GMM and EM questions

Haresh Rengaraj Rajamohan

CDS, NYU

April 28, 2021

Recap: Gaussian Mixture models

- Probabilistic Model for clustering

Question 1: Clustering [1]

Consider the set of training data below, and two clustering algorithms: K-Means, and a Gaussian Mixture Model (GMM) trained using EM. Will these two clustering algorithms produce the same cluster centers (means) for this data set? In one sentence, explain why or why not

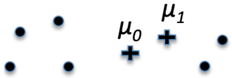
[1] From CMU

[Solution] Question 1: Clustering Comparison

- Both the approaches will find the clusters
- In k-means the center of a cluster is the average of all the elements in the cluster
- In GMM, the centers are weighted average of all the elements in the data.
- So, in GMM, we can expect the right center to be skewed a bit to the left and left center to the right

Question 2: EM basics [2]

Consider applying EM to train a GMM to cluster the data into two clusters. Thr '+' points indicate the current means μ_0, μ_1 of the two components of the mixture after the kth iteration of EM.

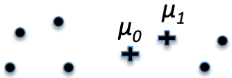


- Draw on the figure the directions in which μ_0 and μ_1 will move during the next M-step
- Will the marginal likelihood of the training data, increase or decrease on the next EM iteration?
  $p(x)$
- Will the estimate of π_0 increase or decrease on the next EM step?

[2] From CMU

[Solution] Question 2: EM basics

Consider applying EM to train a GMM to cluster the data into two clusters. Thr '+' points indicate the current means μ_0, μ_1 of the two components of the mixture after the kth iteration of EM.



- μ_0 moves to the left, and μ_1 moves to the right.
- Increase. Each iteration of the EM algorithm increases to likelihood of the data, unless you happen to be exactly at a local optimum
- It will increase

Question 3: Gaussian Naive Bayes and GMMs [3]

Lets consider the relationship between a Gaussian Naive Bayes (GNB) classifier and the above Gaussian Mixture Model (GMM). It is easy to see that they involve the same probabilistic model. Our usual GNB classifier assumes $p(Y|X)$ is of the form:

$$p(Y|X) = \frac{P(Y)\Pi_i p(X_i|Y)}{p(X)}$$

where Y is a Bernoulli random variable (i.e., $P(Y=0)=\pi_0$). It also assumes each feature X_i is governed by a Gaussian distribution conditioned on Y . For simplicity, letâs assume all features have the same variance, so

$$P(X_i|Y=k) \sim N(\mu_{k,i}, \sigma)$$

[3] From CMU

Question 3: Gaussian Naive Bayes and GMMs continued

Notice this GNB generative model is identical to that of our GMM above (plus the simplifying assumption of identical σs). In other words, both models assume we generate data points by choosing a Y according to π_0, then drawing an X according to a Gaussian conditioned on Y.

- The GNB objective is $argmax_\theta \Pi_j P(x^j, y^j|\theta)$. Give the EM objective for GMM.
- Suppose we have a set of training data in which we have both labeled and unlabeled samples. We have known y values for $x^1, .., x^m$ but have additional unlabeled examples $x^{m+1}, .., x^{m+n}$ without known values for y. Propose a modified EM approach to train in this setting.
- Write down the objective function that your modified EM is maximizing. In your expression, distinguish between the labeled and unlabeled examples.

[Solution] Question 3: Gaussian Naive Bayes and GMMs

- $argmax_{\theta} \Pi_j \left(\sum_y P(x^j, y|\theta) \right)$
- In the E step, for labeled samples use
- $\gamma_{ij} = \delta_{j,y(i)}$ $argmax_{\theta} \Pi_{j=1}^{m} \left(\sum_y P(x^j, y|\theta) \right) \Pi_{j=m+1}^{m+n} \left(P(x^j, y^j|\theta) \right)$, where $\delta_{j,y(i)} = 1(j = y(i))$

Question 4: EM computation [4]

Suppose that we are fitting a Gaussian mixture model for data items consisting of a single real value, x, using $K = 2$ components. We have $N = 5$ training cases, in which the values of x are as follows:

$$5, 15, 25, 30, 40$$

We use the EM algorithm to find the maximum likeihood estimates for the model parameters, which are the mixing proportions for the two components, π_1 and π_1, and the means for the two components, μ_1 and μ_2. The standard deviations for the two components are fixed at 10.

[4] From UToronto

Question 4: EM computation continued

Suppose that at some point in the EM algorithm, the E step found that the responsibilities of the two components for the five data items were as follows:

r_{i1}	r_{i2}
0.2	0.8
0.2	0.8
0.8	0.2
0.9	0.1
0.9	0.1

What values for the parameters π_1, π_2, μ_1, and μ_2 will be found in the next M step of the algorithm?

[Solution] Question 4 EM computation

The new estimates will be

- $\pi_1 = (0.2+0.2+0.8+0.9+0.9)/5 = 0.6$
- $\pi_2 = (0.8+0.8+0.2+0.1+0.1)/5 = 0.4$
- $\mu_1 = (0.2\times 5+0.2\times 15+0.8\times 25+0.9\times 30+0.9\times 40)/(0.2+0.2+0.8+0.9+0.9) = 29$
- $\mu_2 = (0.8\times 5+0.8\times 15+0.2\times 25+0.1\times 30+0.1\times 40)/(0.8+0.8+0.2+0.1+0.1) = 14$

Question 5 Computation Problem [5]

Consider a two-component Gaussian mixture model for univariate data, in which the probability density for an observation, x, is,

$$\frac{1}{2}N(x|\mu, 1) + \frac{1}{2}N(x|\mu, 2^2)$$

Here, $N(x|\mu, \sigma^2)$ denotes the density for x under a univariate normal distribution with mean μ and variance σ^2. Notice that mixing proportions are equal for this mixture model, that the two components have the same mean, and that the standard deviations of the two components are fixed at 1 and 2. There is only one model parameter, μ.

