Gaussian Mixture Models, Expectation Maximization

Instructor: Jessica Wu -- Harvey Mudd College

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Gaussian Mixture Models Overview

Learning Goals

• Describe the differences between $k$-means and GMMs
K-Means: Another View

- Initialize cluster centers
- Assign examples to closest center
- $k$-means assumes spherical clusters
- Update cluster centers

Gaussian Mixture Models

- Assume data came from mixture of Gaussians (elliptical data)
- Assign data to cluster with certain probability (soft clustering)

- Very similar at high-level to $k$-means: iterate between assigning examples and updating cluster centers

Based on slides by David Kauchak
GMM Example

initialize cluster centers  soft cluster examples  update cluster centers
(based on weighted contribution of examples)

keep iterating...

Based on slides by David Kauchak [Images by Chris Bishop, PRML]

Learning GMMs

Learning Goals

• Describe the technical details of GMMs
Univariate Gaussian Distribution

(scalar) random variable $X$
parameters: (scalar) mean $\mu$, (scalar) variance $\sigma^2$

$$X \sim N(\mu, \sigma^2) \quad p(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( \frac{-1}{2\sigma^2} (x - \mu)^2 \right)$$

Multivariate Gaussian Distribution

random variable vector $\mathbf{X} = [X_1, \ldots, X_n]^T$
parameters: mean vector $\mu \in \mathbb{R}^n$
covariance matrix $\Sigma$ (symmetric, positive definite)

$$\mathbf{X} \sim N(\mu, \Sigma) \quad p(\mathbf{x}; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^n|\Sigma|}} \exp \left( -\frac{1}{2} (\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu) \right)$$
Covariance Matrix

Recall for pair of r.v.’s $X$ and $Y$, covariance is defined as
\[
\text{cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]
\]

For $X = [X_1, \ldots, X_n]^T$, covariance matrix summarizes covariances across all pairs of variables:
\[
\Sigma = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T]
\]
\[
\Sigma \text{ is } n \times n \text{ matrix s.t. } \Sigma_{ij} = \text{cov}(X_i, X_j)
\]

GMMs as Generative Model

• There are $k$ components
• Component $j$
  – has associated mean vector $\mu_j$ and covariance matrix $\Sigma_j$
  – generates data from $N(\mu_j, \Sigma_j)$
• Each example $x^{(i)}$ is generated according to following recipe:
  – pick component $j$ at random with probability $\phi_j$
  – sample $x^{(i)} \sim N(\mu_j, \Sigma_j)$

Based on slides by Andrew Moore
GMMs as Generative Model

We are given training set \( \{ x^{(1)}, \ldots, x^{(n)} \} \) (w/o labels)

We model data by specifying joint distribution

\[
p(x^{(i)}, z^{(i)}) = p(x^{(i)} | z^{(i)}) p(z^{(i)})
\]

Here, for \( k \) components,

\[
z^{(i)} \sim \text{Multinomial}(\phi) \quad \quad \phi_j = p(z^{(i)} = j) \quad \quad \phi_j \geq 0, \sum_{j=1}^{k} \phi_j = 1
\]

\[
x^{(i)} | z^{(i)} = j \sim \mathcal{N}(\mu_j, \Sigma_j)
\]

Goals:
- Determine \( z^{(i)} \) (soft cluster assignments)
- Determine model parameters \( \phi_j, \mu_j, \Sigma_j \) \( (1 \leq j \leq k) \)

Note:
- \( z^{(i)} \) are latent r.v.'s (they are hidden/unobserved)
- This is what makes estimation problem difficult

GMM Optimization

Assume supervised setting (known cluster assignments)

MLE for univariate Gaussian

\[
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x^{(i)} \quad \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \hat{\mu})^2
\]

\text{sum over points generated from this Gaussian}

MLE for multivariate Gaussian

\[
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x^{(i)} \quad \hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \hat{\mu})(x^{(i)} - \hat{\mu})^T
\]
GMM Optimization

What if unobserved data?

Now what?

Expectation Maximization

Based on notes by Andrew Ng

Based on slides by Andrew Moore
Expectation Maximization

Learning Goals

• Describe when EM is useful
• Describe the two steps of EM
• Practice EM on a toy problem

Expectation Maximization

• Clever method for maximizing marginal likelihoods
  \[ \arg \max_{\theta} \prod_{i=1}^{n} P(x^{(i)}) = \arg \max_{\theta} \prod_{i=1}^{n} \sum_{j=1}^{k} P(x^{(i)}, z^{(i)} = j) \]

• Excellent approach for unsupervised learning
• Can do “trivial” things (upcoming example)
• One of most general unsupervised approaches with many other uses (e.g. HMM inference)

Overview

• Begin with guess for model parameters
• Repeat until convergence
  – Update latent variables based on our expectations [E-step]
  – Update model parameters to maximize log likelihood [M-step]

Based on notes by Andrew Ng and slides by Andrew Moore
Silly Example

Let events be “grades in a class”

- component 1 = gets an A \( P(A) = \frac{1}{2} \)
- component 2 = gets a B \( P(B) = p \)
- component 3 = gets a C \( P(C) = 2p \)
- component 4 = gets a D \( P(D) = \frac{1}{2} - 3p \) (note \( 0 \leq p \leq 1/6 \))

Assume we want to estimate \( p \) from data. In a given class, there were

- \( a \) A’s, \( b \) B’s, \( c \) C’s, \( d \) D’s.

What is the MLE of \( p \) given \( a, b, c, d \)?

