Unsupervised learning, mixture models

Semester 1, 2021

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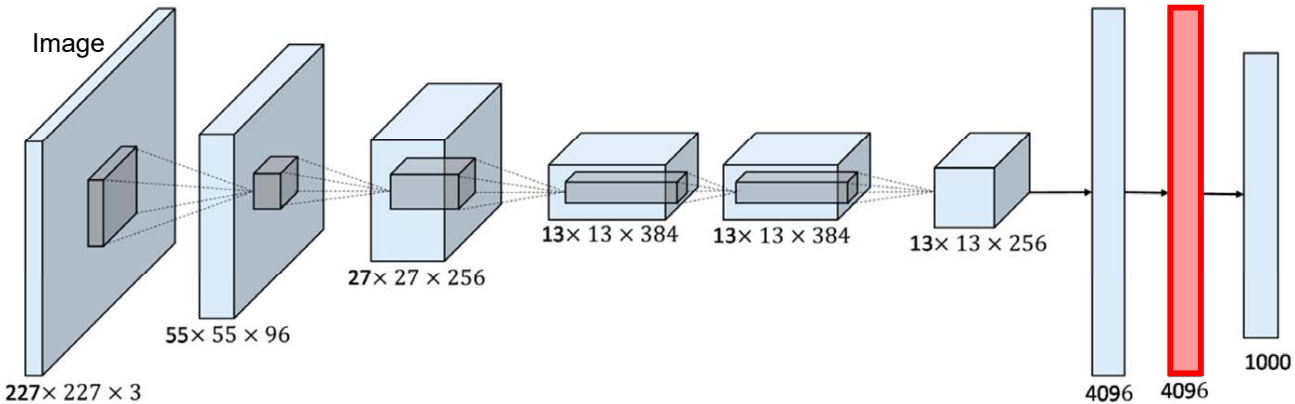
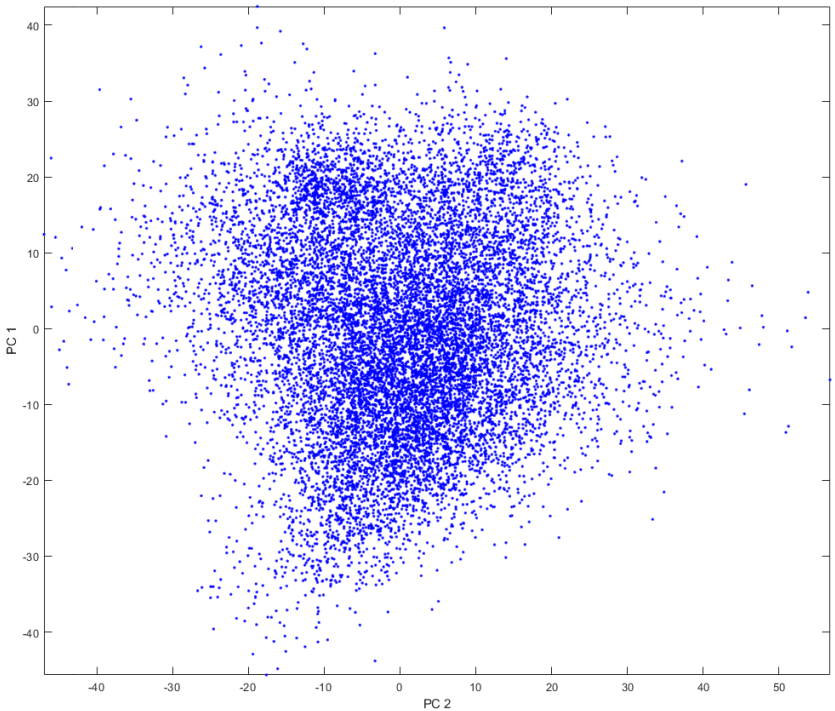
Embeddings, cont.



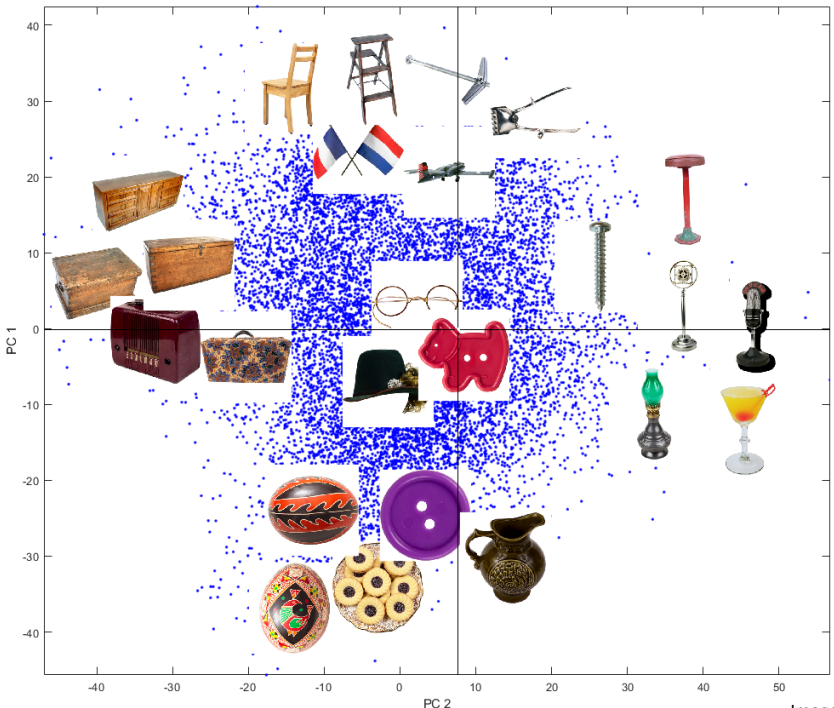
Embedding of an input = the network's response to the input at some layer

Image: Han, Zhong, Cao, & Zhang (2017)

Embeddings, cont.



