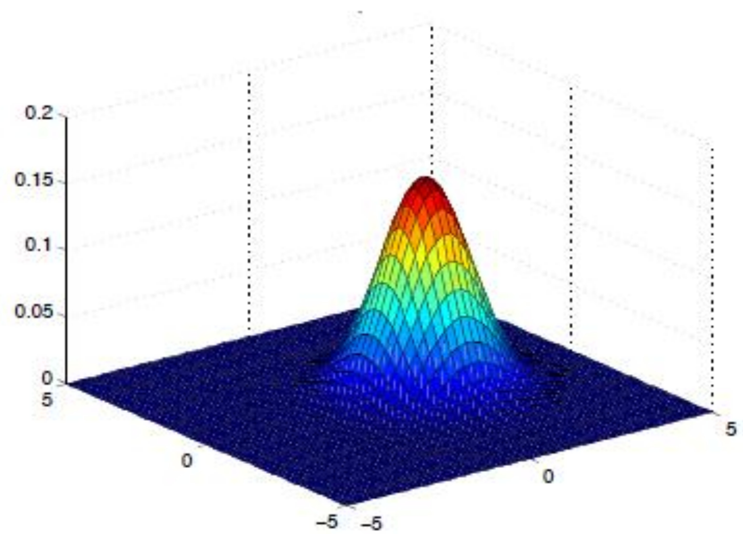


Application: clustering images

Notating a multivariate Gaussian

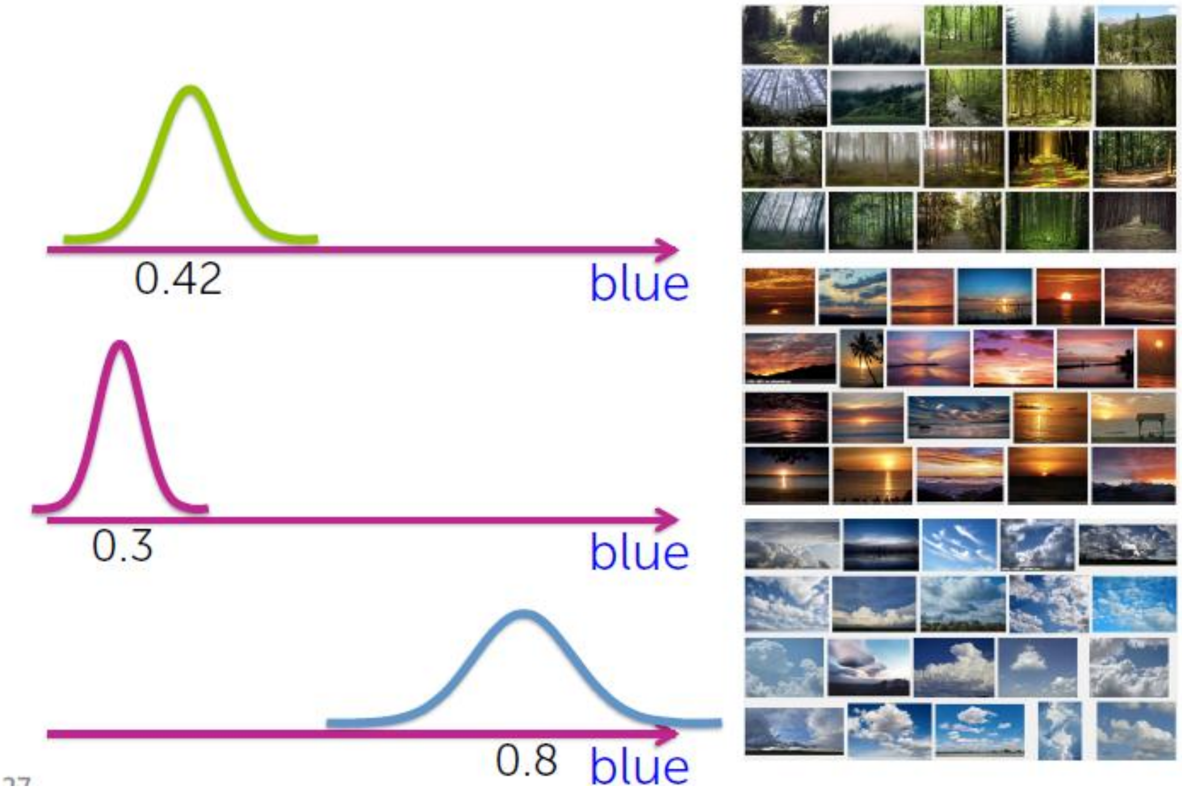
$$\mathcal{N}(\mathbf{x} \mid \underbrace{\boldsymbol{\mu}, \Sigma}_{\text{parameters}})$$

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



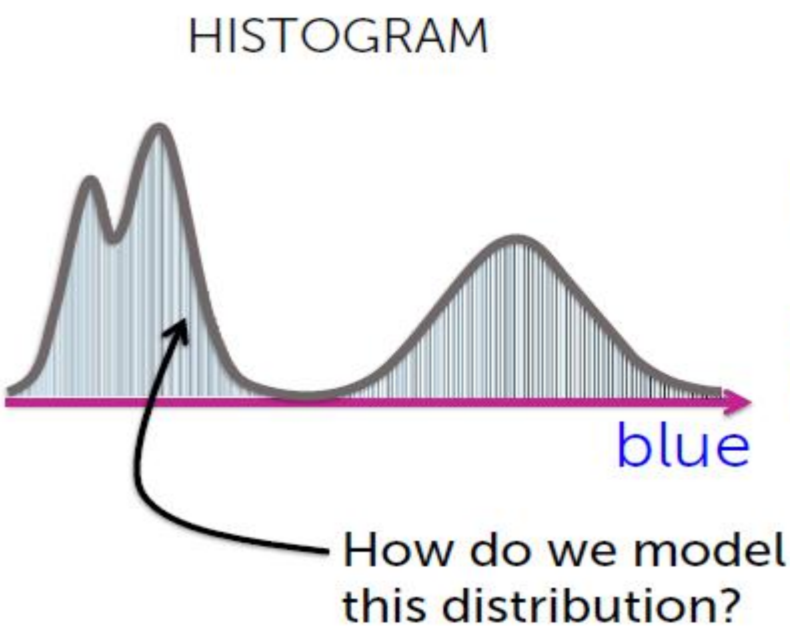
Mixture of Gaussians

Model as Gaussian per category/cluster



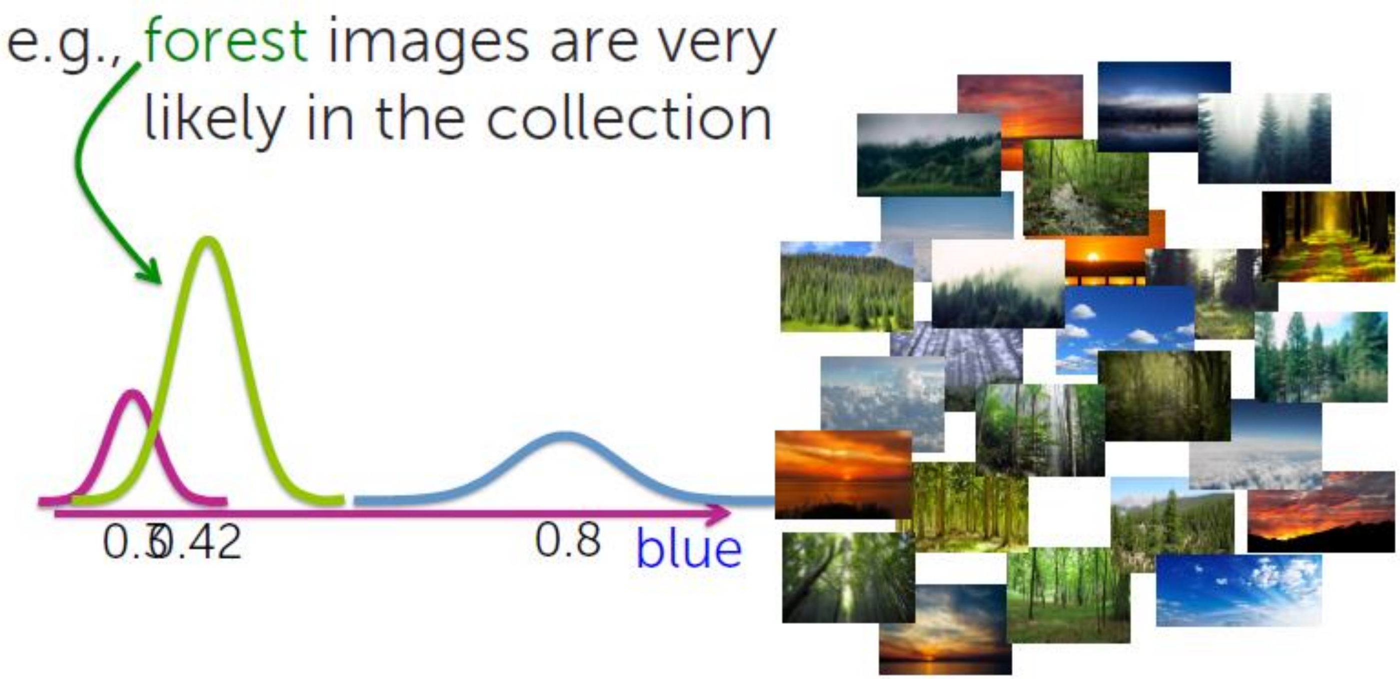
Mixture of Gaussians

Jumble of unlabeled images



Mixture of Gaussians

What if image types not equally represented?



Mixture of Gaussians

Combination of weighted Gaussians

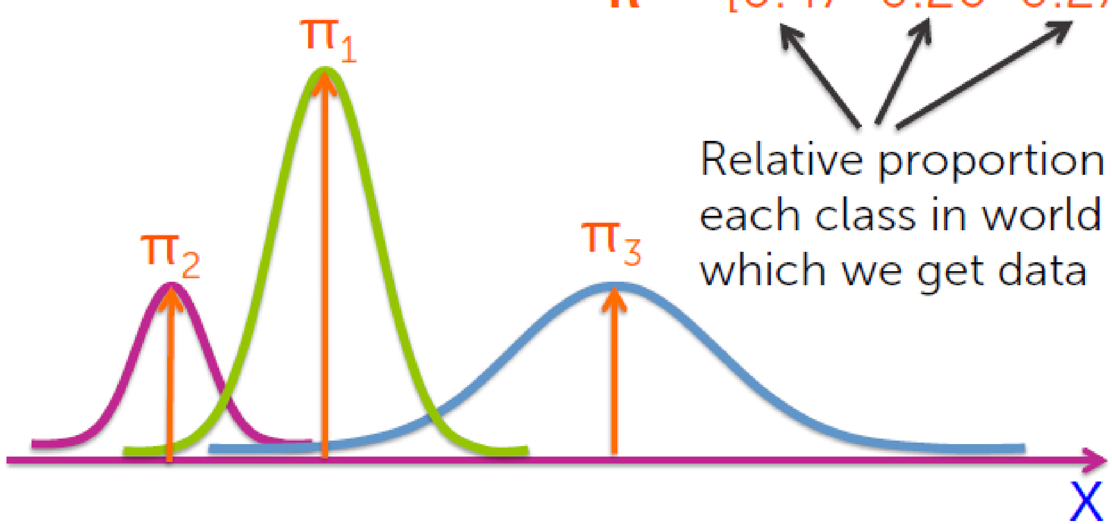
Associate a weight π_k with each Gaussian component

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

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

$$\pi = [\underset{\pi_1}{0.47} \;\; \underset{\pi_2}{0.26} \;\; \underset{\pi_3}{0.27}]$$

