机器学习与数据挖掘

Machine Learning & Data Mining

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Preface

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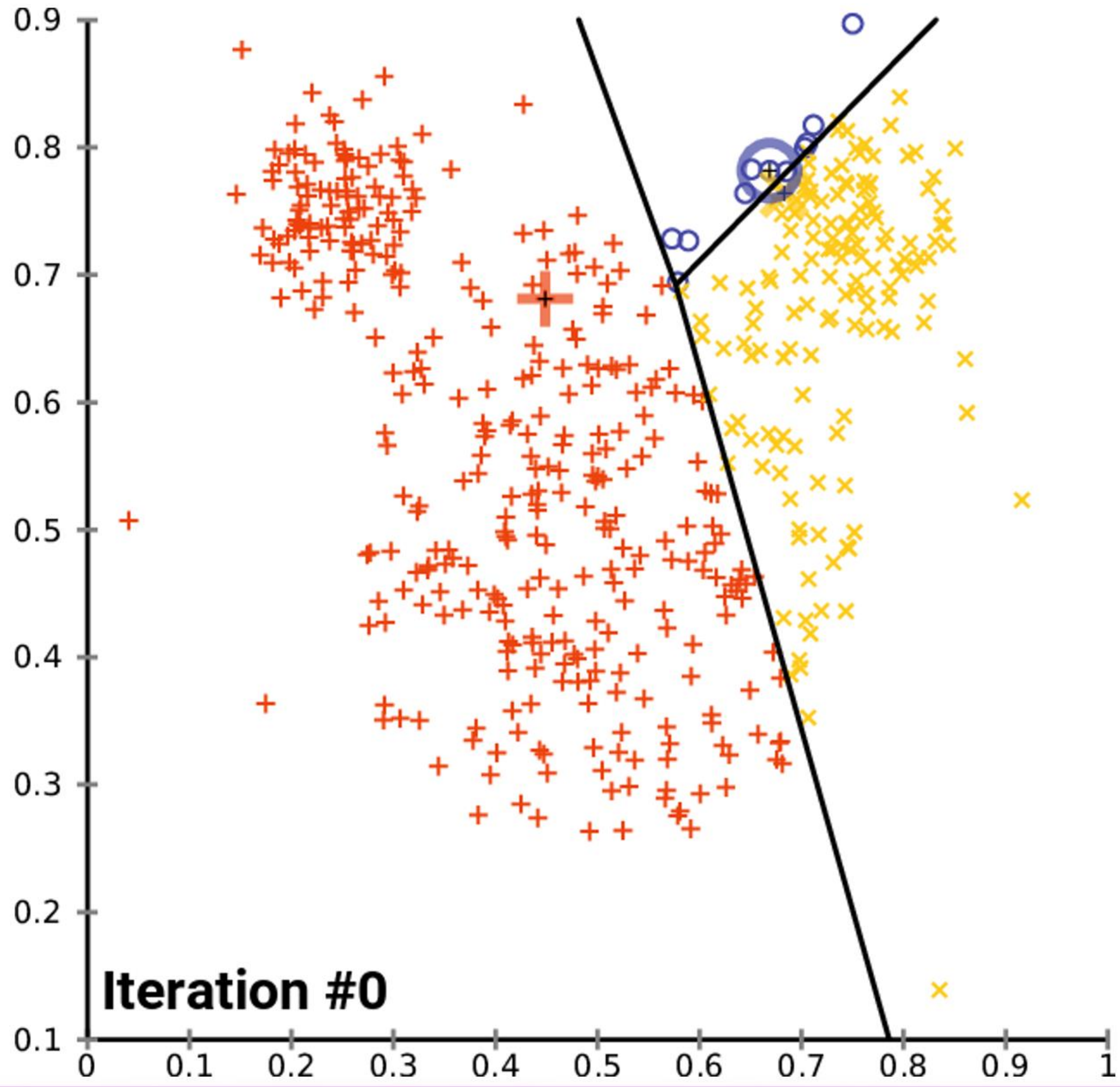

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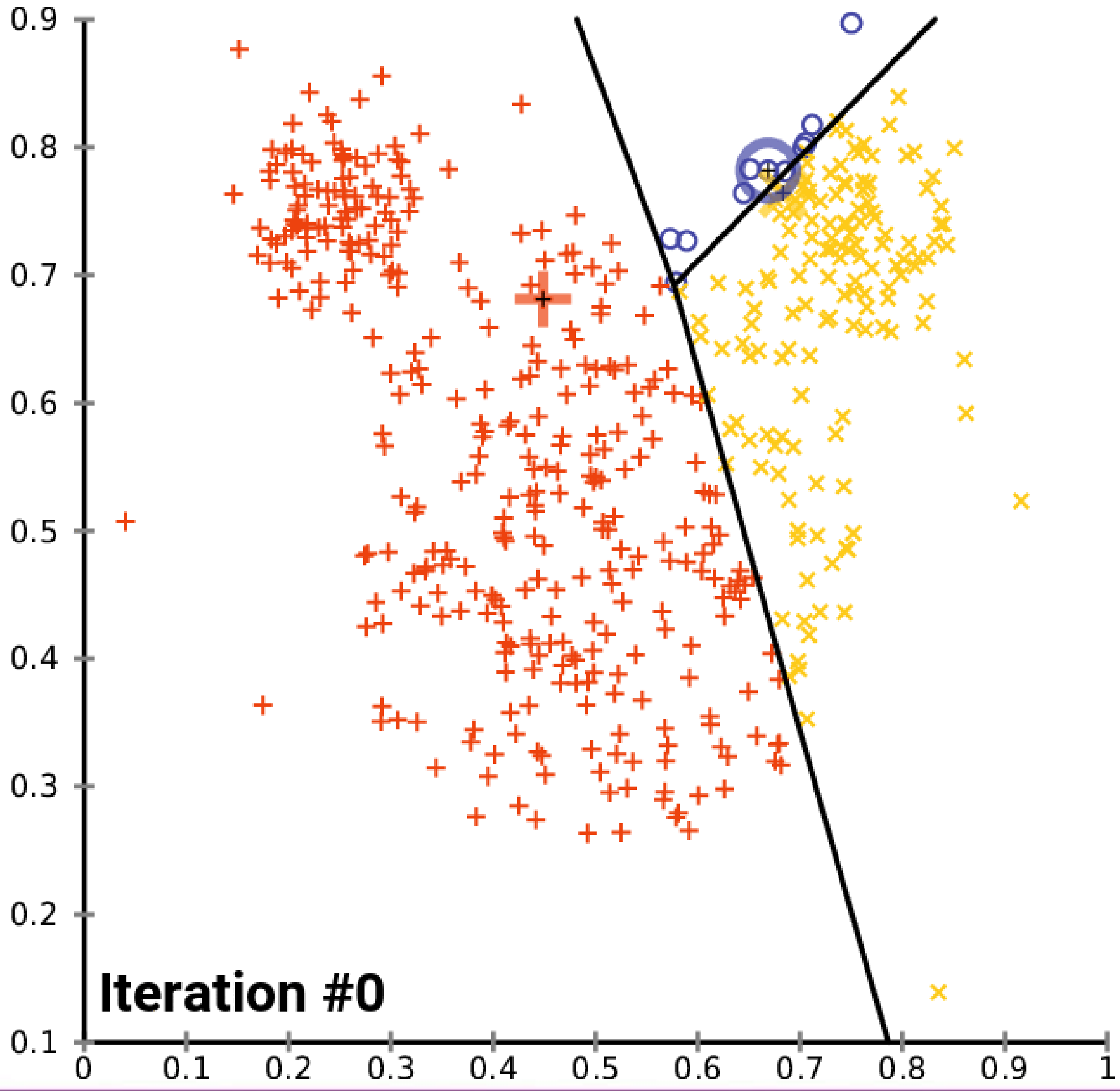
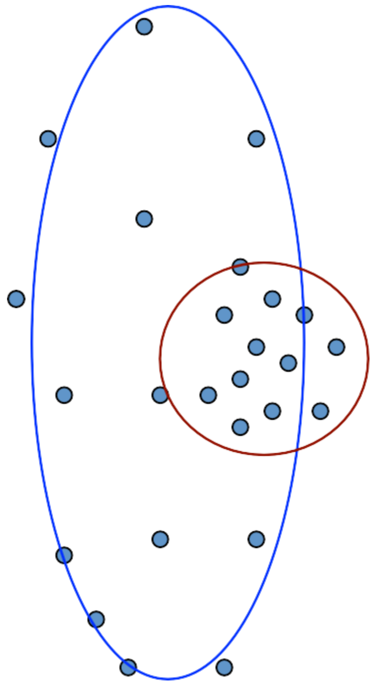