Embeddings, cont.



Images: Hemera Technologies

Embeddings, cont.

Similar images: layer 7

Images: Hemera Technologies

Outline

- Clustering
- Gaussian mixture model and EM algorithm
- Unsupervised evaluation

Clustering

Clustering basics

- Clustering = unsupervised learning; no explicit or implicit definition of class
- Learn structure from data alone
- But you usually bring your own assumptions about what kind of structure you expect in the data:
  - Exclusive or overlapping clusters?
  - Hierarchical clusters?
  - What defines a good “group”?

Deterministic vs. probabilistic

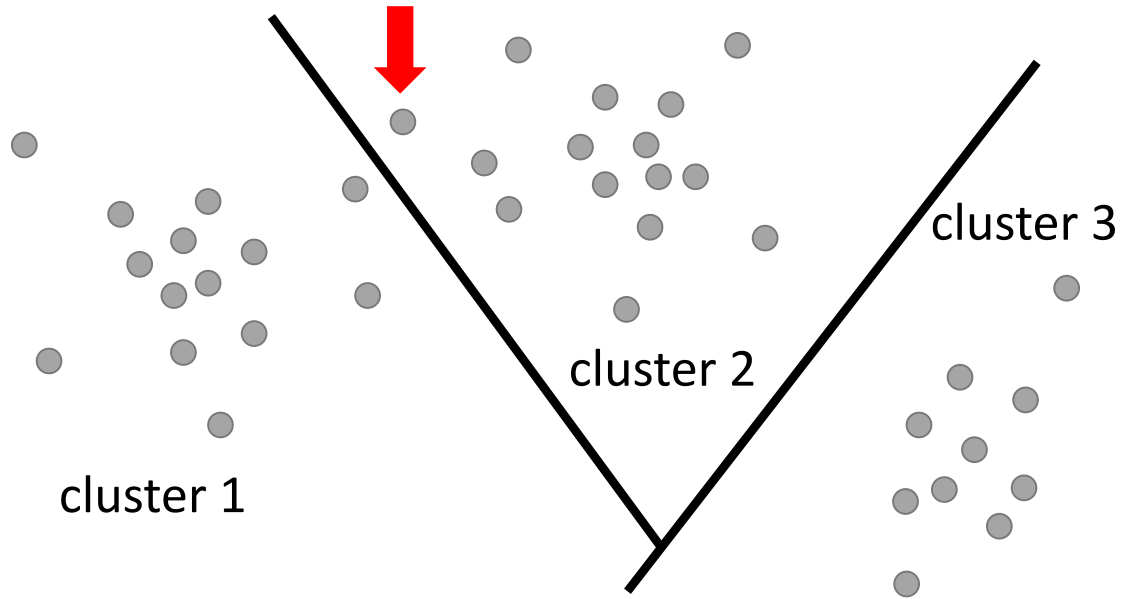
- Deterministic clustering = each instance is a member of one cluster = clusters can't overlap

Instance	Cluster
1	3
2	1
⋮	⋮

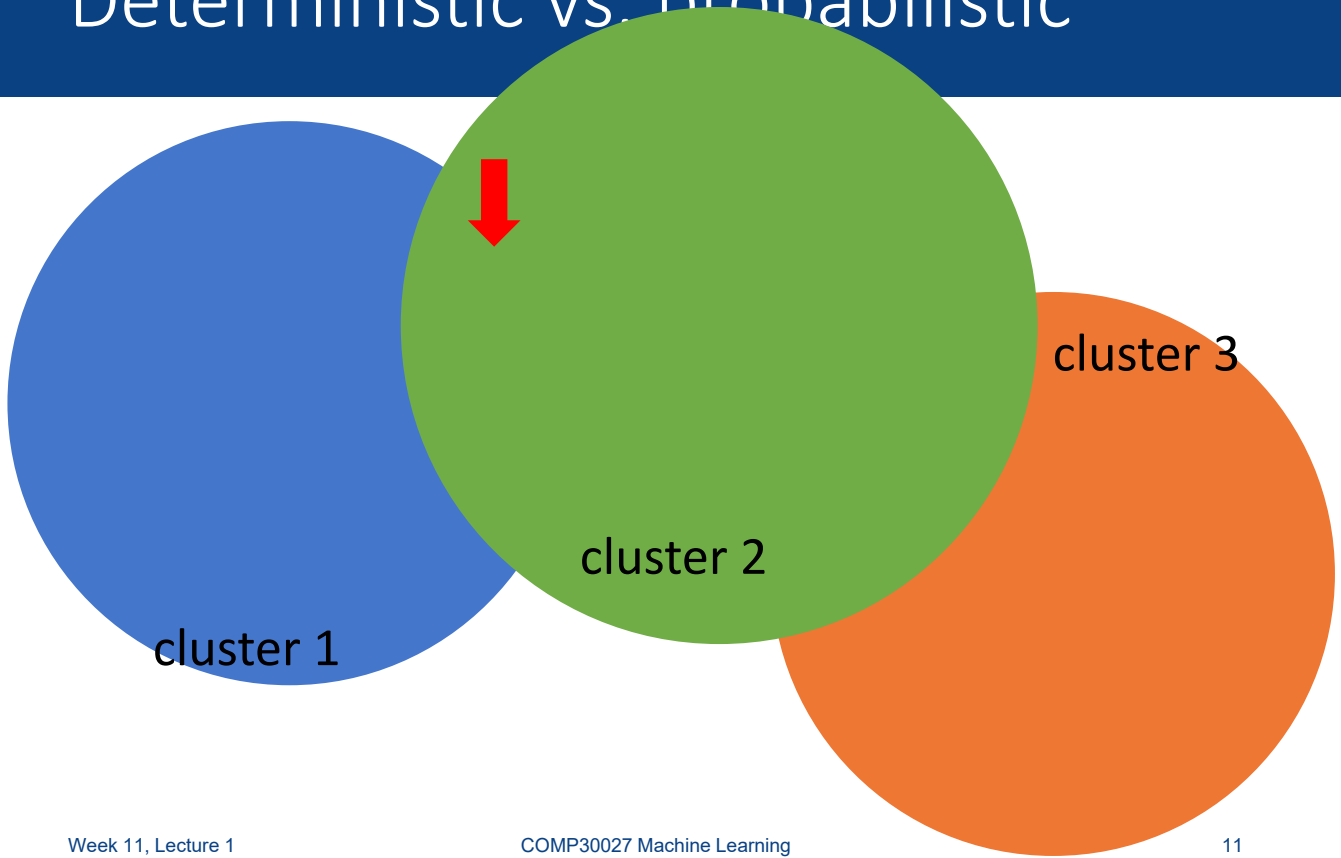
- Probabilistic cluster = each instance has a weight in each class = clusters overlap

