CSC 411: Lecture 13: Mixtures of Gaussians and EM

Richard Zemel, Raquel Urtasun and Sanja Fidler

University of Toronto

Today

- Mixture of Gaussians
- EM algorithm
- Latent Variables

A Generative View of Clustering

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  - Then we adjust the model parameters to maximize the probability that it would produce exactly the data we observed

Gaussian Mixture Model (GMM)

- A Gaussian mixture model 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:

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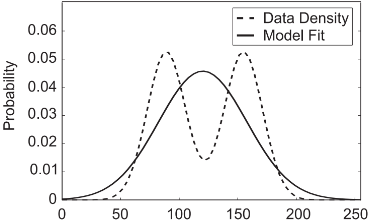
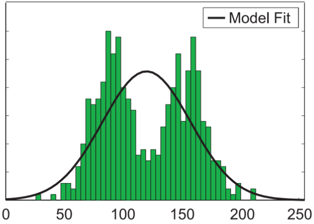
- GMMs are **universal approximators of densities** (if you have enough Gaussians). Even diagonal GMMs are universal approximators.

Visualizing a Mixture of Gaussians – 1D Gaussians

- In the beginning of class, we tried to fit a Gaussian to data:





[Slide credit: K. Kutulakos]

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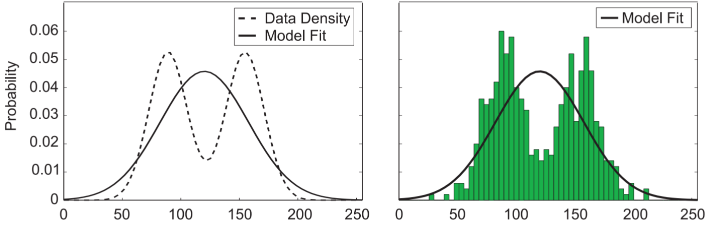
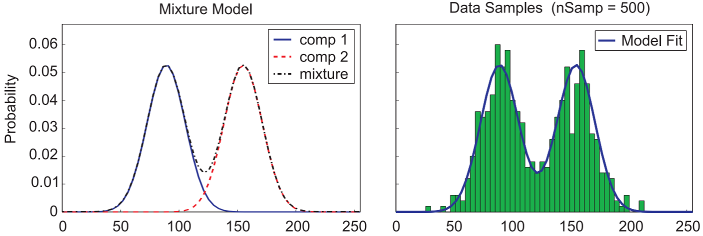


- Now, we are trying to fit a GMM (with $K = 2$ in this example):



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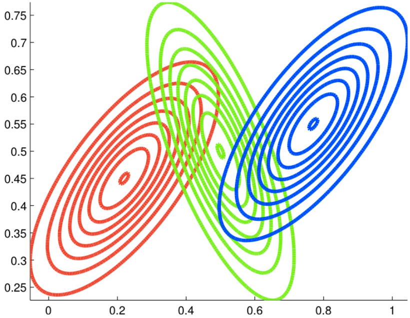

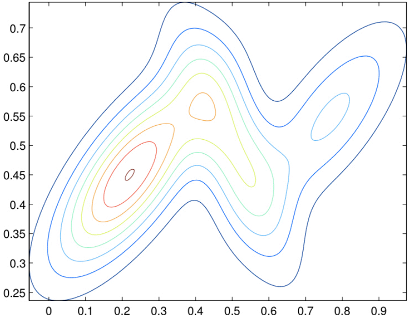

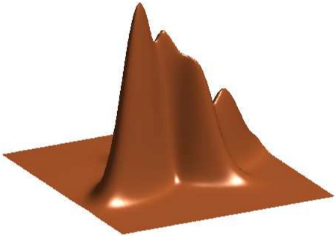

Fitting GMMs: Maximum Likelihood

- Maximum likelihood maximizes

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- Don't forget to satisfy the constraints on π_k

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- Then:

$$
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- In a mixture model, the identity of the component that generated a given datapoint is a latent variable

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- We would get this (check old slides):

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

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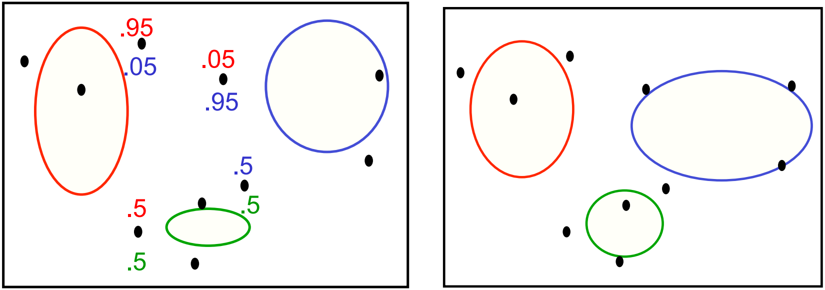