Preface

The Evils of "**Hard Assignments**"?



- Clusters may overlap
- Some clusters may be "wider" than others
- Distances can be deceiving!

Lecture 16:
Expectation Maximization

A Generative View of Clustering

- We need a sensible measure of what it means to cluster the data well
  - This makes it possible to judge different methods
  - It may help us decide on the number of clusters
- An obvious approach is to imagine that the data was produced by a generative model
  - Then we adjust the model parameters to maximize the probability that it would produce exactly the data we observed

Generative Models

- We model the joint distribution as,

$$p(\mathbf{x}, z) = p(\mathbf{x}|z)p(z)$$

- But in unsupervised clustering we do not have the class labels z .
- What can we do instead?

$$p(\mathbf{x}) = \sum_z p(\mathbf{x}, z) = \sum_z p(\mathbf{x}|z)p(z)$$

- This is a mixture model.

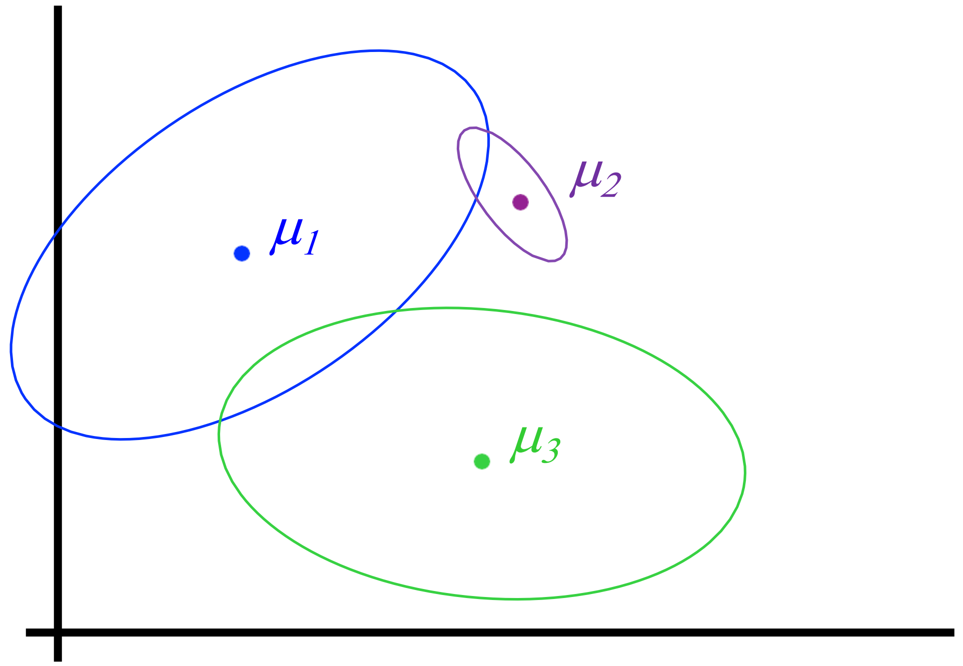
The General GMM assumption

- P(Z): There are k components
- P(X|Z): Each component generates data from a **multivariate Gaussian** with mean μ_i and covariance matrix Σ_i

The General GMM assumption

Each data point is sampled from a ***generative process***:

1. Choose component *i* with probability $P(z=i)$
2. Generate datapoint ~ $N(m_i, \Sigma_i)$



Gaussian Mixture Model (GMM)

Most common mixture model: Gaussian mixture model (GMM)

- A GMM represents a **distribution** as

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

with π_k the mixing coefficients, where:

$$\sum_{k=1}^{K} \pi_k = 1 \quad \text{and} \quad \pi_k \geq 0 \quad \forall k$$

- GMM is a density estimator
- GMMs are **universal approximators of densities** (if you have enough Gaussians). Even diagonal GMMs are universal approximators.
- In general mixture models are very powerful, but harder to optimize

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- GMM is a density estimator

In probability and statistics, density estimation is the construction of an estimate, based on observed data, of an unobservable underlying probability density function.