So if class got

\[
\begin{array}{cccc}
  a & b & c & d \\
  14 & 6 & 9 & 10
\end{array}
\]

Same Problem with Hidden Information

Someone tells us that

- # of high grades (A’s + B’s) = \( h \)
- # of C’s = \( c \)
- # of D’s = \( d \)

What is the MLE of \( p \) now?

We can answer this question circularly:

**EXTRACTION**

If we know value of \( p \), we could compute expected values of \( a \) and \( b \).

**MAXIMIZATION**

If we know expected values of \( a \) and \( b \), we could compute maximum likelihood value of \( p \).

Based on slides by Andrew Moore [Clustering with Gaussian Mixtures]
EM for Our Silly Example

- Begin with initial guess for $p$
- Iterate between Expectation and Maximization to improve our estimates of $p$ and $a$ & $b$

- Define $p^{(t)} = \text{estimate of } p \text{ on } t^{th} \text{ iteration}$
  $b^{(t)} = \text{estimate of } b \text{ on } t^{th} \text{ iteration}$
- Repeat until convergence
  
  **E-step**  
  $b^{(t)} = \frac{p^{(t)}}{\frac{1}{2} + p^{(t)}}h = \mathbb{E}[b|p^{(t)}]$  
  
  **M-step**  
  $p^{(t+1)} = \frac{b^{(t)} + c}{6 \left(b^{(t)} + c + d\right)} = \text{MLE of } p \text{ given } b^{(t)}$

Based on slides by Andrew Moore [Clustering with Gaussian Mixtures]

EM Convergence

- **Good news**: converging to local optima is guaranteed
- **Bad news**: local optima

Aside (idea behind convergence proof)

- likelihood must increase or remain same between each iteration [not obvious]
- likelihood can never exceed 1 [obvious]
- so likelihood must converge [obvious]

In our example, suppose we had  
\[ h = 20, \ c = 10, \ d = 10 \]
\[ p^{(0)} = 0 \]

Error generally decreases by constant factor each time step (e.g. convergence is linear)

<table>
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<tr>
<th>$t$</th>
<th>$p^{(t)}$</th>
<th>$b^{(t)}$</th>
</tr>
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</tr>
<tr>
<td>6</td>
<td>0.0948</td>
<td>3.187</td>
</tr>
</tbody>
</table>

Based on slides by Andrew Moore [Clustering with Gaussian Mixtures]
EM Applied to GMMs
Learning Goals

• Describe how to optimize GMMs using EM

Learning GMMs

Recall $z^{(i)}$ indicates which of $k$ Gaussians each $x^{(i)}$ comes from
If $z^{(i)}$’s were known, maximizing likelihood is easy

$$\ell(\phi, \mu, \Sigma) = \sum_{i=1}^{n} \log P(x^{(i)}|z^{(i)}; \phi, \mu, \Sigma) + \log P(z^{(i)}; \phi)$$

Maximize wrt $\phi, \mu, \Sigma$ gives

$$\phi_j = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I} \left[ z^{(i)} = j \right]$$
fraction of examples assigned to component $j$

$$\mu_j = \frac{\sum_{i=1}^{n} \mathbb{I} \left[ z^{(i)} = j \right] x^{(i)}}{\sum_{i=1}^{n} \mathbb{I} \left[ z^{(i)} = j \right]}$$
mean and covariance of examples assigned to component $j$

$$\Sigma_j = \frac{\sum_{i=1}^{n} \mathbb{I} \left[ z^{(i)} = j \right] (x^{(i)} - \mu_j) (x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} \mathbb{I} \left[ z^{(i)} = j \right]}$$

Based on notes by Andrew Ng
Learning GMMs

Since $z(i)'s$ are not known, use EM!

Repeat until convergence

[E-step] Know model parameters, “guess” values of $z(i)'s$

[M-step] Know class probabilities, update model parameters

Based on notes by Andrew Ng
Learning GMMs

Since \( z^{(i)} \)'s are not known, use EM!

Repeat until convergence

[E-step] Know model parameters, “guess” values of \( z^{(i)} \)'s

for each \( i,j \), set

\[
w_j^{(i)} = p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)
\]

\( w_j^{(i)} \)'s are “soft” guesses for values of \( z^{(i)} \)'s

compute posterior probability using Bayes’ Rule

\[
\frac{p(x^{(i)} | z^{(i)} = j; \mu, \Sigma) p(z^{(i)} = j; \phi)}{\sum_{l=1}^{k} p(x^{(i)} | z^{(i)} = l; \mu, \Sigma) p(z^{(i)} = l; \phi)}
\]

[M-step] Know class probabilities, update model parameters

update parameters

\[
\phi_j = \frac{1}{n} \sum_{i=1}^{n} w_j^{(i)}
\]

\[
\mu_j = \frac{\sum_{i=1}^{n} w_j^{(i)} x^{(i)}}{\sum_{i=1}^{n} w_j^{(i)}}
\]

\[
\Sigma_j = \frac{\sum_{i=1}^{n} w_j^{(i)} (x^{(i)} - \mu_j) (x^{(i)} - \mu_j)^T}{\sum_{i=1}^{n} w_j^{(i)}}
\]

Final Comments

EM is not magic

• Still optimizing non-convex function with lots of local optima
• Computations are just easier (often, significantly so!)

Problems

• EM susceptible to local optima
  \( \Rightarrow \) reinitialize at several different initial parameters

Extensions

• EM looks at maximum log likelihood of data
  \( \Rightarrow \) also possible to look at maximum a posteriori
GMM Exercise

We estimated a mixture of two Gaussians based on two-dimensional data shown below. The mixture was initialized randomly in two different ways and run for three iterations based on each initialization. However, the figures got mixed up. Please draw an arrow from one figure to another to indicate how they follow from each other (you should only draw four arrows).