[5] From UToronto

Question 5 Computation Problem continued

Suppose we wish to estimate the μ parameter by maximum likelihood using the EM algorithm. Answer the following questions regarding how the E step and M step of this algorithm operate, if we have the three data points below:

$$4.0, 4.6, 2.0$$

- Find the responsibilities that will be computed in the E step if the model parameter estimates from the previous M step are $\mu = 4$, $\sigma_1 = 1$, and $\sigma_2 = 2$. Since the responsibilities for the two components must add to one, it is enough to give $r_{i1} = P(component_1 | x_i)$ for $i = 1, 2, 3$.
- Using the responsibilities that you computed in part (a), find the estimate for μ that will be found in the next M step.

[Solution] Question 5 Computation Problem

(A). Using Bayes Rule,

$$P(component\, 1|x) = \frac{\frac{1}{2}N(x|\mu,1)}{\frac{1}{2}N(x|\mu,1)+\frac{1}{2}N(x|\mu,2^2)}$$

Lets apply this to the three observations,

$$r_{11} = \frac{(1/2)0.4}{(1/2)0.4+(1/2)(1/2)0.4} = 2/3$$

$$r_{21} = \frac{(1/2)0.33}{(1/2)0.33+(1/2)(1/2)0.38} = 33/52$$

$$r_{31} = \frac{(1/2)0.05}{(1/2)0.05+(1/2)(1/2)0.24} = 5/17$$

[Solution continued] Question 5 Computation Problem

(B). The expected log likelihood is,

$\sum_{i} \log \sum_{z} p(z)\, p(x|z)$

$$\sum_{i=1}^{3}\left[r_{i1}(-1/2)(x_i-\mu)^2+(1-r_{i1})(-1/2)(x_i-\mu)^2/4\right]$$

Lets differentiate and equate this to 0,

$$\sum_{i=1}^{3}[r_{i1}(x_i-\mu)+(1-r_{i1})(x_i-\mu)/4]=0$$

We get,

$$\hat{\mu}=\frac{\sum_{i=1}^{3}(r_{i1}+(1-r_{i1})/4)x_i}{\sum_{i=1}^{3}(r_{i1}+(1-r_{i1})/4)}=\frac{(3/4)4.0+(151/208)4.6+(25/68)2.0}{(3/4)+(151/208)+(25/68)}$$

Question 6 EM derivation [6]

Lets derive the E-M update rules for a univariate Gaussian mixture model (GMM) with two mixture components. Unlike the GMMs we covered in the course, the mean μ will be shared between the two mixture components, but each component will have its own standard deviation σ_k . The model is defined as follows:

$$z \sim Bernoulli(\theta)$$

$$x|z = k \sim N(\mu, \sigma_k)$$

- Write the density defined by this model (i.e. the probability of x, with z marginalized out)
- E-Step: Compute the posterior probability $r^{(i)} = P(z^{(i)} = 1|x^{(i)})$
- Update rule for μ (σ_k fixed) and σ_k (μ fixed)

[6] From UToronto

[Solution]Question 6 EM derivation

(A).

$$p(x) = \theta N(x; \mu, \sigma_1) + (1-\theta) N(x; \mu, \sigma_0)$$

(B).

$$r^{(i)} = \frac{\theta N(x; \mu, \sigma_1)}{\theta N(x; \mu, \sigma_1) + (1-\theta) N(x; \mu, \sigma_0)}$$

(C).

$$\mu \leftarrow \frac{\sum_{i=1}^{N} x^{(i)} (r^{(i)} \sigma_0^2 + (1 - r^{(i)}) \sigma_1^2)}{\sum_{i=1}^{N} (r^{(i)} \sigma_0^2 + (1 - r^{(i)}) \sigma_1^2)}$$

$$\sigma_1^2 \leftarrow \frac{\sum_{i=1}^{N} r^{(i)} (x^{(i)} - \mu)^2}{\sum_{i=1}^{N} r^{(i)}}$$

Question 7.1 MCQ [7]

Assume you have points that are generated by one of two possible Gaussian distributions. Which of the following are true?

- We know how to get a globally optimal solution by deriving the maximum likelihood estimate analytically
- Using the EM algorithm to solve this problem, we assume that we know from which Gaussian each point originated.
- Once the EM algorithm has converged, we know for certain from which Gaussian each point originated.
- The EM algorithm for this problem guarantees that the likelihood of the data never decreases from one iteration to the next.

[7] from CMU

[Solution] Question 7.1 MCQ

Answer: (d). A - EM doesnt give the globally optimal solution. B - We can start out with one of the Gaussians being more likely for some points, but we dont know for sure. C - After convergence, we only know the probability values of belonging to a particular Gaussian.

Question 7.2 MCQ [8]

Which of the following are true about the EM algorithm as applied to a Gaussian Mixture Model?

- The choice of initial values of parameters of the Gaussian affects the final estimates.
- The algorithm is guaranteed to converge
- The algorithm is guaranteed to converge to a global maxima.
- The estimate of the parameters obtained at the end is the Maximum Likelihood Estimate.

[8] from CMU

[Solution] Question 7.2 MCQ

A and B are true. C - EM doesnt give the globally optimal solution. D - We cannot solve GMM in closed form to get a clean maximum likelihood expression

Coding Exercise

- GMM tutorial