- In general mixture models are very powerful, but harder to optimize

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Most common mixture model: Gaussian mixture model (GMM)

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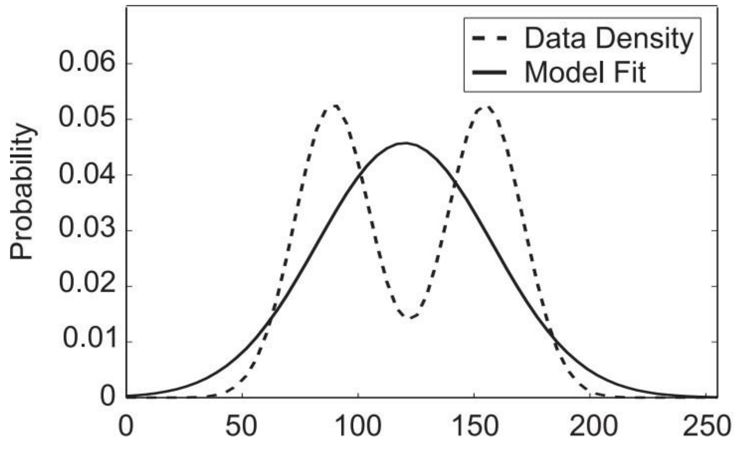
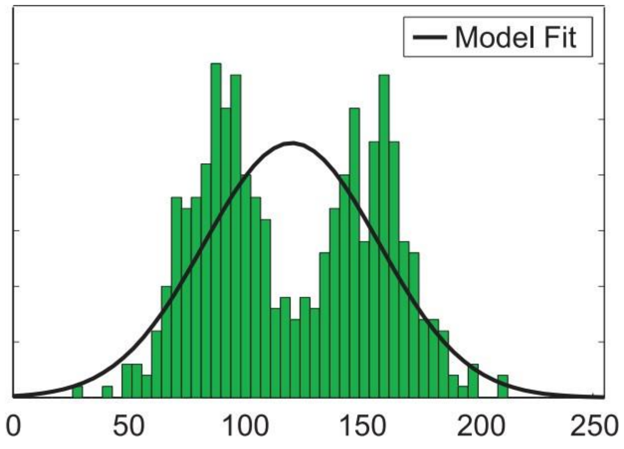
- GMM is a density estimator
- GMMs are **universal approximators of densities** (if you have enough Gaussians).
- In general mixture models are very powerful, but harder to optimize

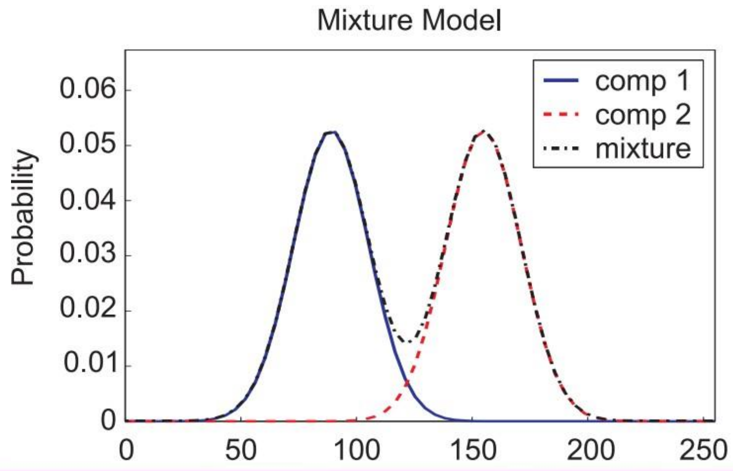
Visualizing a Mixture of Gaussians – 1D Gaussians

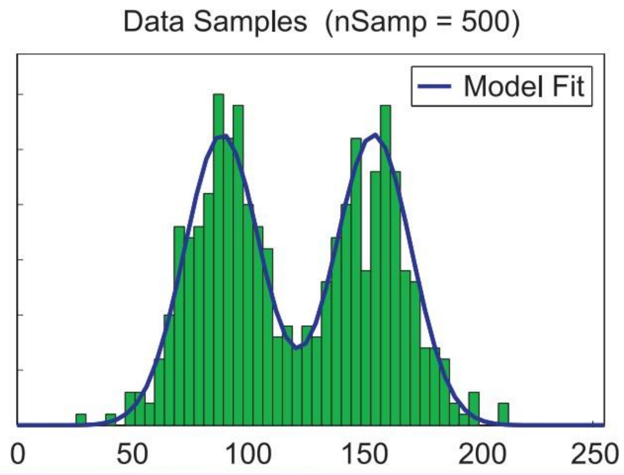
- If you fit a Gaussian to data:





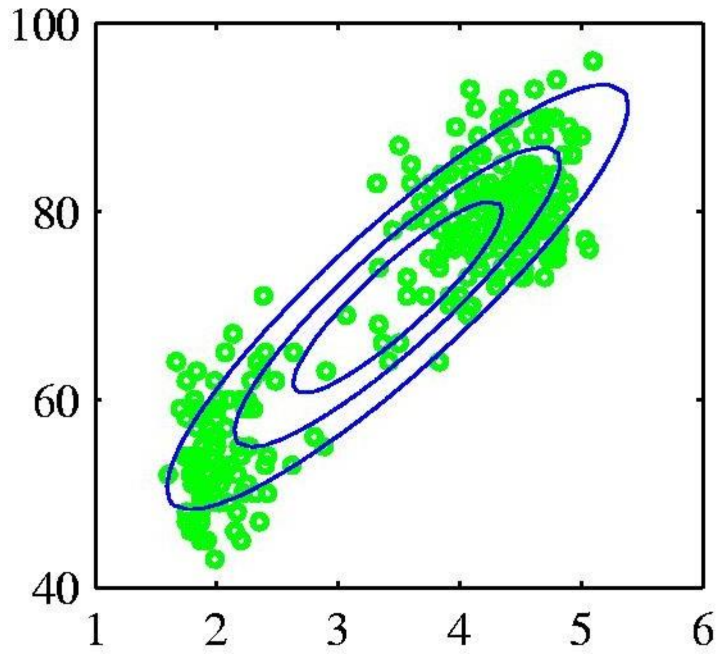
- Now, we are trying to fit a GMM (with $K = 2$ in this example):