Instance	Cluster 1	Cluster 2	Cluster 3
1	0.01	0.87	0.12
2	0.67	0.15	0.18
⋮		⋮	

Deterministic vs. probabilistic



Deterministic vs. probabilistic



Deterministic vs. probabilistic

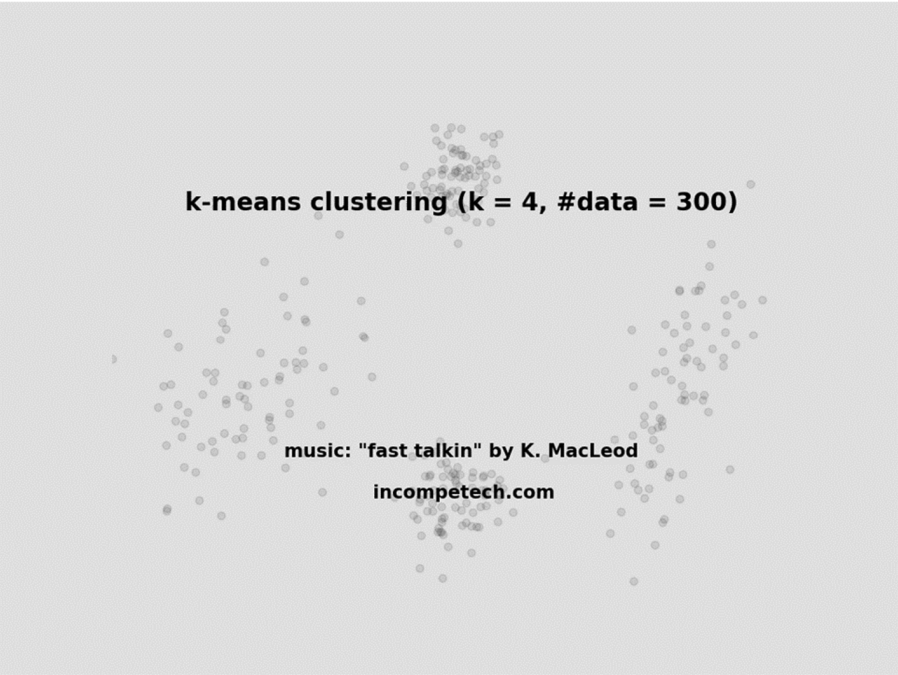
- Why choose one over the other?

K-means clustering

- Given k, the k-means algorithm is implemented as follows (Lloyd's algorithm):

1. Select k points at random as the initial cluster centroids
2. For each instance, compute the distance to each centroid
3. Assign each instance to the cluster with nearest centroid
4. Compute a new centroid for each cluster (centroid = mean of all instances in the cluster)
5. Go to 2, repeat until no instances are reassigned

K-means clustering



https://www.youtube.com/watch?v=5I3Ei69I40s

“Soft” k-means clustering

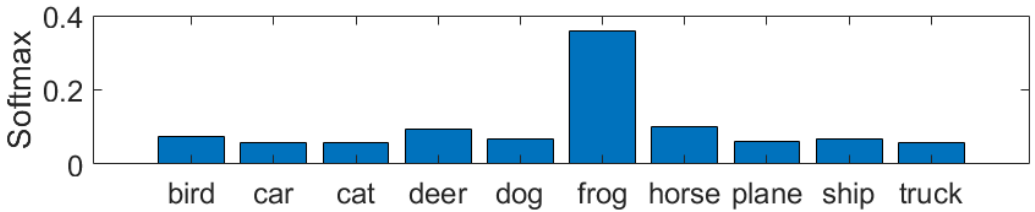
- Is it possible to have a probabilistic (“soft”) version of k-means, where each instance is a member of all clusters, with some probability?
- Solution: use softmax function

$$\sigma(x_i) = \frac{e^{x_i}}{\sum_{i=1}^{k} e^{x_i}}$$

- Example: x = [-0.5, 0, 1.3, 2]
- After softmax: σ = [0.048, 0.079, 0.29, 0.58]

Note on softmax function

- Produces a vector that has the properties of a probability distribution:
  - All values in range 0-1
  - Values sum to 1
- Common application: normalise the output of a multiclass classifier:



- Are these values actual probabilities?