Relative proportion of each class in world from which we get data

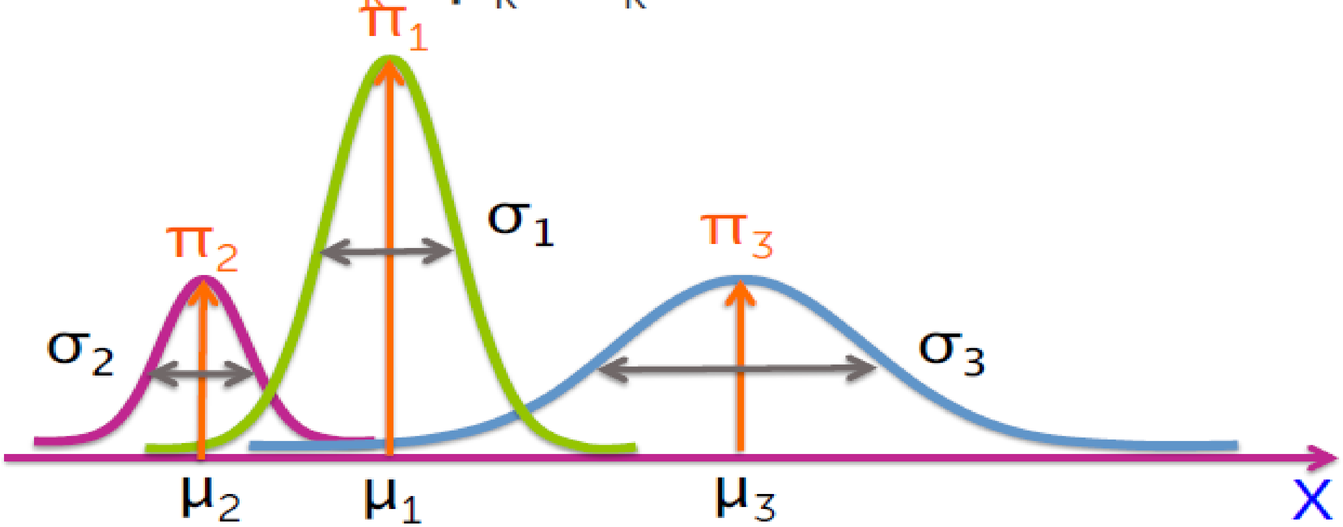


Mixture of Gaussians

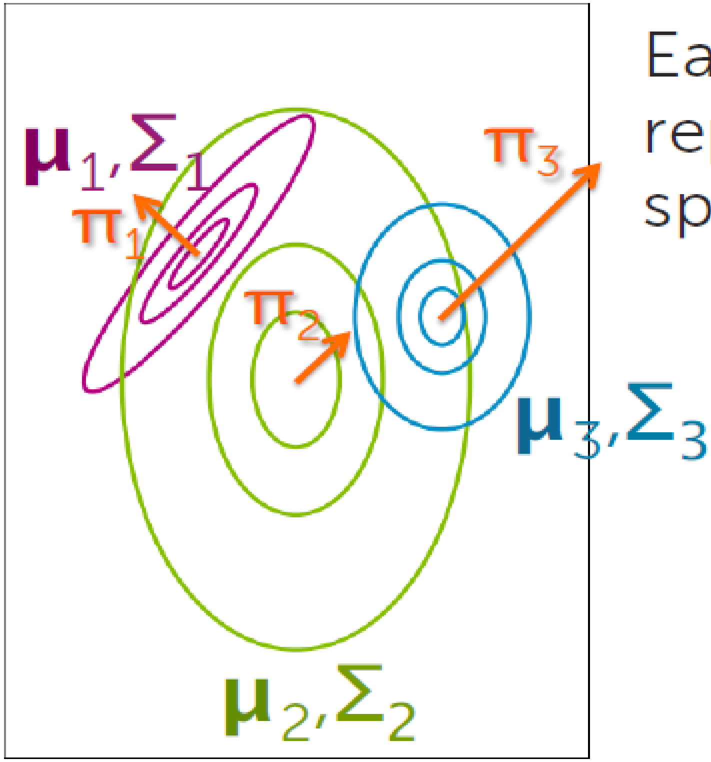
Mixture of Gaussians (1D)

Each mixture component represents a unique cluster specified by:

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



Mixture of Gaussians (general)



Each mixture component represents a unique cluster specified by:

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

Mixture of Gaussians

According to the model…

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

cluster assignment for obs. x_i

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

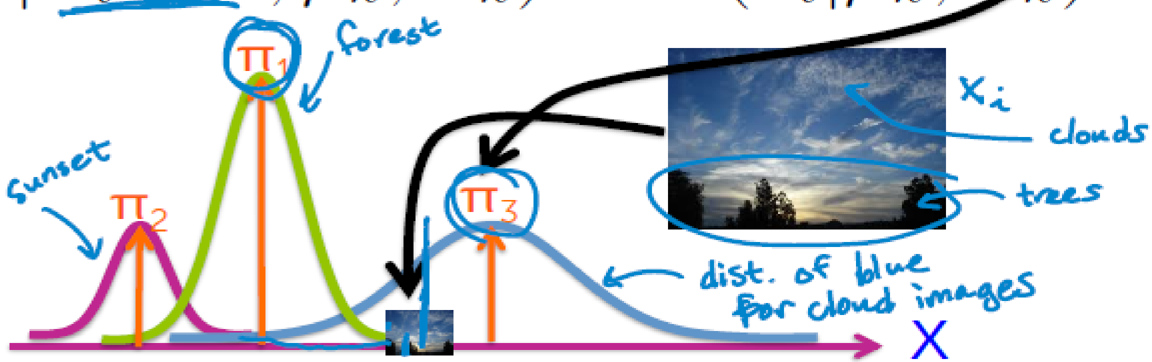
prior

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

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

likelihood

$[RGB]_i$



Application: clustering documents

Discover groups of related documents

Application: clustering documents

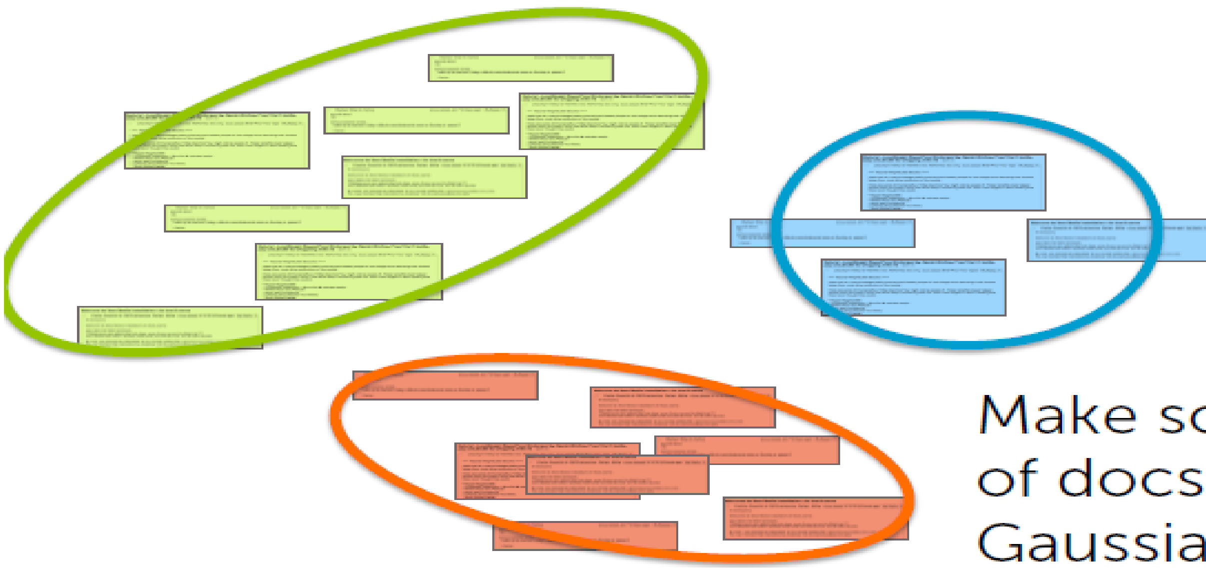
Document representation

$\mathbf{x}_i$ = tf-idf vector

Application: clustering documents

Mixture of Gaussians for clustering documents

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

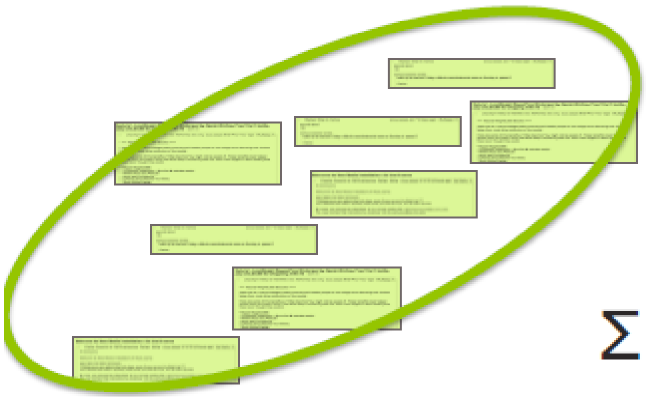


Make soft assignments of docs to each Gaussian

Application: clustering documents

Counting parameters

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



In 2D:

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

Application: clustering documents

Counting parameters

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

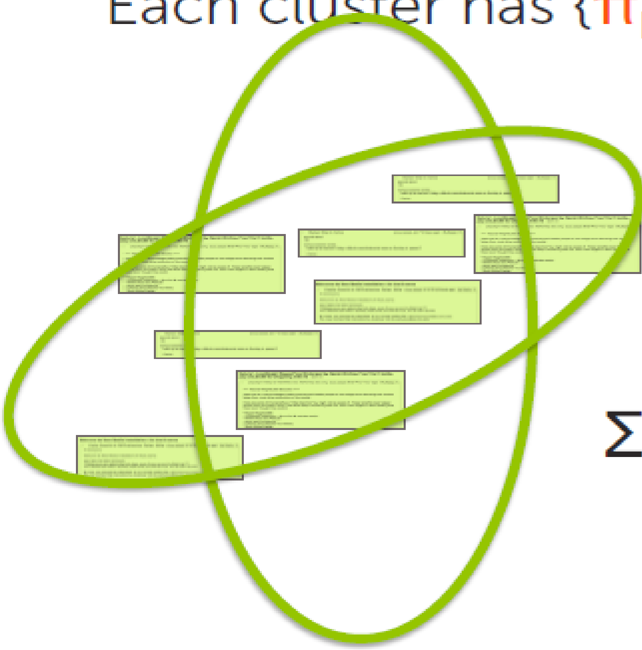
In V (vocab size) dims:

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

Application: clustering documents

Restricting to diagonal covariance

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

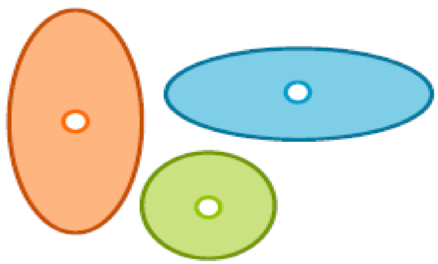


V params

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

Application: clustering documents

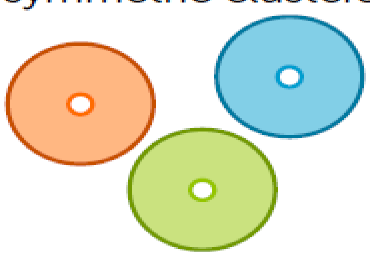
Restrictive assumption, but...