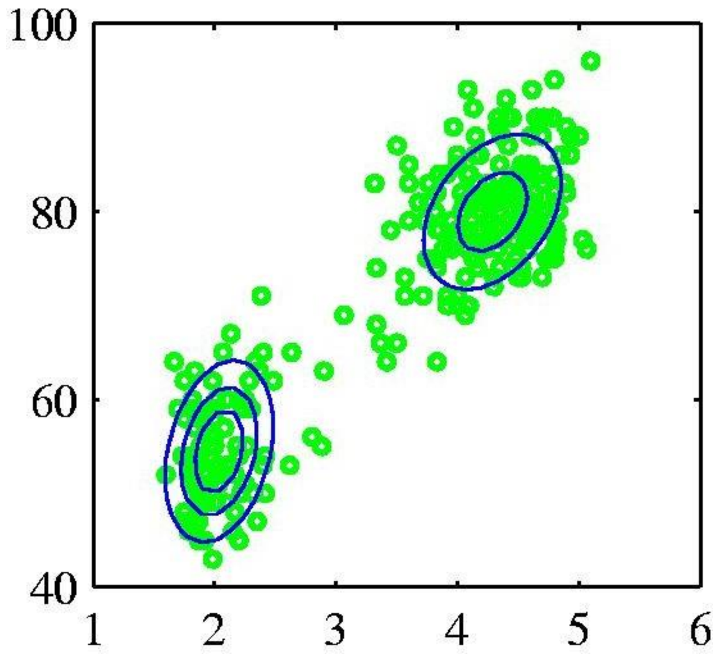


Visualizing a Mixture of Gaussians – 2D Gaussians

Old Faithful Data Set

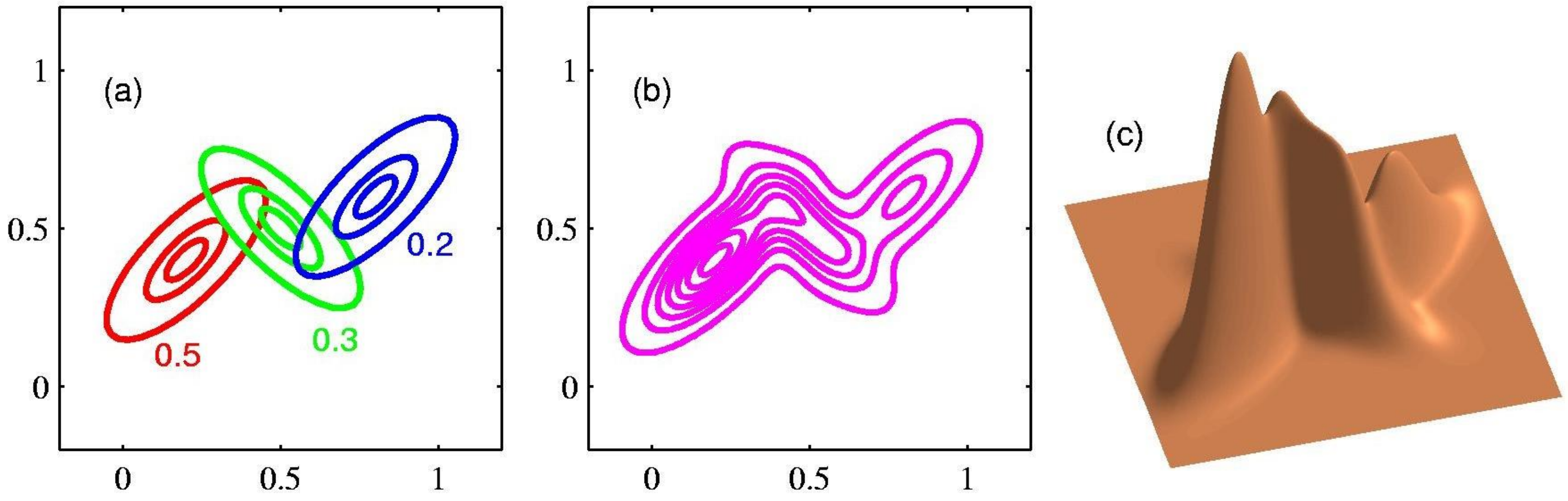


Single Gaussian



Mixture of two Gaussians

Visualizing a Mixture of Gaussians – 2D Gaussians



Fitting GMMs: Maximum Likelihood

- Maximum likelihood maximizes

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k) \right)$$

w.r.t $\Theta = \{\pi_k, \mu_k, \Sigma_k\}$

- How would you optimize this?
- Can we have a closed form update?
- Don't forget to satisfy the constraints on π_k and Σ_k

Latent Variable

- Our original representation had a hidden (latent) variable *z* which would represent which Gaussian generated our observation **x**, with some probability
- Let $z \sim \mathrm{Categorical}(\boldsymbol{\pi})$ (where $\pi_k \geq 0, \quad \sum_k \pi_k = 1$)
- Then:

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(\mathbf{x}, z = k)$$

$$= \sum_{k=1}^{K} \underbrace{p(z = k)}_{\pi_k} \underbrace{p(\mathbf{x}|z = k)}_{\mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}$$

- This breaks a complicated distribution into simple components.

Latent Variable Models

- Some model variables may be unobserved, either at training or at test time, or both
- If occasionally unobserved they are missing, e.g., undefined inputs, missing class labels, erroneous targets
- Variables which are always unobserved are called latent variables, or sometimes hidden variables
- We may want to intentionally introduce latent variables to model complex dependencies between variables – this can actually simplify the model
- Form of divide-and-conquer: use simple parts to build complex models
- In a mixture model, the identity of the component that generated a given datapoint is a latent variable

Back to GMM

- A Gaussian mixture distribution: $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$
- We had: $z \sim \mathrm{Categorical}(\boldsymbol{\pi})$ (where $\pi_k \geq 0$, $\sum_k \pi_k = 1$)
- Joint distribution: $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$
- Log-likelihood:

$$\begin{aligned}\ell(\boldsymbol{\pi}, \mu, \Sigma) = \ln p(\mathbf{X}|\pi, \mu, \Sigma) &= \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)}|\pi, \mu, \Sigma) \\ &= \sum_{n=1}^{N} \ln \sum_{z^{(n)}=1}^{K} p(\mathbf{x}^{(n)}|\, z^{(n)}; \mu, \Sigma) p(z^{(n)}|\, \boldsymbol{\pi})\end{aligned}$$

- Note: We have a hidden variable $z^{(n)}$ for every observation
- General problem: sum inside the log
- How can we optimize this?

Back to GMM

- A Gaussian mixture distribution: $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$
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$$\ell(\boldsymbol{\pi}, \mu, \Sigma) = \ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)}|\pi, \mu, \Sigma)$$

$$= \sum_{n=1}^{N} \ln \sum_{k=1}^{K} p(\mathbf{x}^{(n)}|\, z^{(n)}; \mu, \Sigma) p(z^{(n)}|\, \boldsymbol{\pi})$$

Relation to neural networks!