No. more like a confidence

"Soft" k-means clustering

- Choose random centroids $\mu_1, \mu_2, \ldots, \mu_k$
- Probability instance x_i is in cluster j is:

$$z_{ij} = \frac{\exp\left[-\beta \left\| x_i - \mu_j \right\|\right]}{\sum_\ell \exp\left[-\beta \left\| x_i - \mu_\ell \right\|\right]}$$

distance.

$$\frac{e^{-\beta \|x_i - \mu_j\|}}{\sum_\ell e^{-\beta \|x_i - \mu_\ell\|}}$$

$\beta > 0$, and is the "stiffness" parameter ⇒ how quickly the prob will fall with distance

- Update each of the centroids with a weighted average of all instances:

prob of x_i in cluster j

$$\mu_j = \frac{\sum_i z_{ij} x_i}{\sum_i z_{ij}}$$

- Result: overlapping clusters

Gaussian mixture model and EM algorithm

Finite mixtures

- A **finite mixture** is a distribution composed of *k* component distributions
- Used to represent subgroups or latent factors in a dataset
- **Gaussian mixture model** (GMM) represents a distribution as composed of *k* Gaussian distributions

Expectation maximization

- **Expectation maximisation (EM)** = parameter estimation method with guaranteed "positive" hill-climbing characteristics relative to the gradient of log-likelihood
- Used to estimate (hidden) parameter values, such as cluster membership
- Family of algorithms rather than a specific algorithm

GMM with EM algorithm

- Basic idea: generalization of (soft) k-means
- **E(xpectation) step:**
  - Based on current estimate of the parameters, calculate the log-likelihood of the instances
- **M(aximization) step:**
  - Compute the parameter distribution that maximizes the log-likelihood
- Repeat until convergence

EM log likelihood

- The log likelihood of a given finite mixture is:

$$L = \sum_i log \sum_j P(c_j)P(x_i|c_j)$$

  where each x_i is an instance and each c_j is a class

- This gives an estimate of the "goodness" of the cluster model; guaranteed to increase on each iteration of the EM algorithm
- Convergence: if the change in log likelihood falls below a predefined value, we consider the estimate to have converged

GMM with EM algorithm

- Assume this data is a mixture of two normal distributions
- Each instance is drawn from one of the two distributions; probability of drawing from distribution 1 is γ and from 2 is $(1-\gamma)$
- The probability density can be written as:

$$g(x) = \gamma\phi_{\mu_1,\sigma_1}(x) + (1-\gamma)\phi_{\mu_2,\sigma_2}(x)$$

  where $\phi_{\mu,\sigma}$ is a normal distribution with mean μ and standard deviation σ
- Problem: estimate the parameters $\gamma, \mu_1, \sigma_1, \mu_2, \sigma_2$

GMM with EM algorithm

- We want to find the parameters that maximize the log likelihood of the instances x_i:

$$\sum_{i=1}^{N} \log\left[\gamma \phi_{\mu_1,\sigma_1}(x_i) + (1-\gamma)\phi_{\mu_2,\sigma_2}(x_i)\right]$$

- This is difficult to solve numerically, but if we know which instances come from which generating distribution, the computation is simpler:

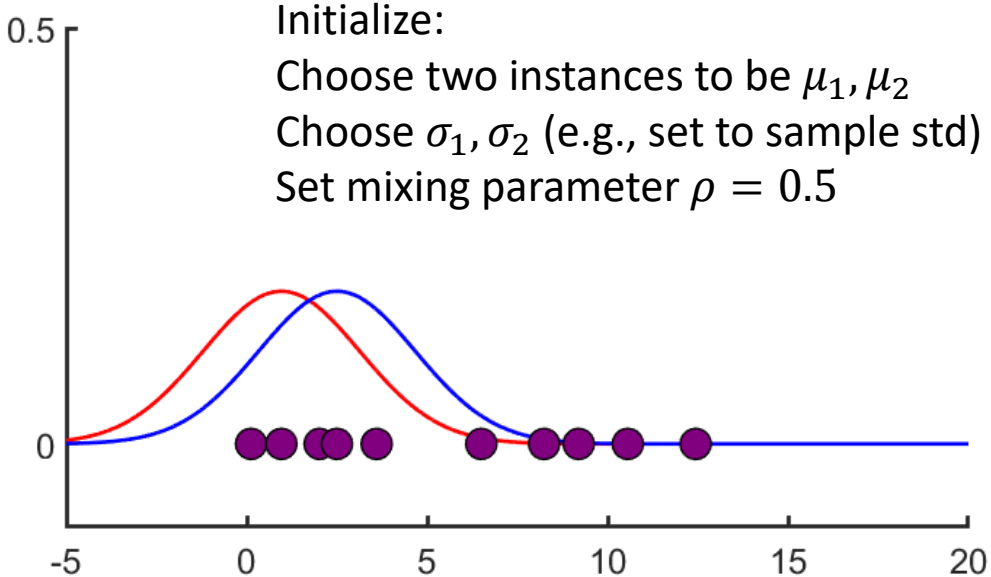
Distribution 1: $\sum_{j \in D_1} \left[\log\left(\phi_{\mu_1,\sigma_1}(x_j)\right) + \log(\gamma)\right]$

Distribution 2: $\sum_{j \in D_2} \left[\log\left(\phi_{\mu_2,\sigma_2}(x_j)\right) + \log(1-\gamma)\right]$

GMM with EM algorithm

- We don't know which distribution produced each instance
- But given some parameters $\gamma, \mu_1, \sigma_1, \mu_2, \sigma_2$ we could estimate how likely each distribution was to have generated each instance
- So, in the iterative EM algorithm:
  - Expectation step: do a soft assignment of instances to each distribution based on current parameters
  - Maximization step: update parameters based on current assignment