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

Still more flexible than k-means

Spherically symmetric clusters



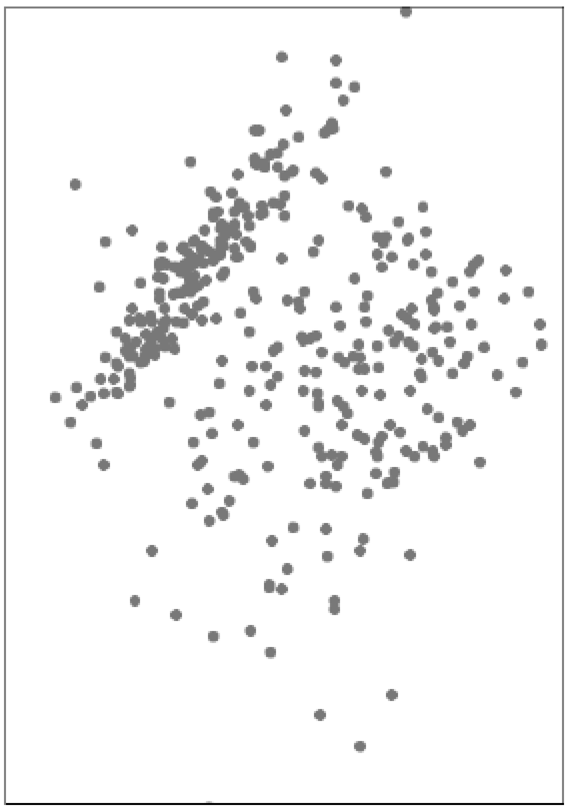
Specify weights...

All clusters have same axis-aligned ellipses

Inferring soft assignments with expectation maximization (EM)

Inferring cluster labels

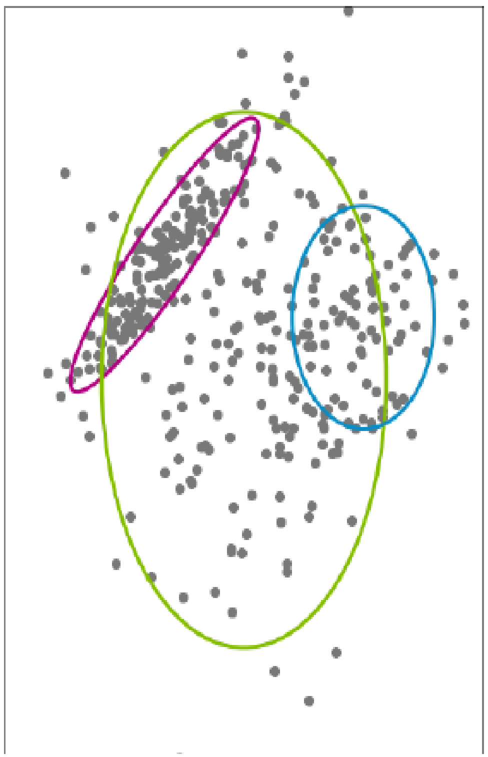
Data



Desired soft assignments

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

Compute responsibilities



$r_i = [r_{i1} \; r_{i2} \; .... \; r_{iK}]$

clusters

fixed values defining the distribution

Responsibility cluster k takes for observation i

"given"

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

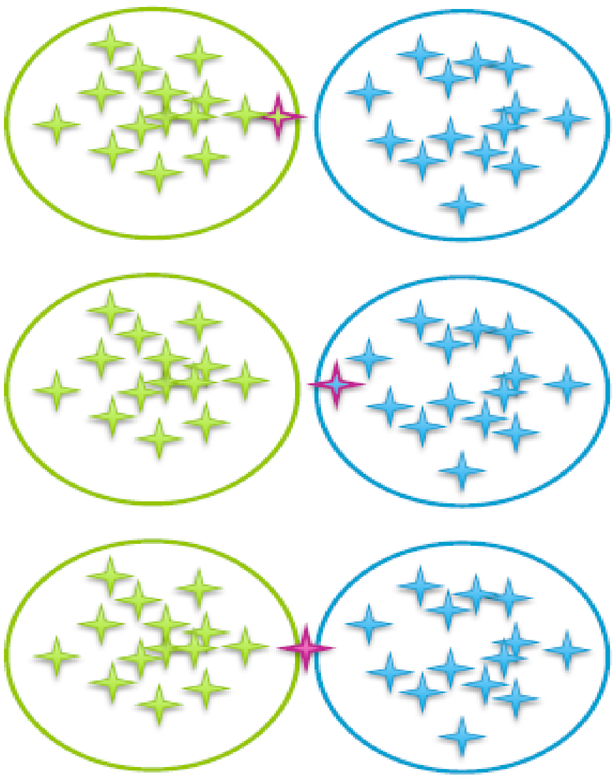
random variable

probability of assignment to cluster k

given model parameters and observed value

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

Responsibilities in pictures



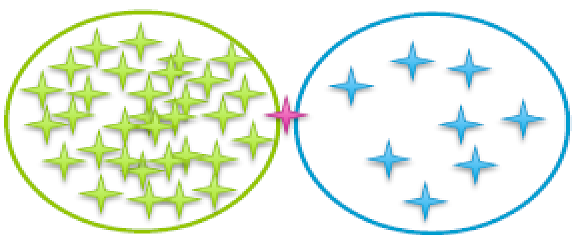
Green cluster takes more responsibility

Blue cluster takes more responsibility

Uncertain... split responsibility

Responsibilities in pictures

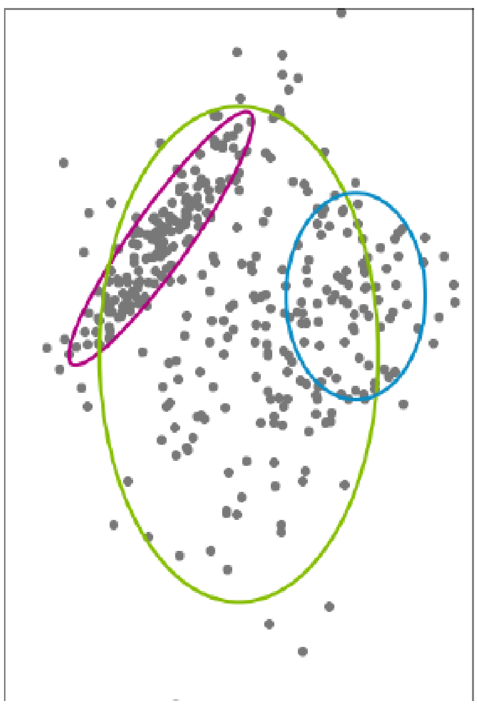
Need to weight by cluster probabilities, not just cluster shapes



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

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

Responsibilities in equations

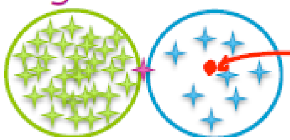


Responsibility cluster k takes for observation i

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

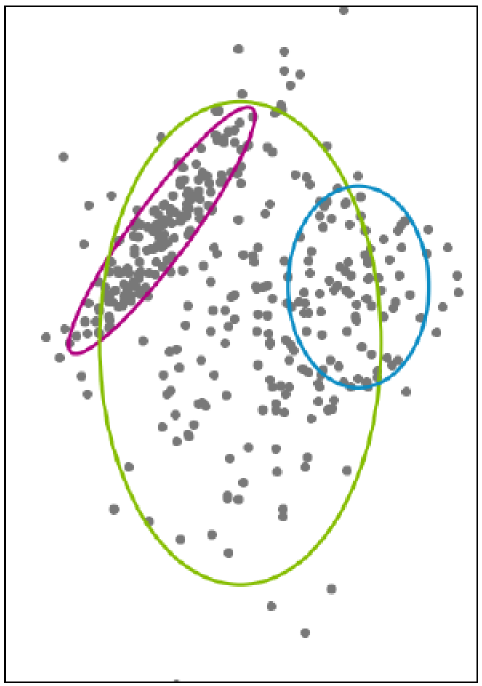
Initial probability of being from cluster k

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



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

Responsibilities in equations



Responsibility cluster k takes for observation i

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

Normalized over all possible cluster assignments

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

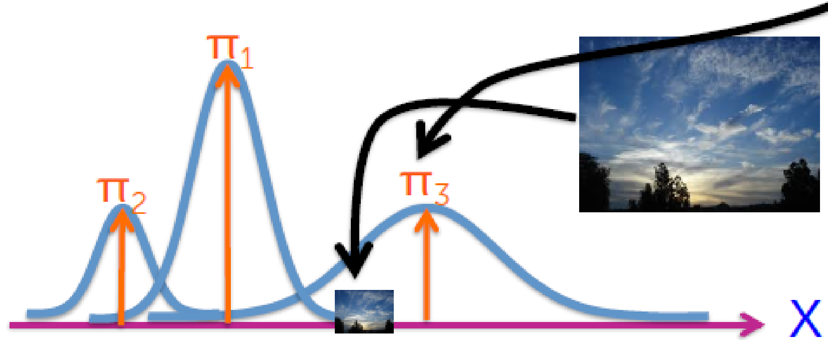
Recall: According to the model...

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

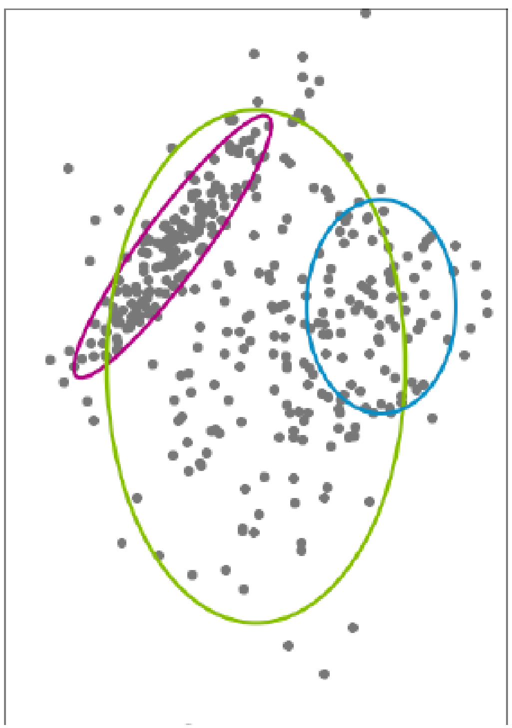
$$p(z_i = k) = \pi_k$$

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

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



Part 1: Summary

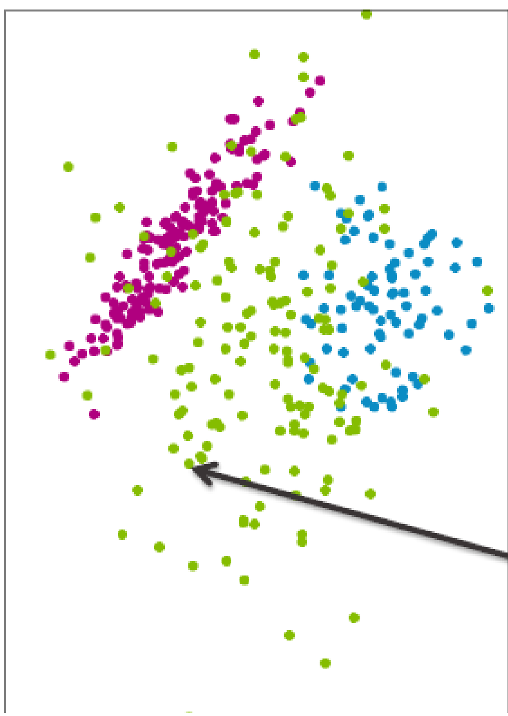


Desired soft assignments (responsibilities) are **easy** to compute when cluster parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$ are known

But, we don't know these!

Imagine we knew the cluster (hard) assignments z_i

Estimating cluster parameters



Imagine we know the cluster assignments

Estimation problem decouples across clusters

Is green point informative of fuchsia cluster parameters?

NO!

Imagine we knew the cluster (hard) assignments z_i

Data table decoupling over clusters

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

Then split into separate tables and consider them independently.