- Note: We have a hidden variable $z^{(n)}$ for every observation
- General problem: sum inside the log
- How can we optimize this?

Maximum Likelihood

- **If we knew** $z^{(n)}$ for every $x^{(n)}$, the maximum likelihood problem is easy:

$$\ell(\boldsymbol{\pi}, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(x^{(n)}, z^{(n)} | \pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)} | z^{(n)}; \mu, \Sigma) + \ln p(z^{(n)} | \boldsymbol{\pi})$$

- We would get this:

$$\mu_k = \frac{\sum_{n=1}^{N} 1_{[z^{(n)}=k]} \mathbf{x}^{(n)}}{\sum_{n=1}^{N} 1_{[z^{(n)}=k]}}$$

$$\Sigma_k = \frac{\sum_{n=1}^{N} 1_{[z^{(n)}=k]} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T}{\sum_{n=1}^{N} 1_{[z^{(n)}=k]}}$$

$$\pi_k = \frac{1}{N} \sum_{n=1}^{N} 1_{[z^{(n)}=k]}$$

How Can We Fit a Mixture of Gaussians?

- Optimization uses the Expectation Maximization algorithm, which alternates between two steps:
  1. E-step: Compute the posterior probability over *z* given our current model - i.e. how much do we think each Gaussian generates each datapoint.
  2. M-step: Assuming that the data really was generated this way, change the parameters of each Gaussian to maximize the probability that it would generate the data it is currently responsible for.

Relation to k-Means

- The K-Means Algorithm:
  1. Assignment step: Assign each data point to the closest cluster
  2. Refitting step: Move each cluster center to the center of gravity of the data assigned to it

Relation to k-Means

- The K-Means Algorithm:
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- The EM Algorithm:
  1. E-step: Compute the posterior probability over *z* given our current model
  2. M-step: Maximize the probability that it would generate the data it is currently responsible for.

Expectation Maximization for GMM Overview

- Elegant and powerful method for finding maximum likelihood solutions for models with latent variables

1. E-step:
   - In order to adjust the parameters, we must first solve the inference problem: Which Gaussian generated each datapoint?
   - We cannot be sure, so it's a distribution over all possibilities.

$$\gamma_k^{(n)} = p(z^{(n)} = k|\mathbf{x}^{(n)}; \pi, \mu, \Sigma)$$

2. M-step:
   - Each Gaussian gets a certain amount of posterior probability for each datapoint.
   - We fit each Gaussian to the weighted datapoints
   - We can derive closed form updates for all parameters

Where does EM come from? I

- Remember that optimizing the likelihood is hard because of the sum inside of the log. Using Θ to denote all of our parameters:

$$\ell(\mathbf{X}, \Theta) = \sum_i \log(P(\mathbf{x}^{(i)}; \Theta)) = \sum_i \log\left(\sum_j P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)\right)$$

- We can use a common trick in machine learning, introduce a new distribution, *q*:

$$\ell(\mathbf{X}, \Theta) = \sum_i \log\left(\sum_j q_j \frac{P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)}{q_j}\right)$$

- Now we can swap them! Jensen's inequality - for concave function (like log)

$$f(\mathbb{E}[x]) = f\left(\sum_i p_i x_i\right) \geq \sum_i p_i f(x_i) = \mathbb{E}[f(x)]$$

Where does EM come from? II

- Applying Jensen's,

$$\sum_i \log\left(\sum_j q_j \frac{P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)}{q_j}\right) \geq \sum_i \sum_j q_j \log\left(\frac{P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)}{q_j}\right)$$

- Maximizing this lower bound will force our likelihood to
- increase. But how do we pick a q_i that gives a good bound?

EM derivation

- We got the sum outside but we have an inequality.

$$\ell(\mathbf{X},\Theta) \geq \sum_i \sum_j q_j \log\left(\frac{P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)}{q_j}\right)$$

- Lets fix the current parameters to Θ^{old} and try to find a good q_i
- What happens if we pick $q_j = p(z^{(i)} = j|x^{(i)}, \Theta^{old})$?

$\frac{P(\mathbf{x}^{(i)}, z^{(i)}; \Theta)}{p(z^{(i)} = j|x^{(i)}, \Theta^{old})} = P(\mathbf{x}^{(i)}; \Theta^{old})$ and the inequality becomes an equality!

- We can now define and optimize

$$\begin{aligned} Q(\Theta) &= \sum_i \sum_j p(z^{(i)} = j|x^{(i)}, \Theta^{old}) \log\left(P(\mathbf{x}^{(i)}, z^{(i)} = j; \Theta)\right) \\ &= \mathbb{E}_{P(z^{(i)}|\mathbf{x}^{(i)}, \Theta^{old})}[\log\left(P(\mathbf{x}^{(i)}, z^{(i)}; \Theta)\right)] \end{aligned}$$

- We ignored the part that doesn't depend on Θ

EM derivation

- So, what just happened?
- Conceptually: We don't know $z^{(i)}$ so we average them given the current model.
- Practically: We define a function