GMM with EM algorithm



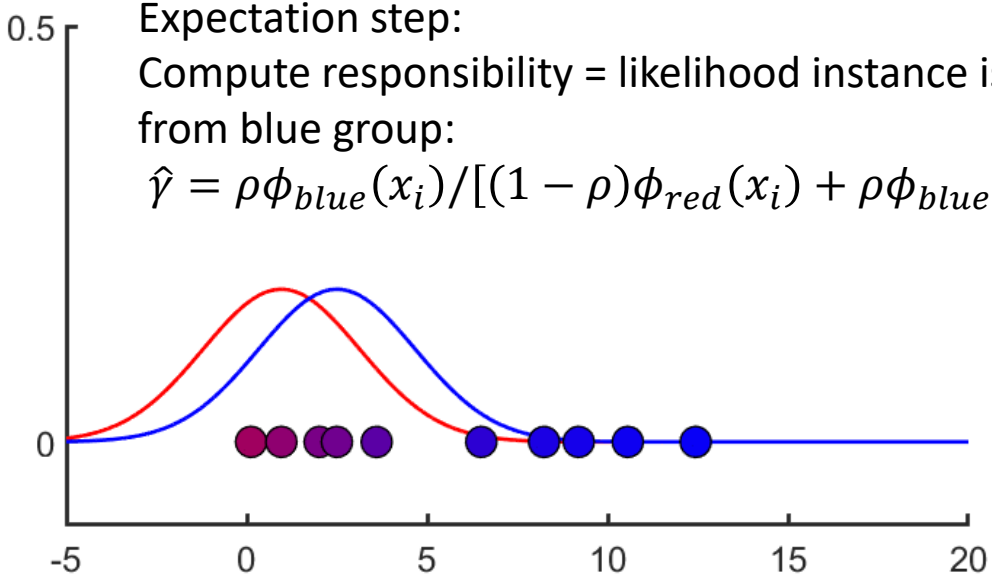
Initialize:

Choose two instances to be μ_1, μ_2

Choose σ_1, σ_2 (e.g., set to sample std)

Set mixing parameter $\rho = 0.5$

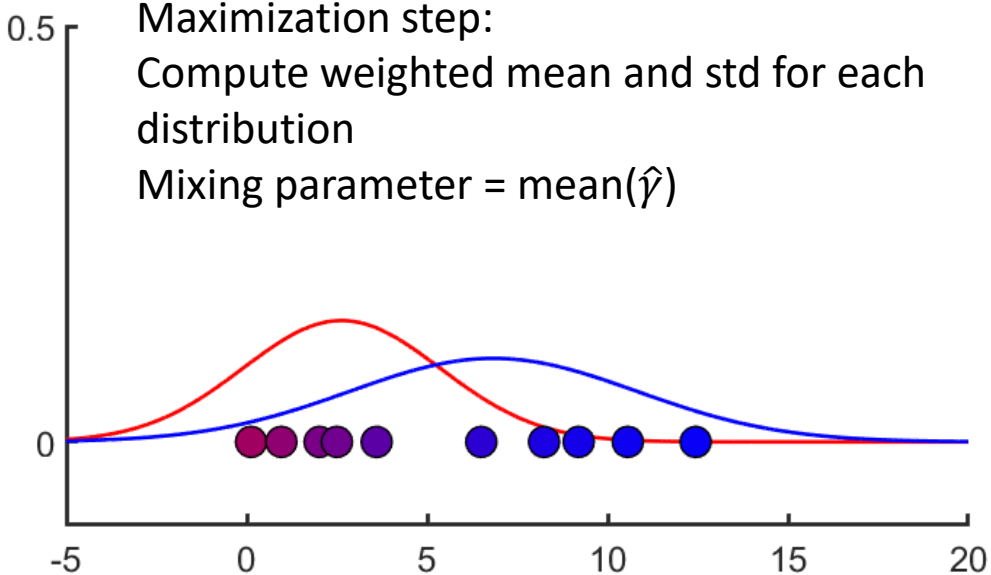
GMM with EM algorithm



Expectation step:
Compute responsibility = likelihood instance is from blue group:

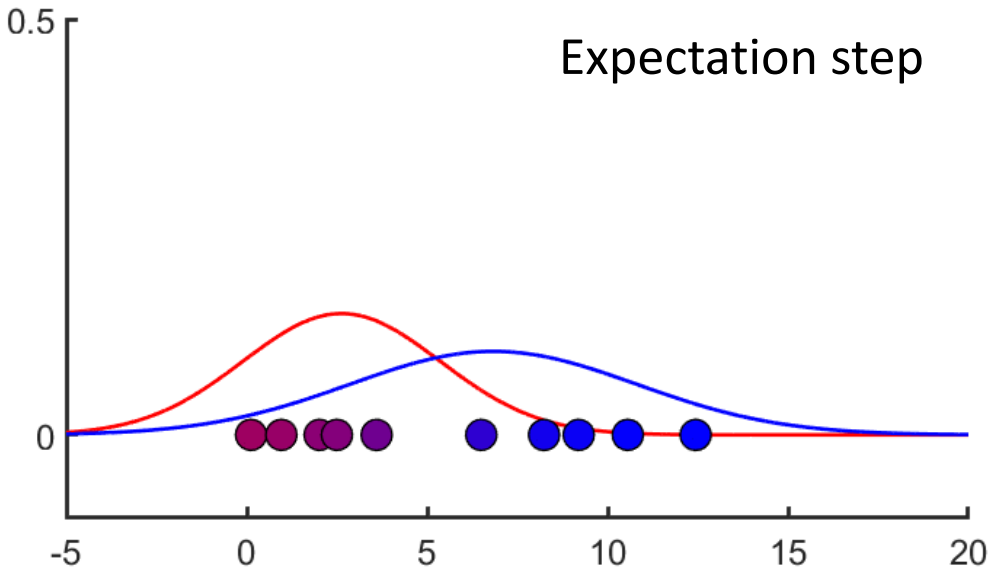
$$\hat{\gamma} = \rho\phi_{blue}(x_i)/[(1-\rho)\phi_{red}(x_i) + \rho\phi_{blue}(x_i)]$$