Imagine we knew the cluster (hard) assignments z_i

Maximum likelihood estimation

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

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

maximum likelihood estimation (MLE)

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

Imagine we knew the cluster (hard) assignments z_i

Mean/covariance MLE

sum these vectors

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

divide by 3 (the total # of obs.)

denotes "estimate"

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

← average data points in cluster k

# of obs. in cluster

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

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

Imagine we knew the cluster (hard) assignments z_i

Cluster proportion MLE

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

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

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

obs in cluster k

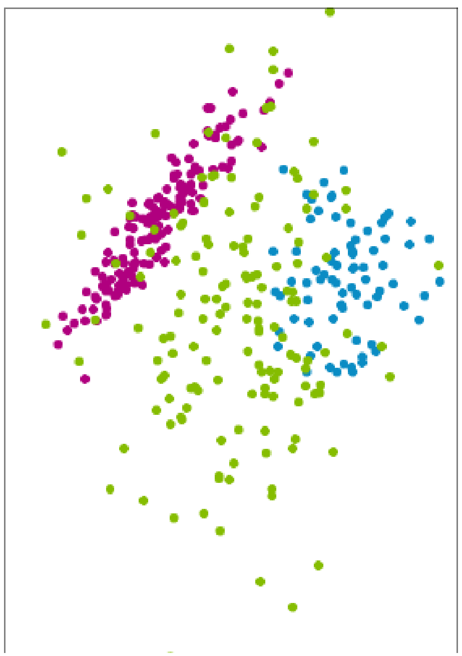
$$\hat{\pi}_k = \frac{N_k}{N}$$

total # of obs

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

Imagine we knew the cluster (hard) assignments z_i

Part 2a : Summary



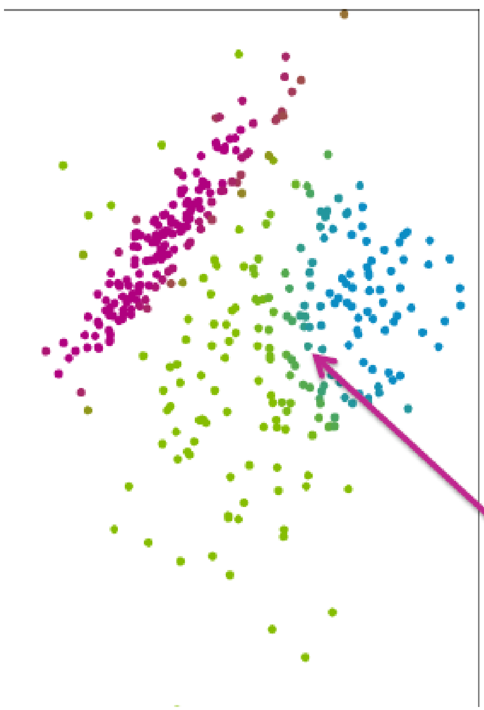
needed to compute soft assignments

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}?

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}?

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

52% chance this obs is in cluster 3

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

Maximum likelihood estimation from soft assignments

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

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

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

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

Cluster-specific location/shape MLE

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

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

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

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

Total weight in cluster k
= effective # obs

Compute cluster parameter estimates with weights on each row operation

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

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

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

Total weight in cluster:

1.242	**2.8**	**2.42**

Total weight in dataset: 6

datapoints N

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

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

Total weight in cluster k = effective # obs

Estimate cluster proportions from relative weights

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

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

Hard assignments have:

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

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

One-hot encoding of cluster assignment

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

Equating the estimates…

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

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

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

only add x_i if i in k ($r_{ik}=1$) $\rightarrow \frac{1}{N_k} \sum_{i \text{ in } k} x_i$ ✓

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

✓

same as above

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

Part 2b: Summary

Still straightforward to compute cluster parameter estimates from soft assignments

Expectation maximization (ME)

An iterative algorithm

Motivates an iterative algorithm:

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

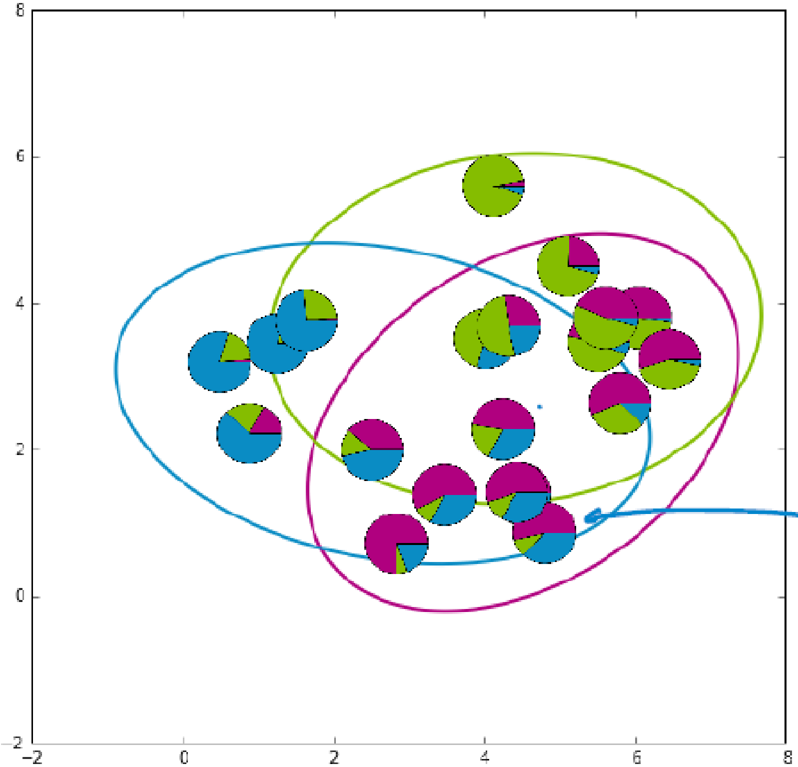
$$\hat{r}_{ik} = \frac{\hat{\pi}_k N(x_i \mid \hat{\mu}_k, \hat{\Sigma}_k)}{\sum_{j=1}^{K} \hat{\pi}_j N(x_i \mid \hat{\mu}_j, \hat{\Sigma}_j)}$$

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

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

Expectation maximization (ME)

EM for mixtures of Gaussians in pictures – initialization



Initialize

iter counter

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

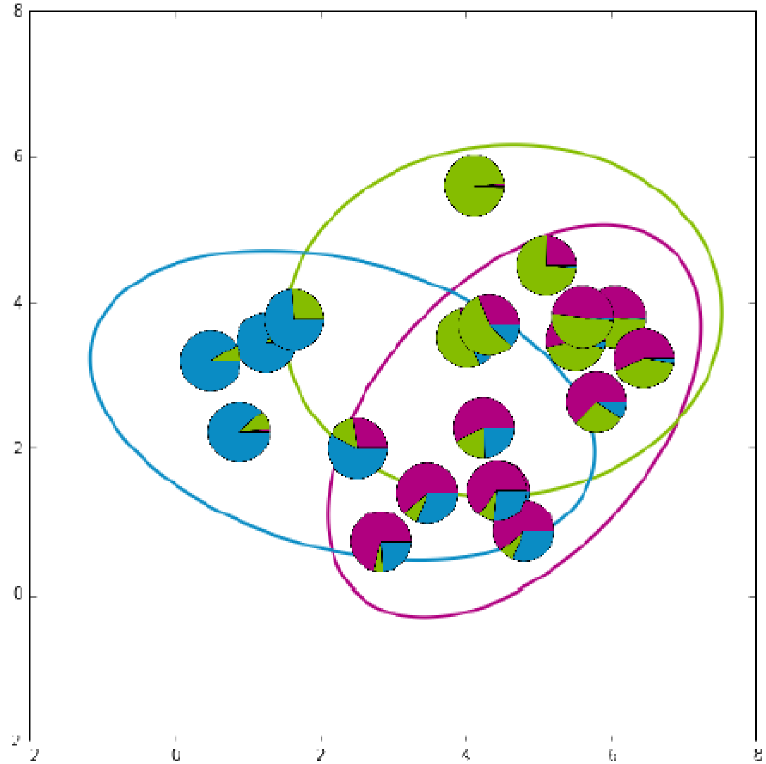
Then compute

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

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

Expectation maximization (ME)

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



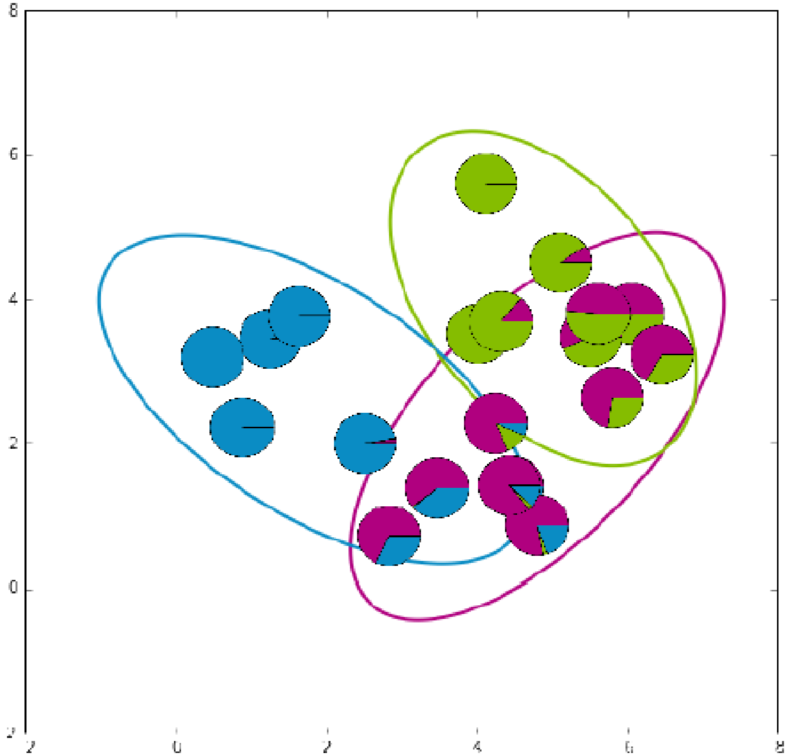
Maximize likelihood
given soft assign. $r_{ik}^{(1)}$

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

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

Expectation maximization (ME)

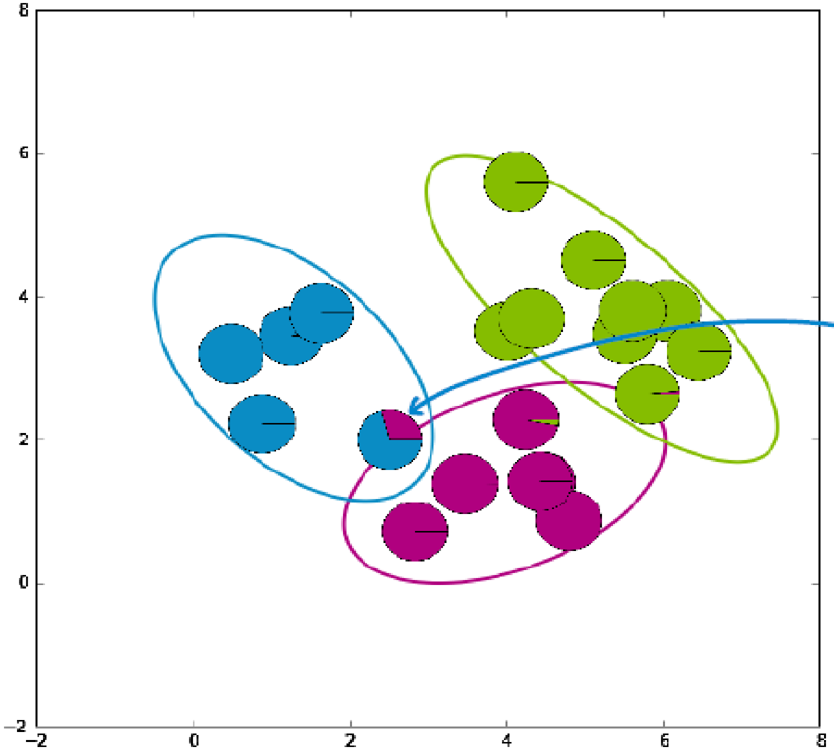
EM for mixtures of Gaussians
in pictures – after 2^{nd} iteration



rinse
+
repeat
until convergence

Expectation maximization (ME)