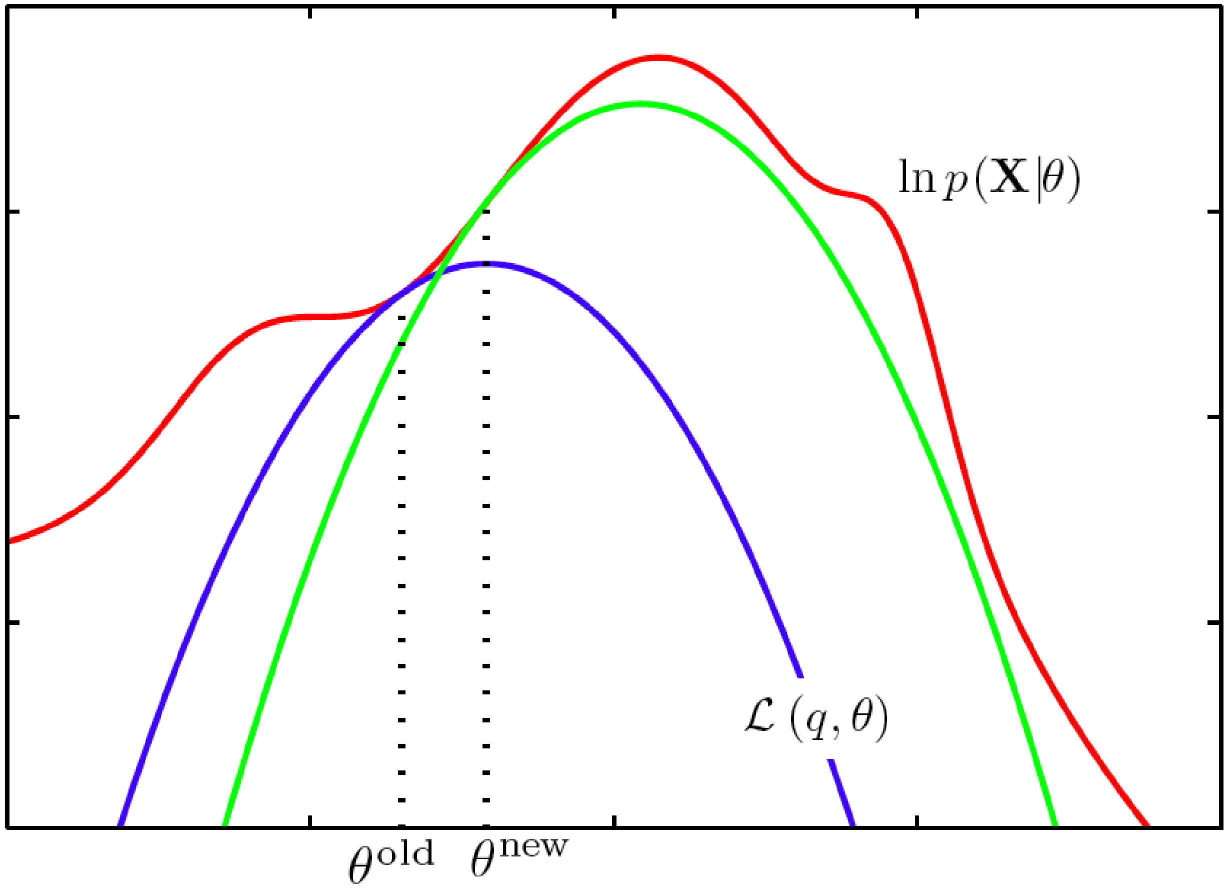
  $Q(\Theta) = \mathbb{E}_{P(z^{(i)}|\mathbf{x}^{(i)},\Theta^{old})}[\log\left(P(\mathbf{x}^{(i)}, z^{(i)}; \Theta)\right)]$ that lower bounds the desired function and is equal at our current guess.

- If we now optimize Θ we will get a better lower bound!

$$\log(P(\mathbf{X}|\Theta^{old})) = Q(\Theta^{old}) \leq Q(\Theta^{new}) \leq \log(P(\mathbf{X}|\Theta^{new}))$$

- We can iterate between expectation step and maximization step and the lower bound will always improve (or we are done)

Visualization of the EM Algorithm



- The EM algorithm involves alternately computing a lower bound on the log likelihood for the current parameter values and then maximizing this bound to obtain the new parameter values.

General EM Algorithm

1. Initialize Θ^{old}
2. E-step: Evaluate $p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$ and compute

$$Q(\Theta, \Theta^{old}) = \sum_{z} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\Theta)$$

3. M-step: Maximize

$$\Theta^{new} = arg \max_{\Theta} Q(\Theta, \Theta^{old})$$

4. Evaluate log likelihood and check for convergence (or the parameters). If not converged, $\Theta^{old} = \Theta^{new}$, Go to step 2

GMM E-Step: Responsibilities

Lets see how it works on GMM:

- Conditional probability (using Bayes rule) of **z** given **x**

$$
\begin{aligned}
\gamma_k = p(z=k|\mathbf{x}) &= \frac{p(z=k)p(\mathbf{x}|z=k)}{p(\mathbf{x})} \\
&= \frac{p(z=k)p(\mathbf{x}|z=k)}{\sum_{j=1}^{K} p(z=j)p(\mathbf{x}|z=j)} \\
&= \frac{\pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j, \Sigma_j)}
\end{aligned}
$$

- γ_k can be viewed as the responsibility of cluster *k* towards **x**

GMM E-Step

- Once we computed $\gamma_k^{(i)} = p(z^{(i)} = k|\mathbf{x}^{(i)})$ we can compute the expected likelihood

$$\begin{aligned}
&\mathbb{E}_{P(z^{(i)}|\mathbf{x}^{(i)})}\left[\sum_i \log(P(\mathbf{x}^{(i)}, z^{(i)}|\Theta))\right] \\
= &\sum_i \sum_k \gamma_k^{(i)} \left(\log(P(z^i = k|\Theta)) + \log(P(\mathbf{x}^{(i)}|z^{(i)} = k, \Theta))\right) \\
= &\sum_i \sum_k \gamma_k^{(i)} \left(\log(\pi_k) + \log(\mathcal{N}(\mathbf{x}^{(i)}; \mu_k, \Sigma_k))\right) \\
= &\sum_k \sum_i \gamma_k^{(i)} \log(\pi_k) + \sum_k \sum_i \gamma_k^{(i)} \log(\mathcal{N}(\mathbf{x}^{(i)}; \mu_k, \Sigma_k))
\end{aligned}$$

- We need to fit k Gaussians, just need to weight examples by γ_k

GMM M-Step

- Need to optimize

$$\sum_k \sum_i \gamma_k^{(i)} \log(\pi_k) + \sum_k \sum_i \gamma_k^{(i)} \log(\mathcal{N}(\mathbf{x}^{(i)}; \mu_k, \Sigma_k))$$

- Solving for μ_k and Σ_k is like fitting k separate Gaussians but with weights $\gamma_k^{(i)}$

- Solution is similar to what we have already seen:

$$\begin{aligned}
\mu_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} \mathbf{x}^{(n)} \\
\Sigma_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T \\
\pi_k &= \frac{N_k}{N} \quad \text{with} \quad N_k = \sum_{n=1}^{N} \gamma_k^{(n)}
\end{aligned}$$

EM Algorithm for GMM

- Initialize the means μ_k , covariances Σ_k and mixing coefficients π_k
- Iterate until convergence:

  E-step: Evaluate the responsibilities given current parameters

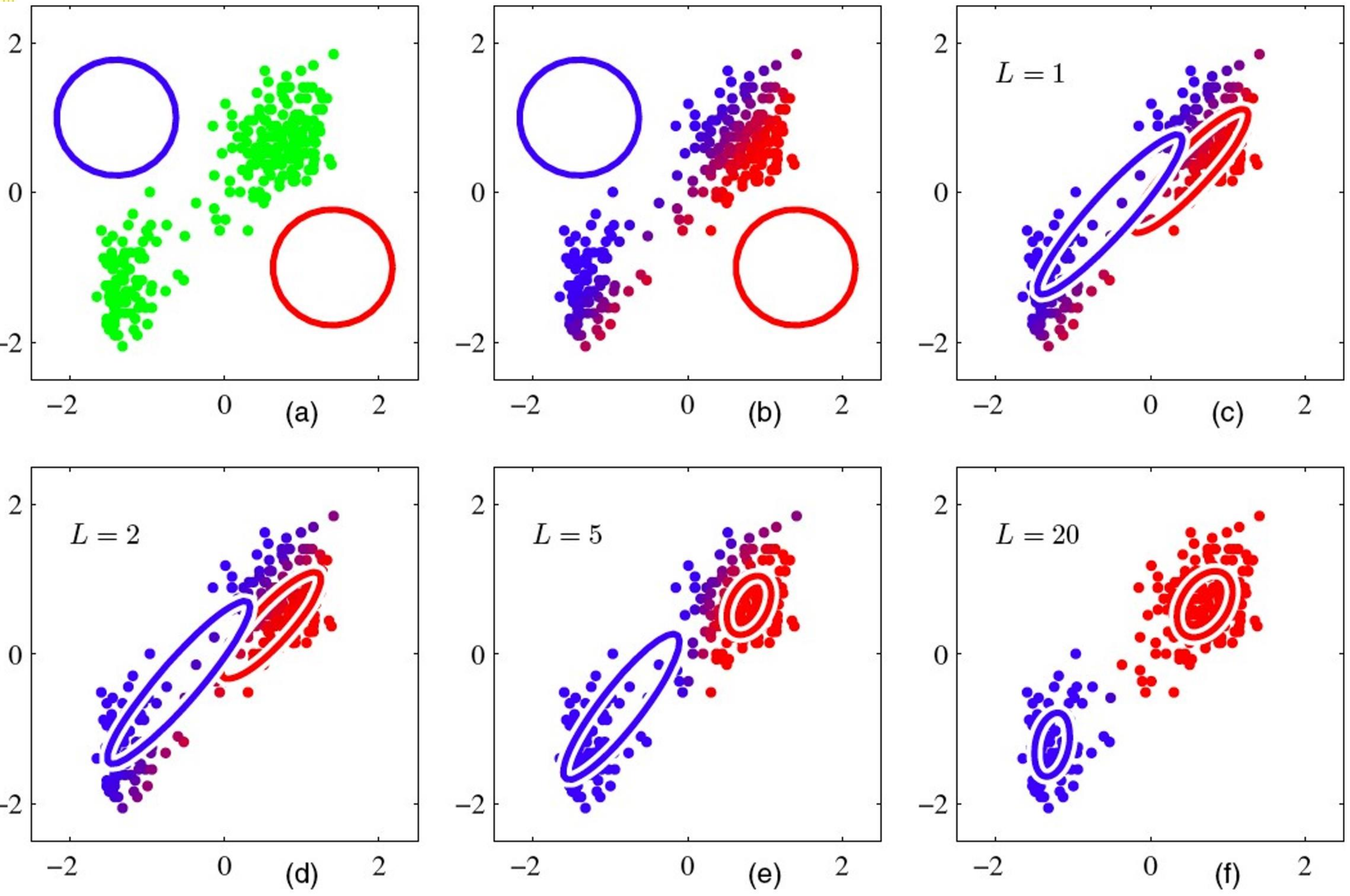
$$\gamma_k^{(n)} = p(z^{(n)}|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\mu_j, \Sigma_j)}$$

  M-step: Re-estimate the parameters given current responsibilities

$$\begin{aligned}
\mu_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} \mathbf{x}^{(n)} \\
\Sigma_k &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T \\
\pi_k &= \frac{N_k}{N} \quad \text{with} \quad N_k = \sum_{n=1}^{N} \gamma_k^{(n)}
\end{aligned}$$

  Evaluate log likelihood and check for convergence

$$\ln p(\mathbf{X}|\pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k) \right)$$


(a)
(b)
L = 1
(c)
L = 2
(d)
L = 5
(e)
L = 20
(f)

Mixture of Gaussians vs. K-means

- EM for mixtures of Gaussians is just like a soft version of K-means, with fixed priors and covariance
- Instead of hard assignments in the E-step, we do soft assignments based on the softmax of the squared Mahalanobis distance from each point to each cluster.
- Each center moved by weighted means of the data, with weights given by soft assignments
- In K-means, weights are 0 or 1

EM alternative approach *

- Our goal is to maximize

$$p(\mathbf{X}|\Theta) = \sum_{\mathbf{z}} p(\mathbf{X}, \mathbf{z}|\Theta)$$

- Typically optimizing $p(\mathbf{X}|\Theta)$ is difficult, but $p(\mathbf{X}, \mathbf{Z}|\Theta)$ is easy
- Let $q(\mathbf{Z})$ be a distribution over the latent variables. For any distribution $q(\mathbf{Z})$ we have

$$\ln p(\mathbf{X}|\Theta) = \mathrm{L}(q, \Theta) + KL(q||p(\mathbf{Z}|\mathbf{X}, \Theta))$$

where

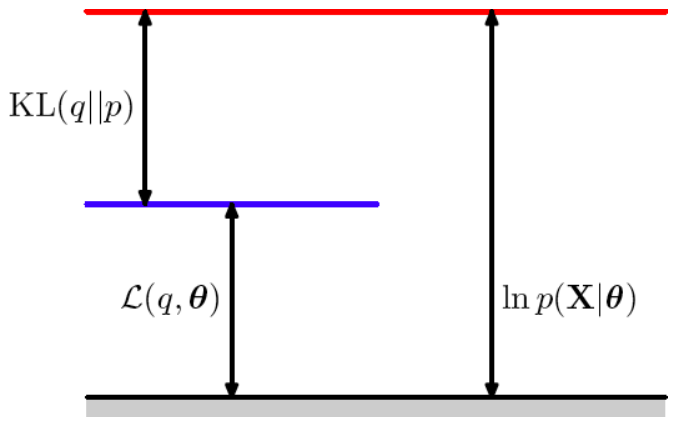
$$\begin{aligned} \mathcal{L}(q, \Theta) &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{q(\mathbf{Z})} \right\} \\ KL(q||p) &= -\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \Theta)}{q(\mathbf{Z})} \right\} \end{aligned}$$