GMM with EM algorithm

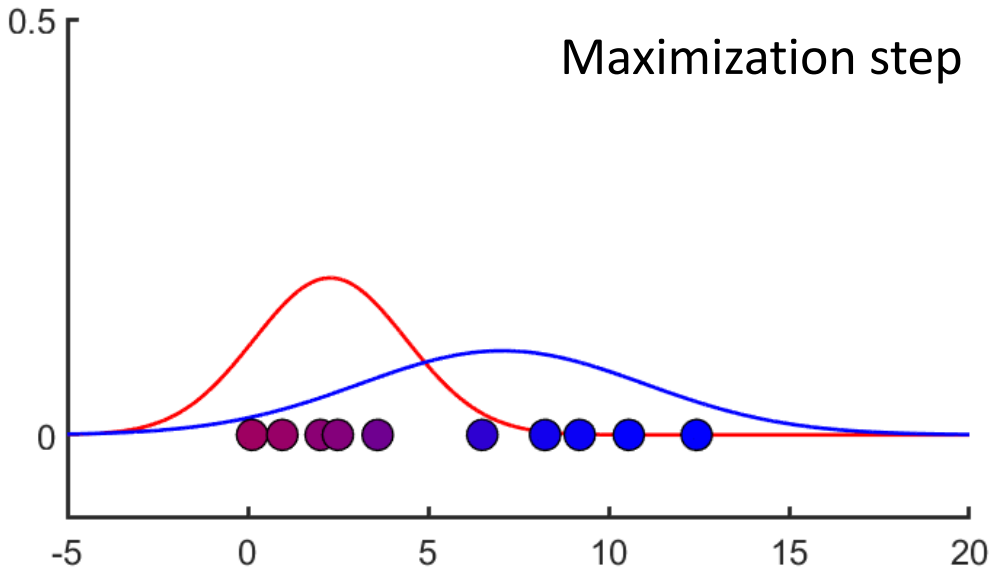


Maximization step:
Compute weighted mean and std for each distribution
Mixing parameter = mean($\hat{\gamma}$)