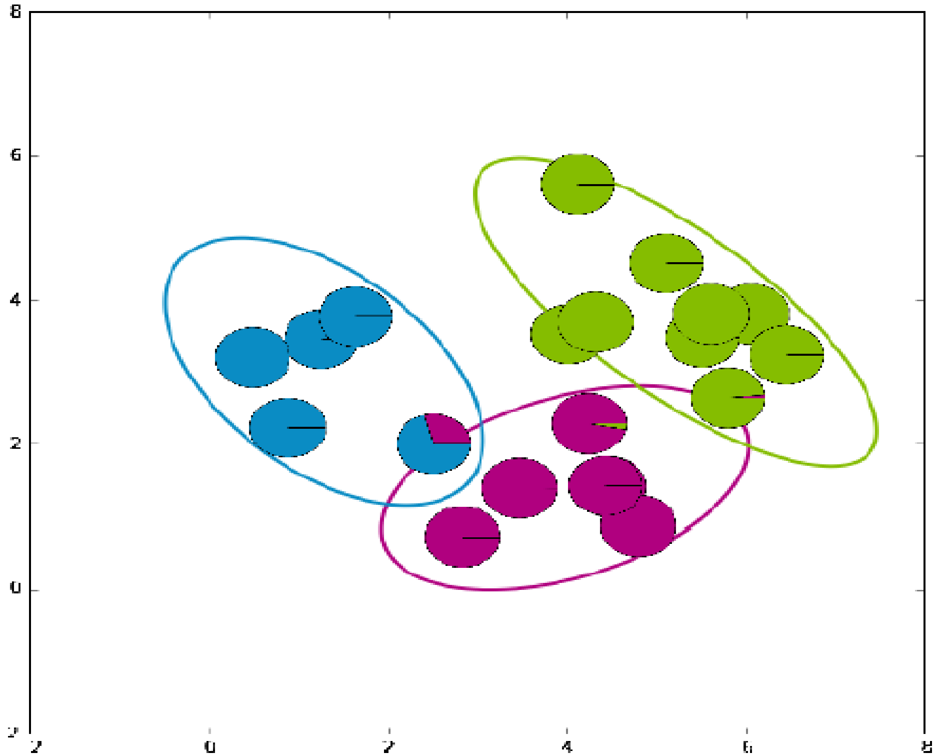
EM for mixtures of Gaussians in pictures – converged solution



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

Expectation maximization (ME)

EM for mixtures of Gaussians in pictures - replay



Expectation maximization (ME)

Convergence of EM

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

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

Expectation maximization (ME)

Initialization

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

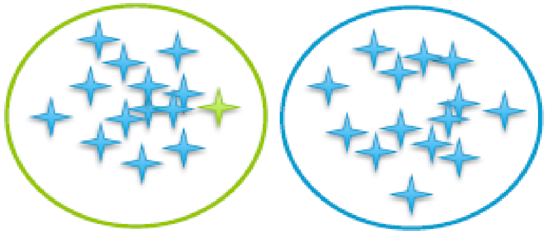
Expectation maximization (ME)

Overfitting of MLE

Maximizing likelihood can overfit to data

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

- What parameter values maximize likelihood?



Set center equal to point and shrink variance to 0

Likelihood goes to ∞ !

Expectation maximization (ME)

Overfitting in high dims

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

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

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

Expectation maximization (ME)

Simple regularization of M-step for mixtures of Gaussians

Simple fix: Don’t let variances → 0!

Add small amount to diagonal of covariance estimate

Alternatively, take Bayesian approach and place prior on parameters.

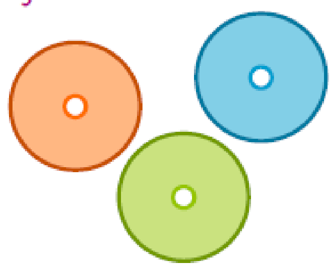
Similar idea, but all parameter estimates are “smoothed” via cluster pseudo-observations.

Relationship to k-means

Consider Gaussian mixture model with

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

Spherically symmetric clusters



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

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

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

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

Expectation maximization (ME)

Infinitesimally small variance EM = k-means

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

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

Infinitesimally small

Decision based on distance to nearest cluster center

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

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

Mixed membership models for documents

Clustering model

So far, clustered articles into groups

Clustering goal: discover groups of related docs

Clustering model

Are documents about just one thing?

Is this article just about science?

Clustering model

Soft assignments capture uncertainty

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

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

Soft assignments

Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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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.

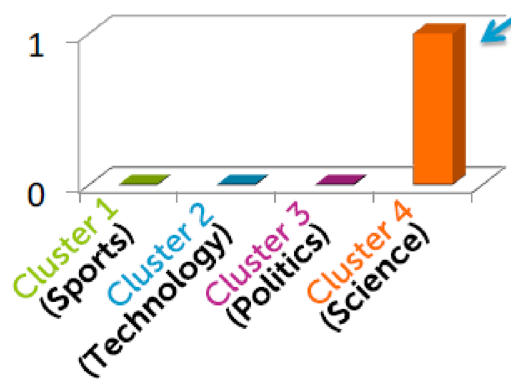
Keywords: Bayesian nonparametric, EEG, factorial hidden Markov model, graphical model, time series

1. Introduction

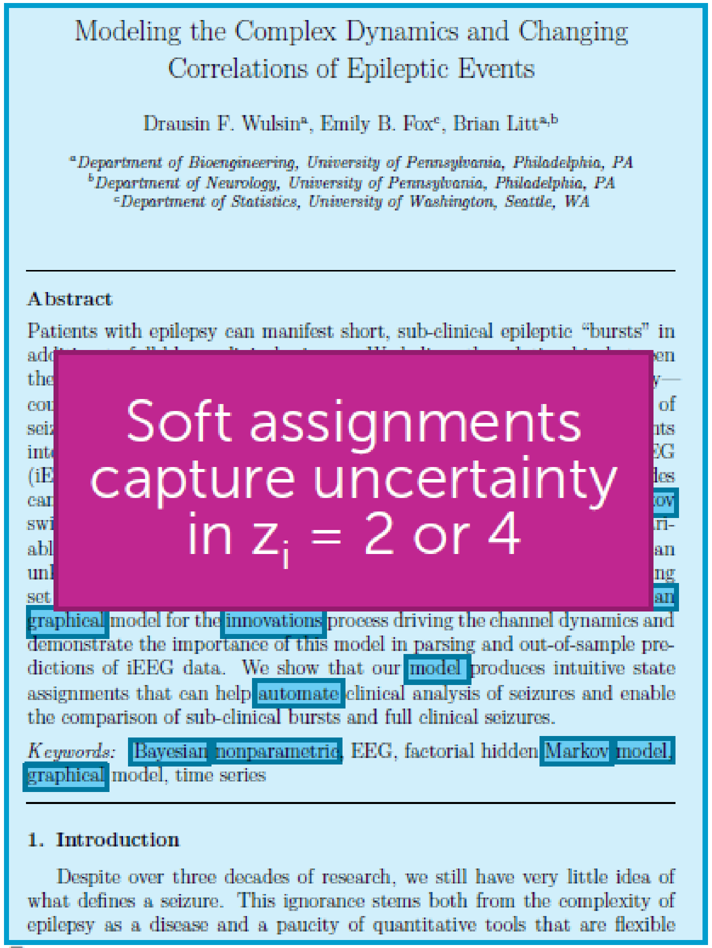
Despite over three decades of research, we still have very little idea of what defines a seizure. This ignorance stems both from the complexity of epilepsy as a disease and a paucity of quantitative tools that are flexible

Encoding of cluster membership $z_i = 4$

Based on science related words, maybe doc in cluster 4



Soft assignments


Modeling the Complex Dynamics and Changing Correlations of Epileptic Events

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

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

Abstract

Patients with epilepsy can manifest short, sub-clinical epileptic “bursts” in ...

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

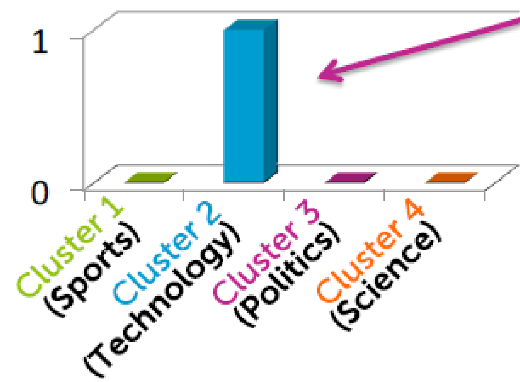
1. Introduction

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



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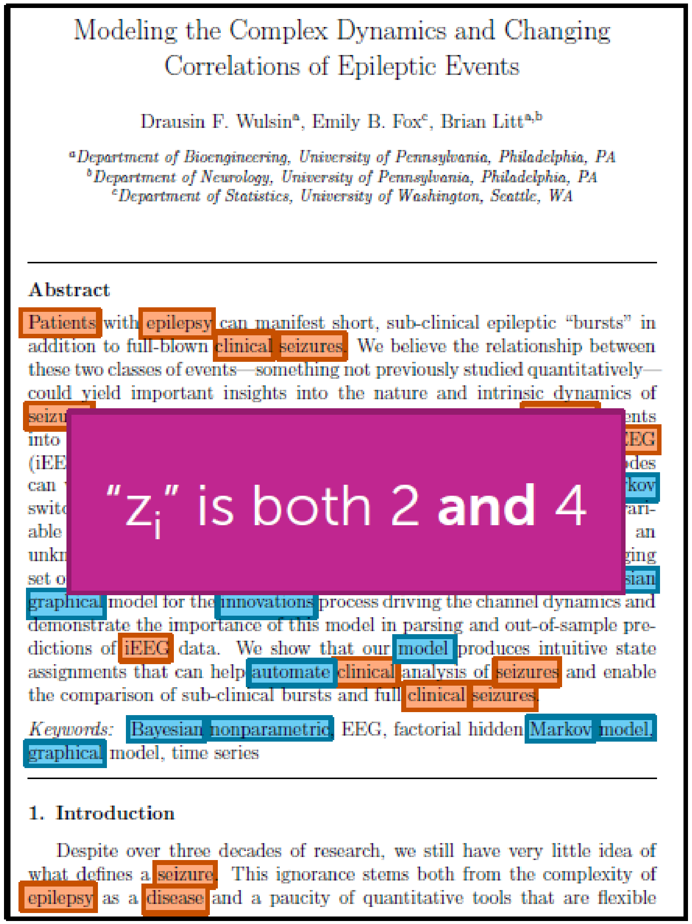
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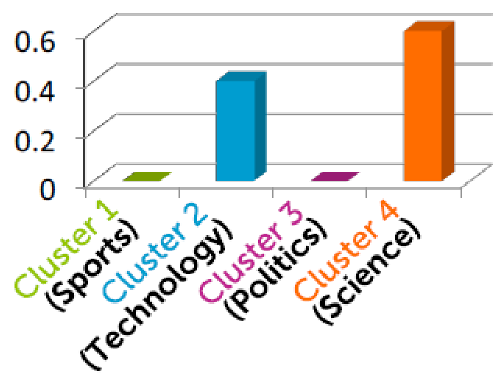
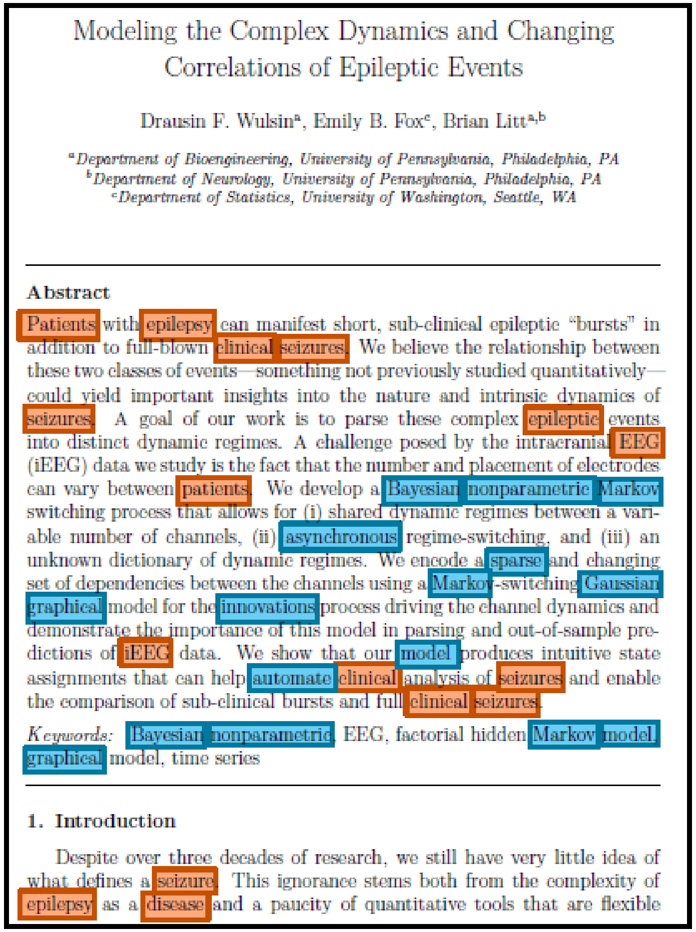
“z_i” is both 2 **and** 4