EM alternative approach *

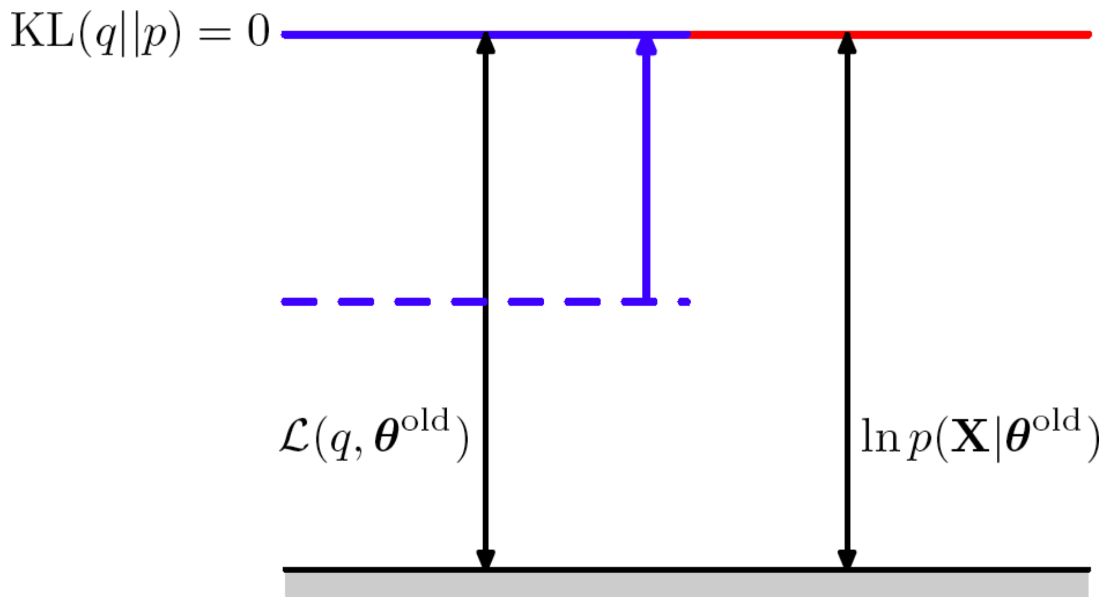
- The KL-divergence is always positive and have value 0 only if $q(Z) = p(\mathbf{Z}|\mathbf{X}, \Theta)$

- Thus $L(q, \Theta)$ is a lower bound on the likelihood

$$L(q, \Theta) \leq \ln p(\mathbf{X}|\Theta)$$

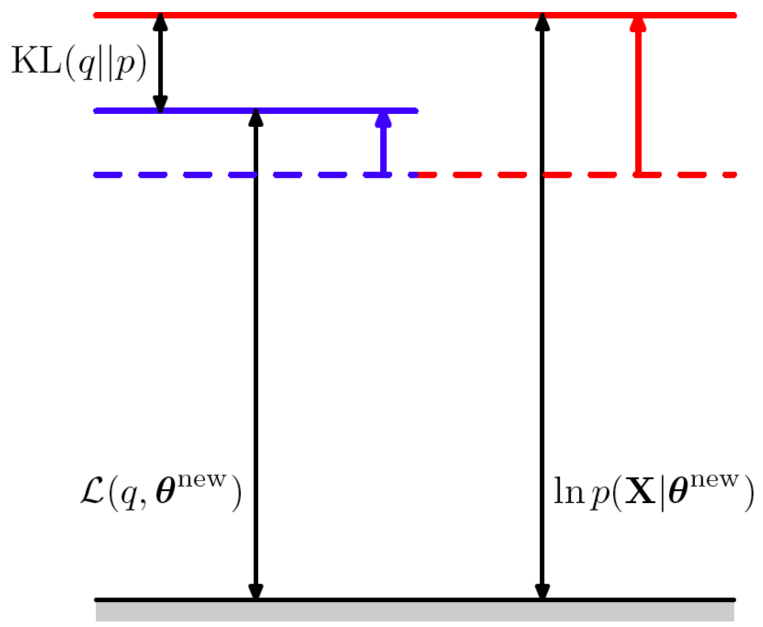

$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

Visualization of E-step


$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$

- The *q* distribution equal to the posterior distribution for the current parameter values Θ^{old} , causing the lower bound to move up to the same value as the log likelihood function, with the KL divergence vanishing.

Visualization of M-step


$\mathrm{KL}(q||p)$
$\mathcal{L}(q,\boldsymbol{\theta}^{\mathrm{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{new}})$

- The distribution $q(\mathbf{Z})$ is held fixed and the lower bound $L(q, \Theta)$ is maximized with respect to the parameter vector Θ to give a revised value Θ^{new}. Because the KL divergence is nonnegative, this causes the log likelihood $\ln p(\mathbf{X}|\Theta)$ to increase by at least as much as the lower bound does.

E-step and M-step *

$$\ln p(\mathbf{X}|\Theta) = \mathcal{L}(q,\Theta) + KL(q||p(\mathbf{Z}|\mathbf{X},\Theta))$$

- In the E-step we maximize q(Z) w.r.t the lower bound L(q;old)
- This is achieved when $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\Theta^{old})$
- The lower bound L is then

$$\begin{aligned}\mathcal{L}(q,\Theta) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \ln p(\mathbf{X},\mathbf{Z}|\Theta) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \ln p(\mathbf{Z}|\mathbf{X},\Theta^{old}) \\ &= Q(\Theta,\Theta^{old}) + \text{const}\end{aligned}$$

- with the content the entropy of the *q* distribution, which is independent of Θ
- In the M-step the quantity to be maximized is the expectation of the complete data log-likelihood
- Note that Θ is only inside the logarithm and optimizing the complete data likelihood is easier

GMM Recap

- A probabilistic view of clustering - Each cluster corresponds to a different Gaussian.
- Model using latent variables.
- General approach, can replace Gaussian with other distributions (continuous or discrete)
- More generally, mixture model are very powerful models, universal approximator
- Optimization is done using the EM algorithm.

EM Recap

- A general algorithm for optimizing many latent variable models.
- Iteratively computes a lower bound then optimizes it.
- Converges but maybe to a local minima.
- Can use multiple restarts.
- Can initialize from k-means
- Limitation - need to be able to compute $P(z \mid \mathbf{x}; \Theta)$, not possible for more complicated models.

Acknowledges

Slides from:

- CSC 411 Fall 2018 Machine Learning and Data Mining, Toronto University
- David Sontag, New York University

Thank you!

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