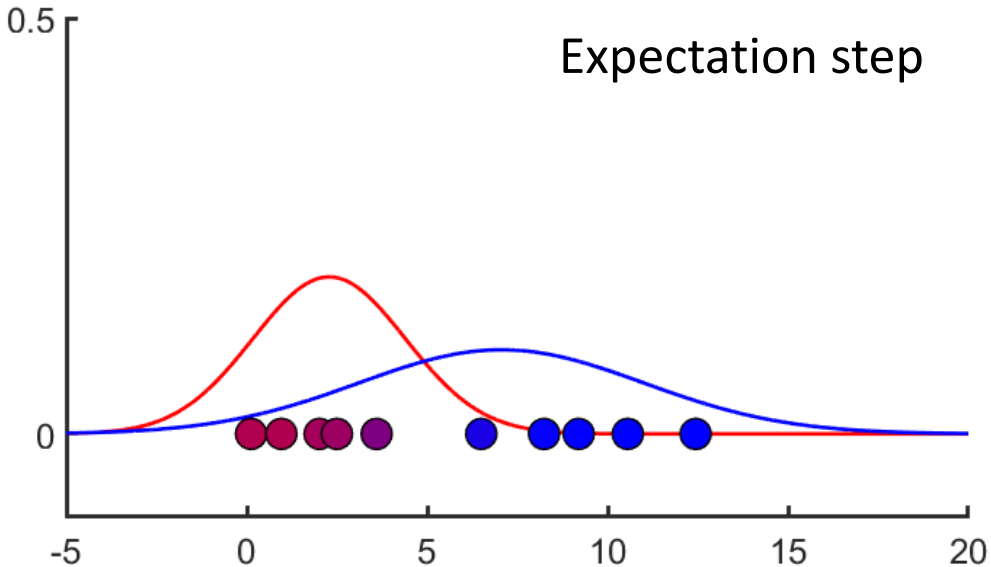
GMM with EM algorithm



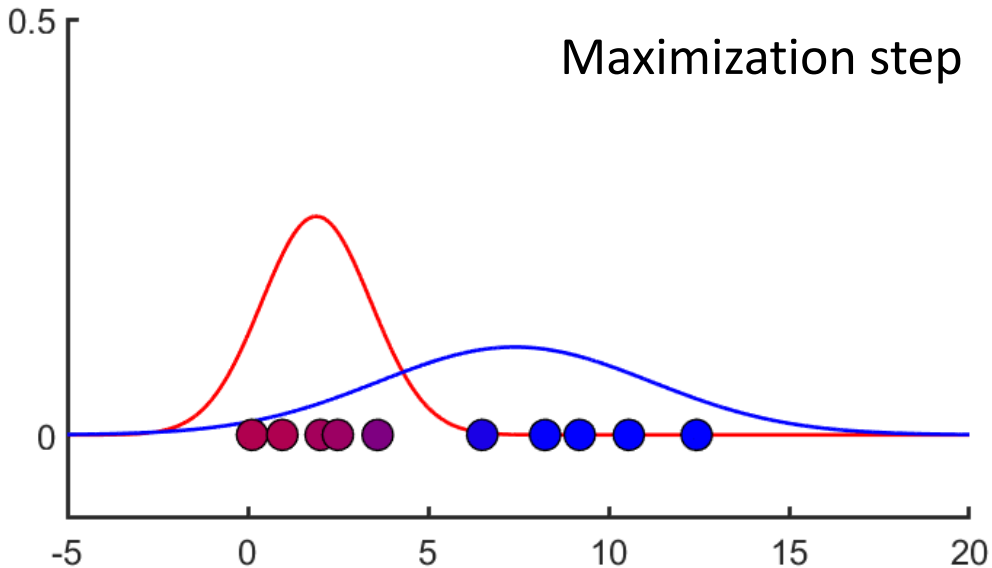
GMM with EM algorithm



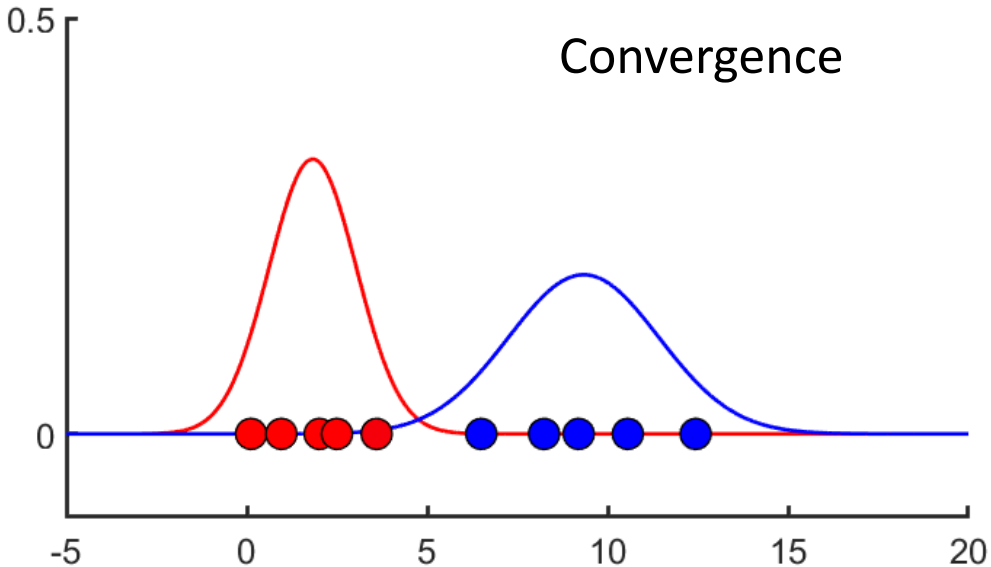
GMM with EM algorithm



GMM with EM algorithm



GMM with EM algorithm



EM algorithm

- Advantages greedy algorithm
  - Guaranteed "positive" hill-climbing behaviour
  - Fast to converge
  - Results in probabilistic cluster assignment
- Disadvantages
  - Has an element of randomness – final model may differ depending on initial parameters
  - Can get stuck in a local maximum; not guaranteed to find the maximum-likelihood solution
  - The number of clusters (k) must be assumed

Unsupervised evaluation

Why do unsupervised learning?

reduce dimensionality

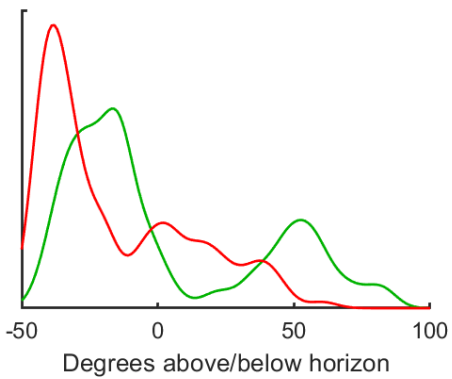
- Map high-dimensional data to a smaller set of clusters or latent factors
- Discover relationships / trends in data
- Model probability density function for probabilistic models (e.g., naïve Bayes)

Example: KDE naïve Bayes

- Naïve Bayes classifier chooses the class that maximizes the posterior probability:

$$\hat{c} = \arg\max_{c_j \in C} P(c_j) \prod_i P(x_i | c_j)$$

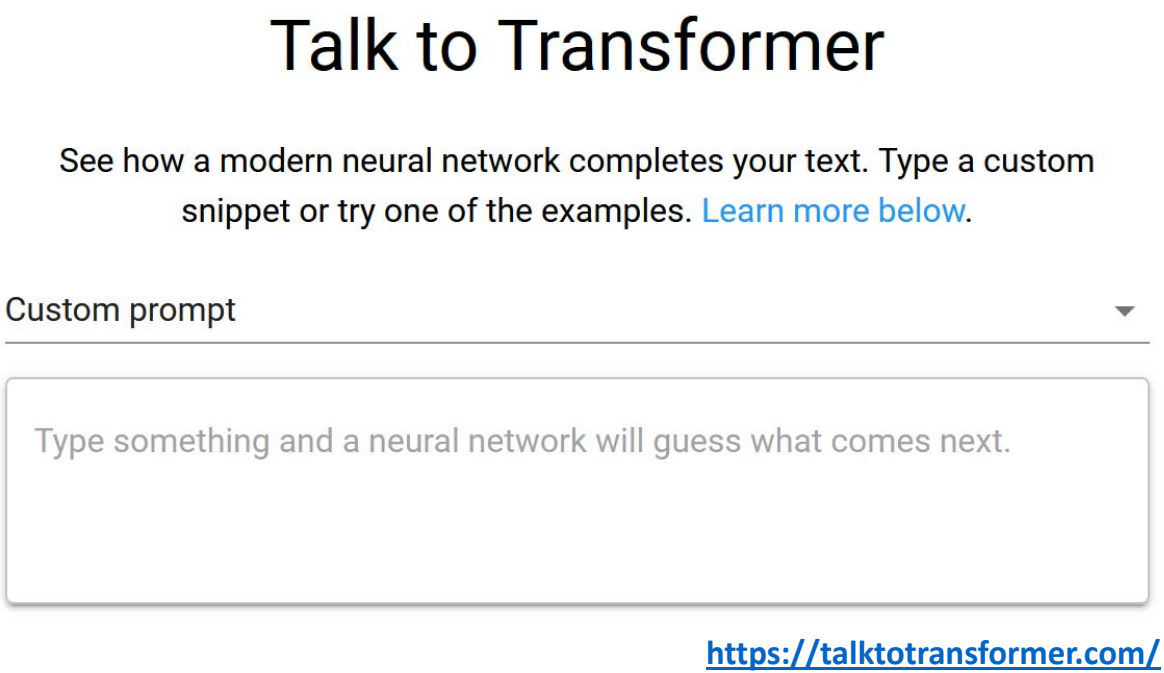
- Likelihood $P(x_i | c_j)$ can be computed by KDE:



Why do unsupervised learning?