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



Mixed membershio models



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Mixed membership models

Want to discover a **set** of memberships

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

Building alternative model

An alternative document clustering model

(Back to clustering, not mixed membership modeling)

Building an alternative model

So far, we have considered...

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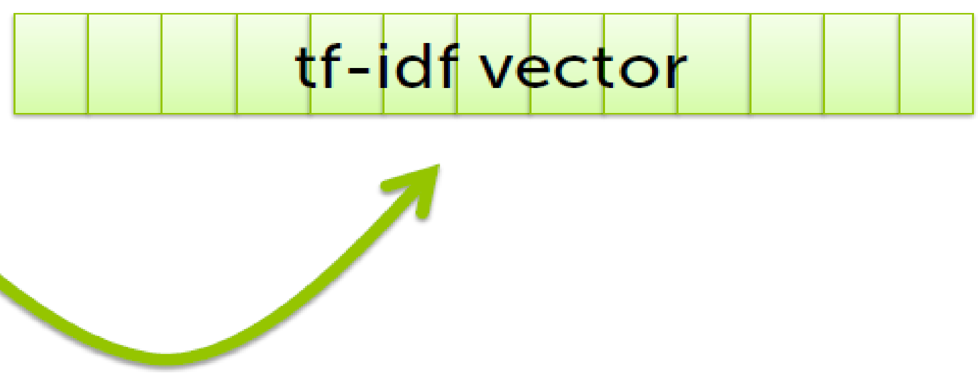
$\mathbf{x}_i$ =



Building an alternative model

Bag-of-words representation

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

multiset

= unordered set of words with duplication of unique elements mattering

Model for „bag-of-words”

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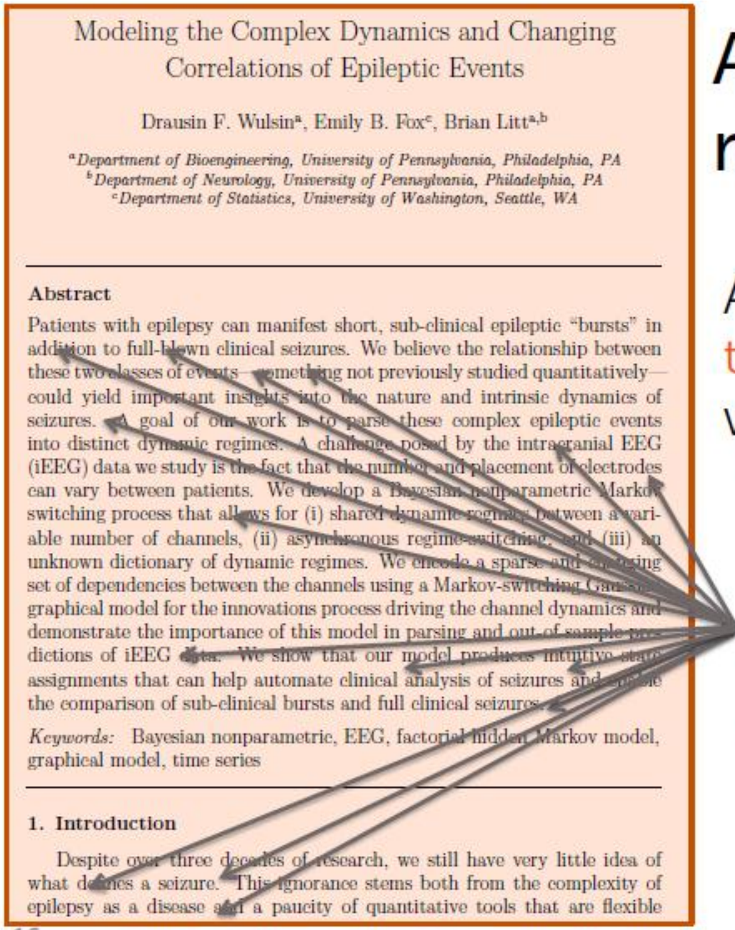
A model for bag-of-words representation

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

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

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

Model for „bag-of-words”



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A model for bag-of-words representation

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

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

words in vocab

Model for „bag-of-words”

Topic-specific word probabilities

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

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

...

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

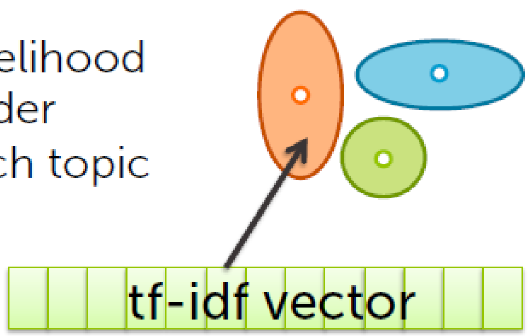
Model for „bag-of-words”

Comparing and contrasting

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

Likelihood under each topic

Previously:



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

Now:

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...}

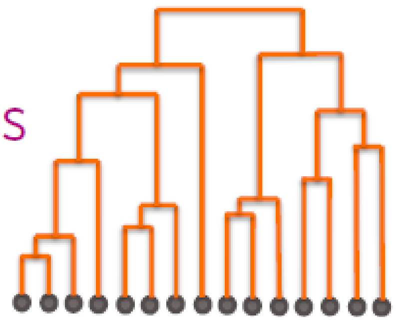
compute likelihood of the **collection of words** in doc under each **topic distribution**

Hierarchical clustering

Why hierarchical clustering

- Avoid choosing # clusters beforehand

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

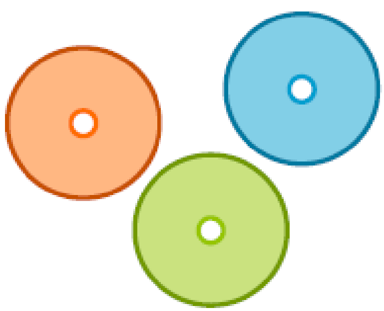


- Most algorithms allow user to choose any distance metric
  - k-means restricted us to Euclidean distance

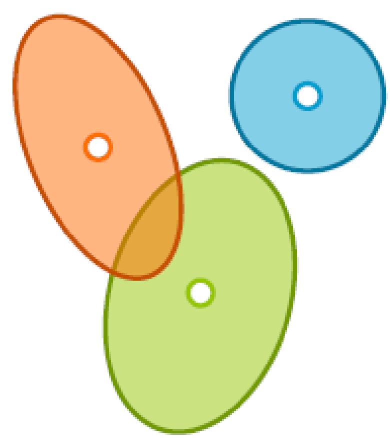
Why hierarchical clustering

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

k-means: spherical clusters



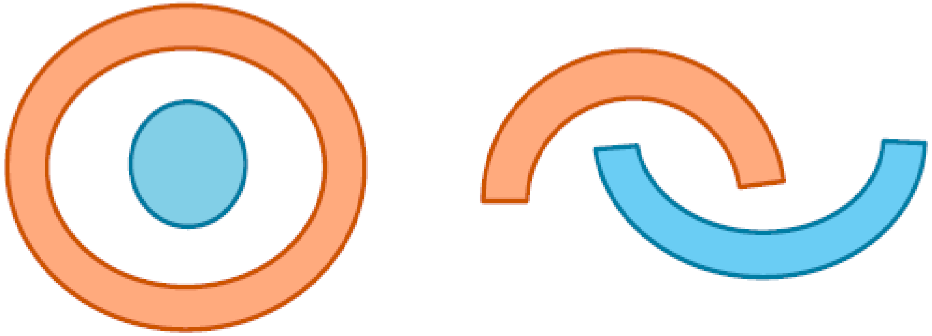
Gaussian mixtures: ellipsoids



Why hierarchical clustering

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

What about these?