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   - We can derive closed form updates for all parameters

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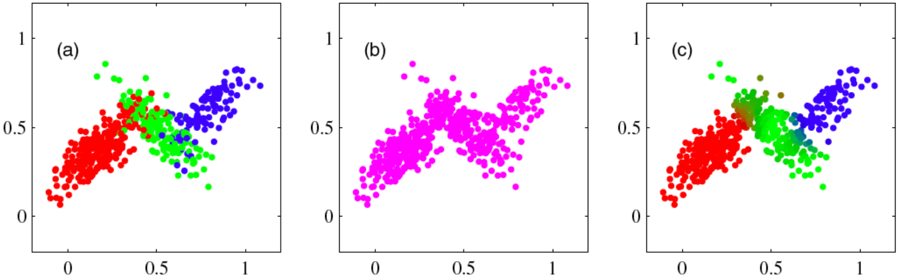

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- γ_k can be viewed as the responsibility

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- Set derivatives to 0:

$$\frac{\partial \ln p(\mathbf{X}|\pi, \mu, \Sigma)}{\partial \mu_k} = 0 = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j, \Sigma_j)} \Sigma_k(\mathbf{x}^{(n)} - \mu_k)$$

M-Step: Estimate Parameters

- Log-likelihood:

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

- Set derivatives to 0:

$$\frac{\partial \ln p(\mathbf{X}|\pi,\mu,\Sigma)}{\partial \mu_k} = 0 = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k,\Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\mu_j,\Sigma_j)} \Sigma_k(\mathbf{x}^{(n)} - \mu_k)$$

- We used:

$$\mathcal{N}(\mathbf{x}|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^d|\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\right)$$

and:

$$\frac{\partial(\mathbf{x}^T A\mathbf{x})}{\partial \mathbf{x}} = \mathbf{x}^T(A + A^T)$$

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- We just take the center-of gravity of the data that the Gaussian is responsible for
- Just like in K-means, except the data is weighted by the posterior probability of the Gaussian.
- Guaranteed to lie in the convex hull of the data (Could be big initial jump)

M-Step (variance, mixing coefficients)

- We can get similarly expression for the variance

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma_k^{(n)} (\mathbf{x}^{(n)} - \mu_k)(\mathbf{x}^{(n)} - \mu_k)^T$$

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- Note that this is not a closed form solution of the parameters, as they depend on the responsibilities $\gamma_k^{(n)}$, which are complex functions of the parameters
- But we have a simple iterative scheme to optimize

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

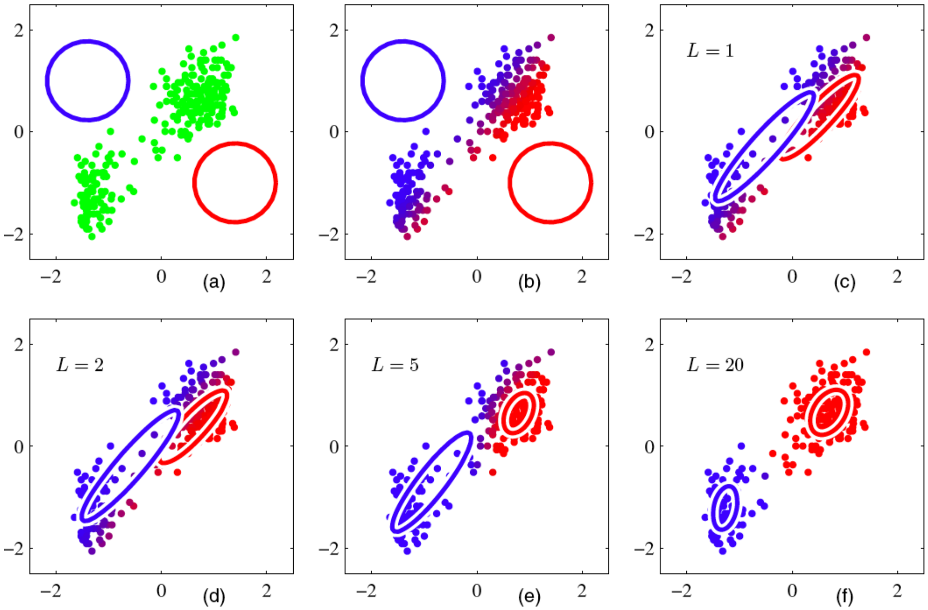
$$\gamma_k^{(n)} = p(z^{(n)}|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\mu_j, \Sigma_j)}$$

  - 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

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



2
0
−2
−2
0
2
(a)
(b)
(c)
(d)
(e)
(f)
$L = 1$
$L = 2$
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- In K-means, weights are 0 or 1

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- In the M-step we maximize w.r.t Θ

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

General EM Algorithm

1. Initialize Θ^{old}
2. E-step: Evaluate $p(\mathbf{Z}|\mathbf{X}, \Theta^{old})$
3. M-step:
$$\Theta^{new} = arg \max_{\Theta} Q(\Theta, \Theta^{old})$$
where
$$Q(\Theta, \Theta^{old}) = \sum_{z} p(\mathbf{Z}|\mathbf{X}, \Theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\Theta)$$
4. Evaluate log likelihood and check for convergence (or the parameters). If not converged, $\Theta^{old} = \Theta$, Go to step 2

- Beyond this slide, read if you are interested in more details

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  - But we know that the posterior will change after updating the parameters.
- A good way to show that this is OK is to show that there is a single function that is improved by both the E-step and the M-step.
  - The function we need is called Free Energy.