- Map high-dimensional data to a smaller set of clusters or latent factors
- Discover relationships / trends in data
- Model probability density function for probabilistic models (e.g., naïve Bayes)
- Generate new samples from the modelled probability distribution

Example: Text generation



https://talktotransformer.com/

Unsupervised learning: Evaluation

- No “ground truth” labels – how to tell if a model is correct, or if one model is better than another?
  - Subjective evaluation
  - Check similarity of clusters over multiple iterations
  - Cross-validation: train on a subset of data and see how well the model predicts held-out data
  - Supervised evaluation: if labels are available, compare how well the discovered clusters match the labels
- Ideally, the evaluation measure should be independent of the objective function used in the learning problem

Unsupervised cluster evaluation

- High cluster cohesion: instances in a given cluster should be closely related to each other

$$cohesion(C_i) = \frac{1}{\sum_{\mathbf{x},\mathbf{y} \in C_i} proximity(\mathbf{x}, \mathbf{y})}$$

→ distance measure
↘ mean near

- High cluster separation: instances in different clusters should be distinct from each other

$$separation(C_i, C_j) = \sum_{x \in C_i, y \in C_{j \neq i}} proximity(\mathbf{x}, \mathbf{y})$$

want high distance

Cluster compactness

- One way to evaluate the quality of clusters (especially for k-means) is sum of squared errors (SSE):

$$SSE = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} proximity(\mathbf{x}, \mathbf{c_i})^2$$

  where $\mathbf{c_i}$ is the centroid of cluster C_i

- Proximity measure is often Euclidean for numeric data, or Hamming for nominal

Sum of squared errors: Example

Cluster 1 centroid:				
sunny	**mild**	**high**	**no**	
sunny	hot	high	no	$1^2 = 1$
sunny	hot	high	yes	$2^2 = 4$
overcast	hot	high	no	$2^2 = 4$
rainy	mild	high	no	$1^2 = 1$
sunny	mild	high	no	0
overcast	mild	high	yes	$2^2 = 4$
rainy	mild	high	yes	$2^2 = 4$

Cluster 2 centroid:			
overcast	**cool**	**normal**	**yes**
rainy	cool	normal	yes
overcast	cool	normal	yes
sunny	cool	normal	no
overcast	mild	normal	no
sunny	mild	normal	yes
overcast	hot	normal	no
rainy	cool	normal	no

$SSE_1 = 18$

$SSE_2 = 20$

$SSE = SSE_1 + SSE_2 = 38$

Supervised cluster evaluation

- If labels are available, evaluate the degree to which class labels are consistent within a cluster and different across clusters

want purity high
entropy low.

$$purity = \sum_{i=1}^{k} \frac{|C_i|}{N} \max_j P_i(j)$$

$$entropy = \sum_{i=1}^{k} \frac{|C_i|}{N} H(x_i)$$

where x_i is the distribution of class labels in cluster i

Supervised cluster evaluation

- Example: calculate the entropy and purity of following cluster output

Cluster	Play = yes	Play = no	Entropy	Purity
1	4	0	0	1
2	4	4	1	0.5

$-\frac{4}{4}\log\frac{4}{4} + 0\log 0 = 0$

$$entropy = -1\log(1) - 0\log(0) = 0$$

$$entropy = -0.5\log(0.5) - 0.5\log(0.5) = 1$$

most common lable

$$purity = \max(1,0) = 1$$

$$purity = \max(0.5,0.5) = 0.5$$

Supervised cluster evaluation

- Example: calculate the entropy and purity of following cluster output

Cluster	Play = yes	Play = no	Entropy	Purity
1	4	0	0	1
2	4	4	1	0.5
Total:			**0.67**	**0.67**

weighted average

$$entropy = \left(\frac{4}{12}\right)0 + \left(\frac{8}{12}\right)1 = 0.67$$

$$purity = \left(\frac{4}{12}\right)1 + \left(\frac{8}{12}\right)0.5 = 0.67$$

Supervised cluster evaluation

- Example: calculate the entropy and purity of following cluster output

Cluster	Play = yes	Play = no	Entropy	Purity
1	2	0	0	1
2	6	4	0.97	0.6

$$entropy = -1\log(1) - 0\log(0) = 0$$

$$entropy = -0.6\log(0.6) - 0.4\log(0.4) = 0.97$$

$$purity = \max(1,0) = 1$$

$$purity = \max(0.6,0.4) = 0.6$$

Supervised cluster evaluation

- Example: calculate the entropy and purity of following cluster output

Cluster	Play = yes	Play = no	Entropy	Purity
1	2	0	0	1
2	6	4	0.97	0.6
Total:			**0.81**	**0.67**

$$entropy = \left(\frac{2}{12}\right)0 + \left(\frac{10}{12}\right)0.97 = 0.81$$

$$purity = \left(\frac{2}{12}\right)1 + \left(\frac{10}{12}\right)0.6 = 0.67$$

Summary

- Unsupervised learning = finding structure in unlabelled data
- Methods to fit probability distributions to data:
  - Gaussian mixture
  - Kernel density estimation
- Expectation-maximization (EM) algorithm: family of algorithms to find maximum likelihood parameters for a model

finite mixture

unsupervised learning