CSC 4020 Fundamentals of Machine Learning:

Gaussian Mixture Models

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Apirl 26/28

[Slide credit: Mengye Ren and Matthew MacKay]

A Generative View of Clustering

- Last time: hard and soft k-means algorithm
- This lecture: statistical formulation of clustering $\rightarrow$ principled, justification for updates
- 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 Recap

- 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**

Gaussian Mixture Model (GMM)

Most common mixture model: **Gaussian mixture model** (GMM)

- A GMM represents a **distribution** as

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

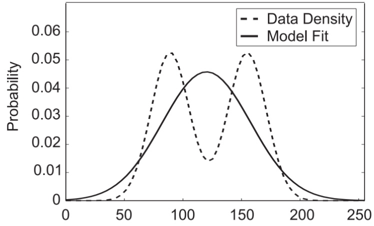
  with π_k the **mixing coefficients**, where:

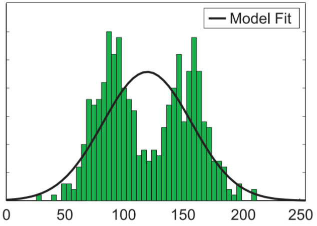
$$\sum_{k=1}^{K} \pi_k = 1 \quad \text{and} \quad \pi_k \geq 0 \quad \forall k$$

- 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

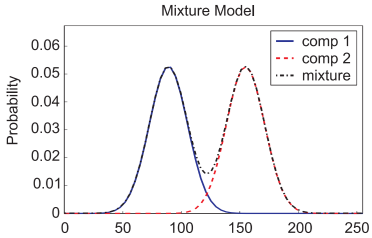
Visualizing a Mixture of Gaussians – 1D Gaussians

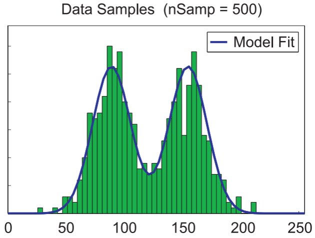
- If you fit a Gaussian to data:





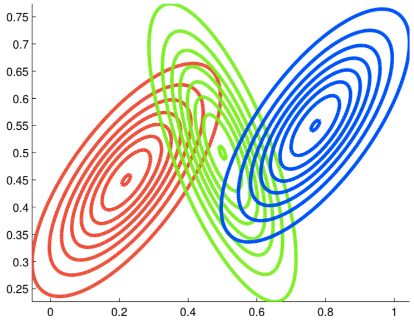
- Now, we are trying to fit a GMM (with $K = 2$ in this example):

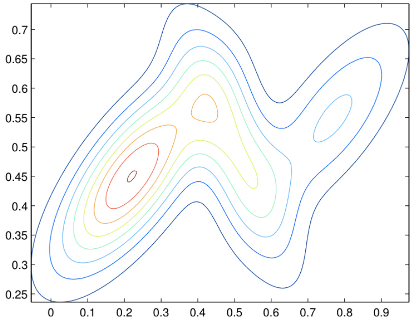


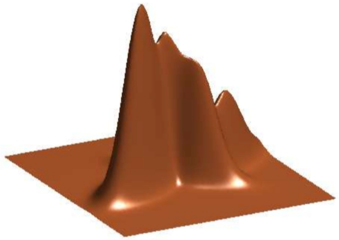


[Slide credit: K. Kutulakos]

Visualizing a Mixture of Gaussians – 2D Gaussians







Fitting GMMs: Maximum Likelihood

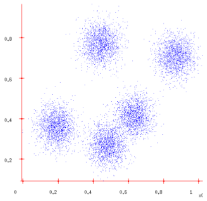
- Maximum likelihood maximizes

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

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

- Problems:
  - **Singularities**: Arbitrarily large likelihood when a Gaussian explains a single point
  - **Identifiability**: Solution is invariant to permutations
  - Non-convex
- 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 $\mathbf{x}$, with some probability
- Let $z \sim \mathrm{Categorical}(\boldsymbol{\pi})$ (where $\pi_k \geq 0$, $\sum_k \pi_k = 1$)
- Then:

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

- This breaks a complicated distribution into simple components - the price is the hidden variable.

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: $z \sim \text{Categorical}(\boldsymbol{\pi})$ (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?

Maximum Likelihood

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

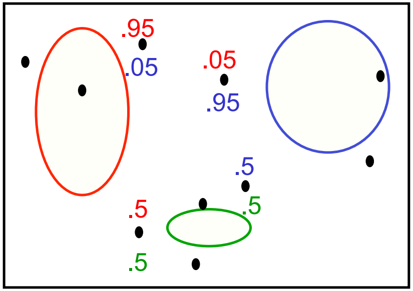
$$\ell(\boldsymbol{\pi}, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(x^{(n)}, z^{(n)} | \pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln p(\mathbf{x}^{(n)} |\, z^{(n)}; \mu, \Sigma) + \ln p(z^{(n)} |\, \boldsymbol{\pi})$$

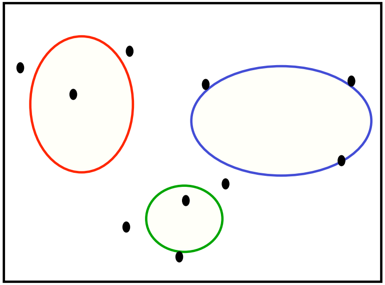
- We have been optimizing something similar for Gaussian bayes classifiers
- We would get this:

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

Intuitively, 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
- 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

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

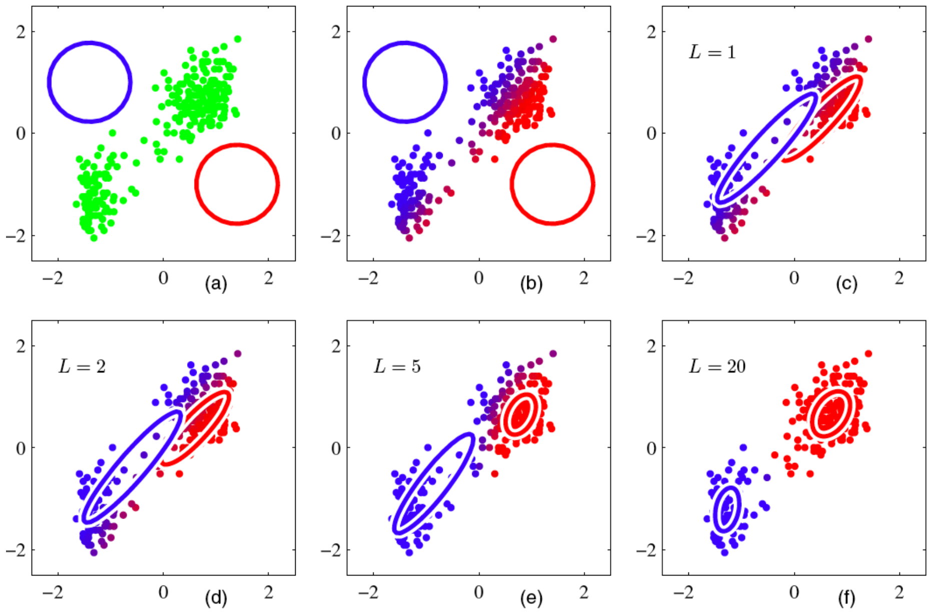
$$\gamma_k^{(n)} = p(z^{(n)}|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}^{(n)}|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}^{(n)}|\mu_j, \Sigma_j)}$$

  - **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)
−2
0
2

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

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.

Where does EM come from?

- In the next lecture, we'll see a principled justification of the EM algorithm and describe how it can be applied to general latent variable models