Why EM converges

- Free energy F is a cost function that is reduced by both the E-step and the M-step.

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- The entropy term encourages "soft" assignments. It would be happiest spreading the assignment probabilities for each datapoint equally between all the Gaussians.

Free Energy

- 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

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

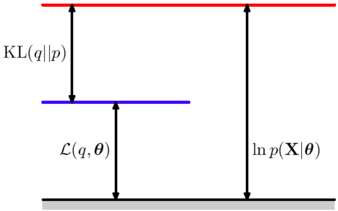
where

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

More on Free Energy

- Since the KL-divergence is always positive and have value 0 only if $q(Z) = p(\mathbf{Z}|\mathbf{X}, \Theta)$
- Thus $\mathcal{L}(q, \Theta)$ is a lower bound on the likelihood

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



E-step and M-step

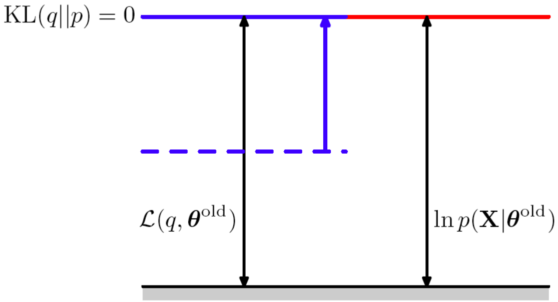
$$\ln p(\mathbf{X}|\Theta) = \mathcal{L}(q, \Theta) + KL(q||p(\mathbf{Z}|\mathbf{X}, \Theta))$$

- In the E-step we maximize w.r.t $q(\mathbf{Z})$ the lower bound $\mathcal{L}(q, \Theta)$
- Since $\ln p(\mathbf{X}|\theta)$ does not depend on $q(\mathbf{Z})$, the maximum $\mathcal{L}$ is obtained when the KL is 0
- This is achieved when $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \Theta)$
- The lower bound $\mathcal{L}$ is then

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

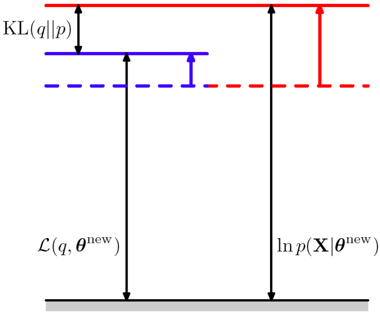
  with the content the entropy of the q distribution, which is independent of Θ
- In the M-step the quantity to be maximized is the expectation of the complete data log-likelihood
- Note that Θ is only inside the logarithm and optimizing the complete data likelihood is easier

Visualization of E-step



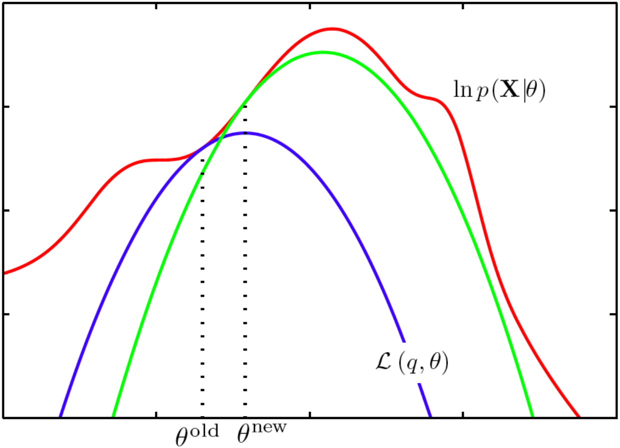
- The q distribution equal to the posterior distribution for the current parameter values Θ^{old}, causing the lower bound to move up to the same value as the log likelihood function, with the KL divergence vanishing.

Visualization of M-step



- The distribution $q(\mathbf{Z})$ is held fixed and the lower bound $\mathcal{L}(q, \Theta)$ 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.

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. See the text for a full discussion.

Summary: EM is coordinate descent in Free Energy

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

- The E-step minimizes F by finding the best distribution over hidden configurations for each data point.
- The M-step holds the distribution fixed and minimizes F by changing the parameters that determine the energy of a configuration.