Two main types of algorithms

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

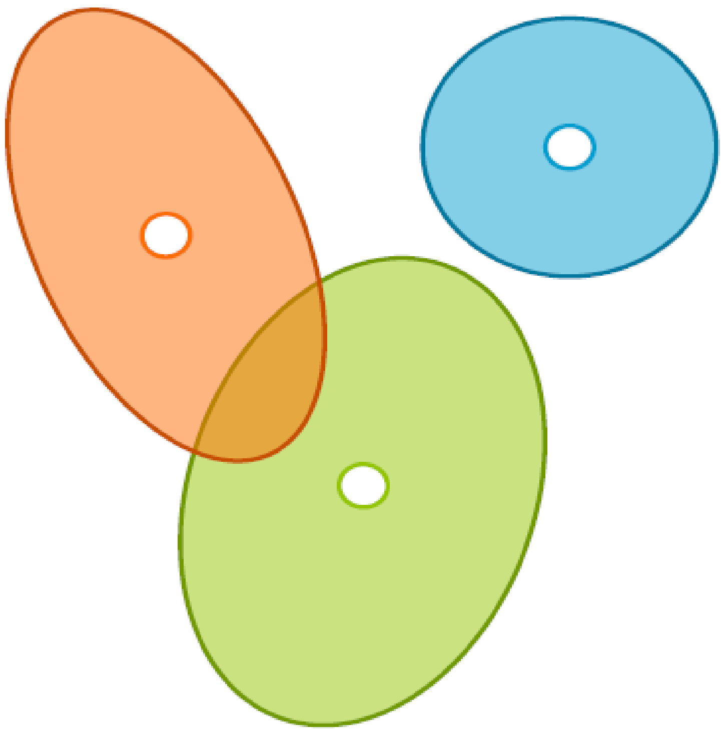
– Example: recursive k-means

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

– Example: single linkage

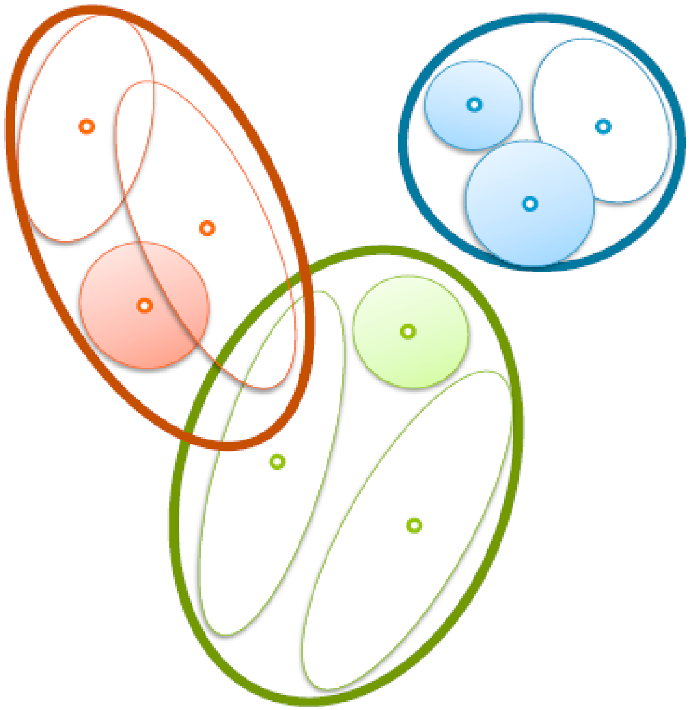
Divisive clustering

Divisive in pictures – level 1

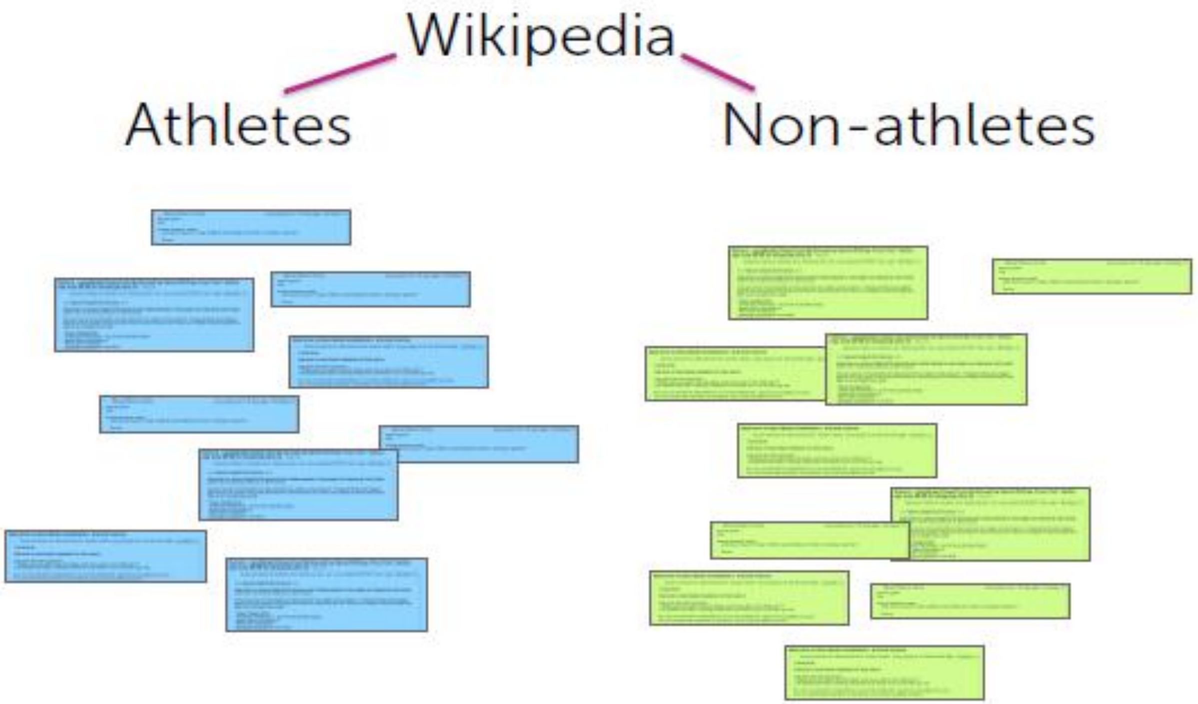


Divisive clustering

Divisive in pictures – level 2



Divisive: Recursive k-means



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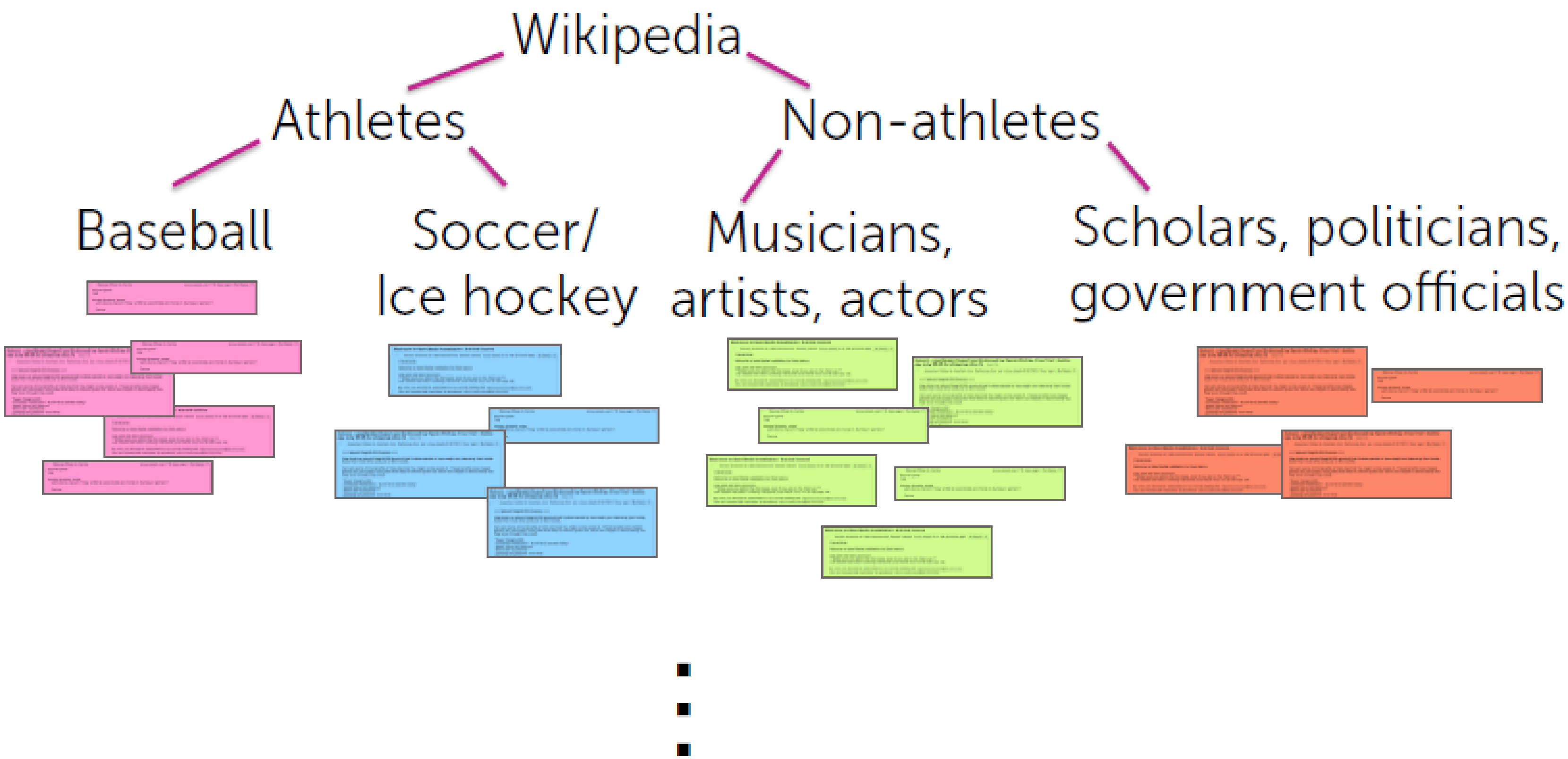
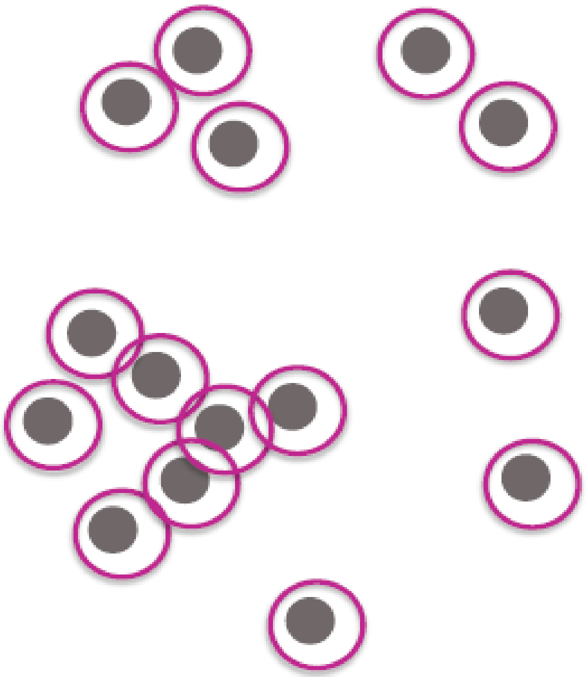


Divisive: choices to be made

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

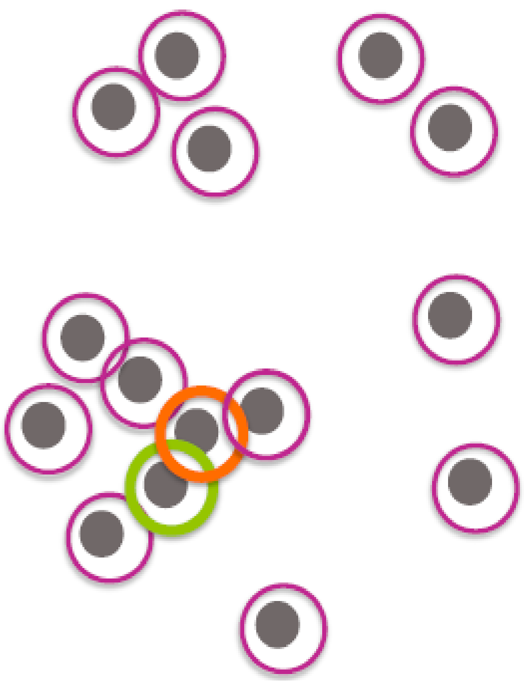
Aglomerative: Single linkage

1. Initialize each point to be its own cluster



Aglomerative: Single linkage

2. Define distance between clusters to be:



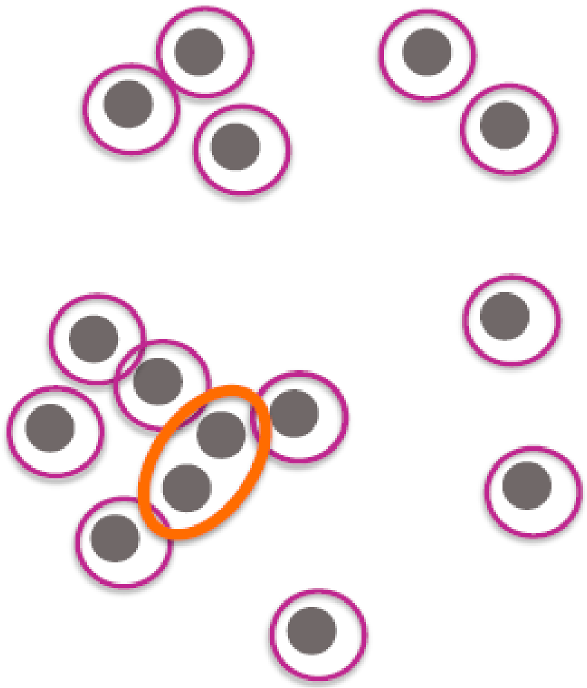
$$\text{distance}(C_1,C_2) = \boxed{\min_{\substack{x_i \text{ in } C_1,\\ x_j \text{ in } C_2}} d(\mathbf{x}_i, \mathbf{x}_j)}$$

specified pairwise distance function

Linkage criteria

Aglomerative: Single linkage

3. Merge the two closest clusters



Aglomerative: Single linkage

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

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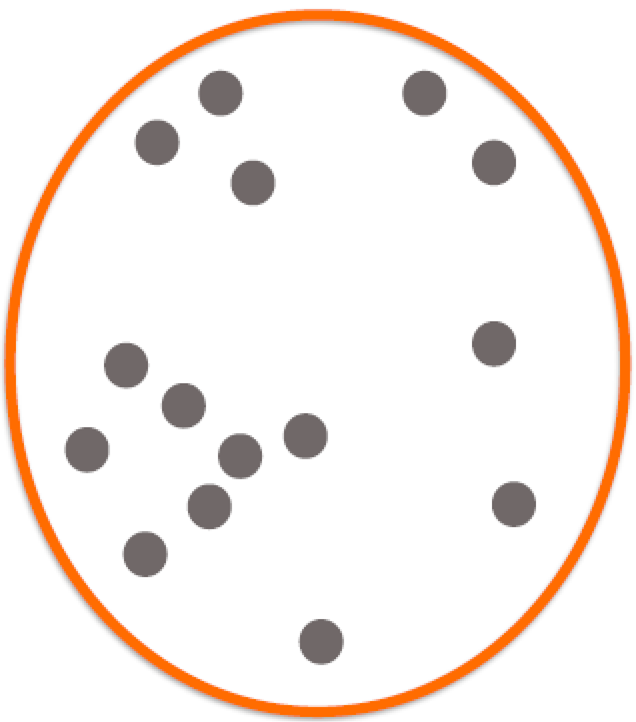
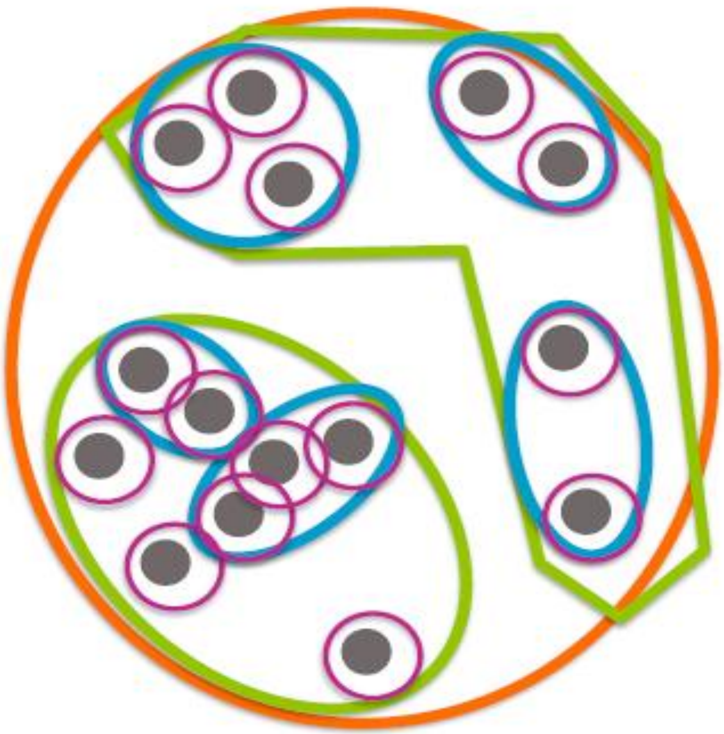


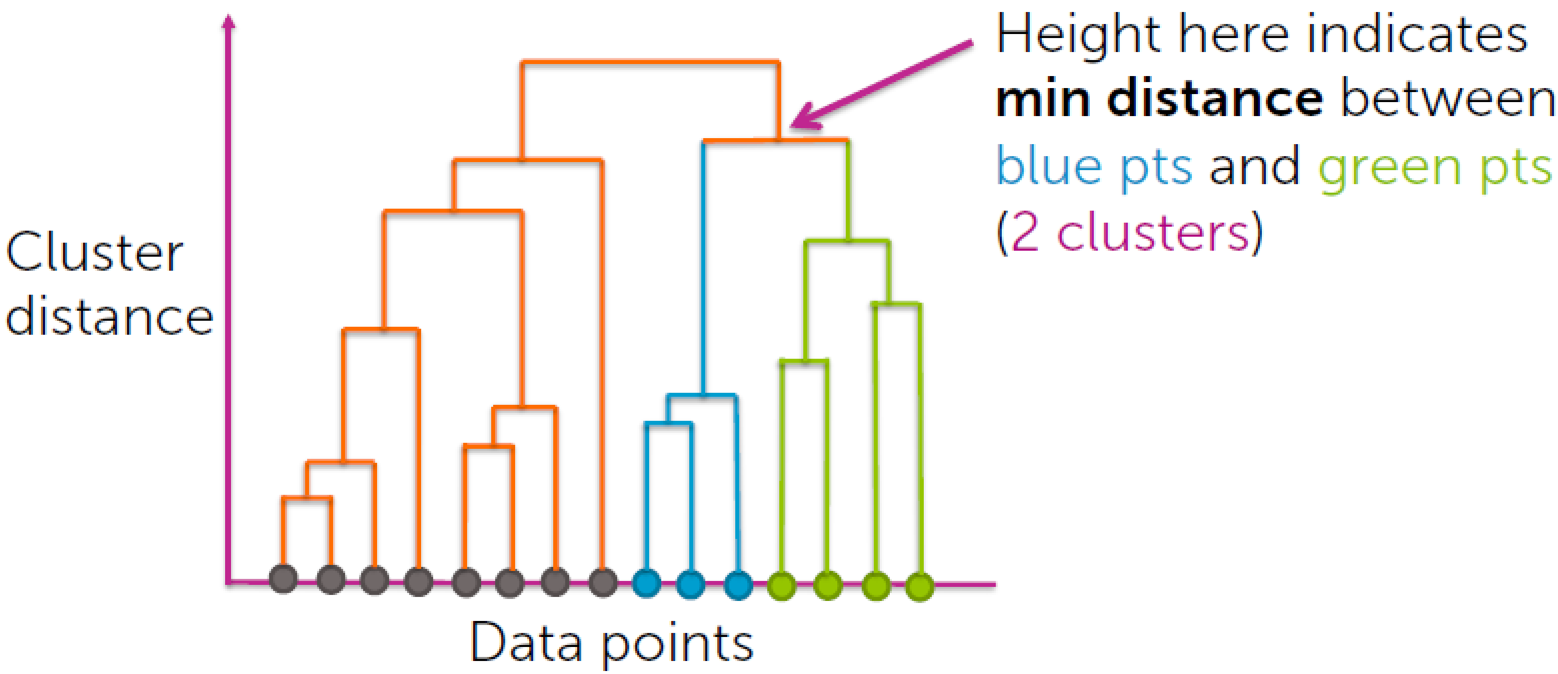
Cluster of clusters

Just like our picture for divisive clustering...



The dendrogram

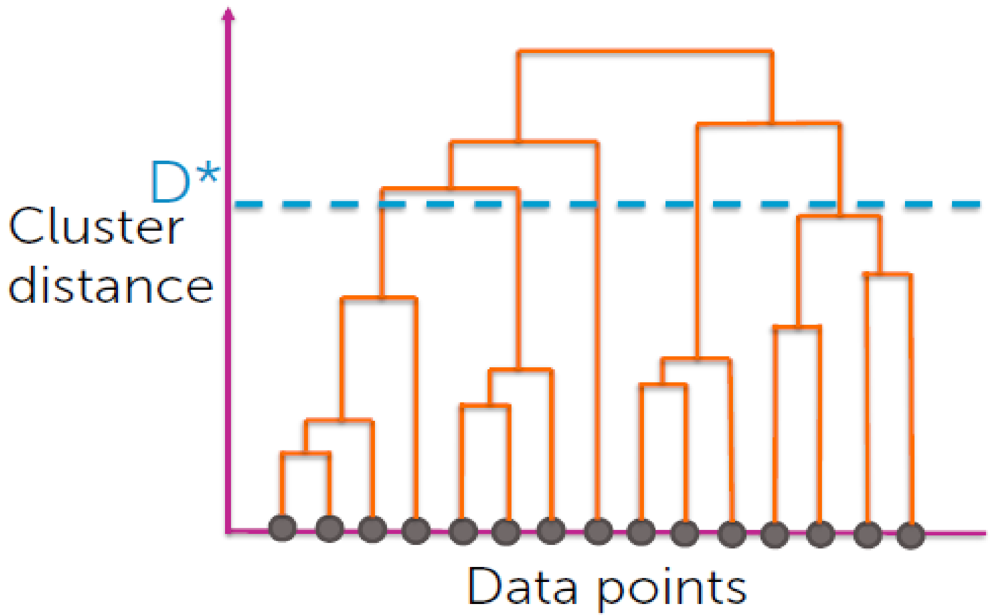
- x axis shows data points (carefully ordered)
- y-axis shows distance between pair of clusters



Extracting a partition

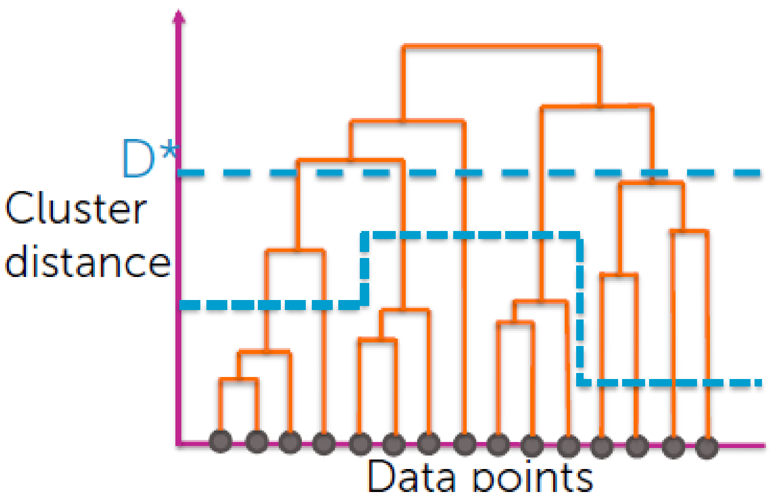
Choose a distance D* at which to cut dendogram

Every branch that crosses D* becomes a separate cluster



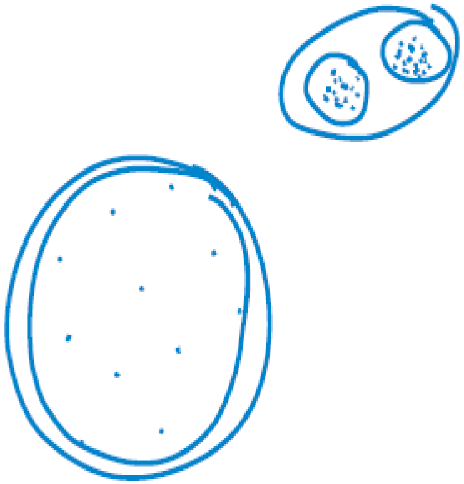
Agglomerative: choices to be made

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



More on cutting dendrogram

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



Computational considerations

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

datapoints

- Smart implementations use triangle inequality to rule out candidate pairs

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