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Unit 4 Unsupervised Learning (2

Course > weeks)

> Homework 5 > 3. EM Algorithm

# 3. EM Algorithm

Extension Note: Homework 4 due date has been extended by 1 day to August 17 23:59UTC.

Consider the following mixture of two Gaussians:

$$p\left(x; heta
ight)=\pi_{1}\mathcal{N}\left(x;\mu_{1},\sigma_{1}^{2}
ight)+\pi_{2}\mathcal{N}\left(x;\mu_{2},\sigma_{2}^{2}
ight)$$

This mixture has parameters  $heta=\{\pi_1,\pi_2,\mu_1,\mu_2,\sigma_1^2,\sigma_2^2\}$ . They correspond to the mixing proportions, means, and variances of each Gaussian. We initialize  $\theta$  as  $\theta_0 = \{0.5, 0.5, 6, 7, 1, 4\}$ .

We have a dataset  ${\cal D}$  with the following samples of x:  $x^{(0)}=-1$ ,  $x^{(1)}=0$ ,  $x^{(2)}=4$ ,  $x^{(3)}=5$ ,  $x^{(4)}=6$ .

We want to set our parameters  $\theta$  such that the data log-likelihood  $l\left(\mathcal{D};\theta\right)$  is maximized:

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Recall that we can do this with the EM algorithm. The algorithm optimizes a lower bound on the log-likelihood, thus iteratively pushing the data likelihood upwards. The iterative algorithm is specified by two steps applied successively:

1. E-step: infer component assignments from current  $\theta_0 = \theta$  (complete the data)

$$p\left(y=k\mid x^{(i)}
ight):=p\left(y=k\mid x^{(i)}; heta_{0}
ight), ext{ for } k=1,2, ext{ and } i=0,\ldots,4.$$

2. M-step: maximize the expected log-likelihood

$$ilde{l}\left(D; heta
ight) := \sum_{i} \sum_{k} p\left(y = k \mid x^{(i)}
ight) \log rac{p\left(x^{(i)}, y = k; heta
ight)}{p\left(y = k \mid x^{(i)}
ight)}$$

with respect to  $\theta$  while keeping  $p(y = k \mid x^{(i)})$  fixed.

To see why this optimizes a lower bound, consider the following inequality:

$$\log p\left(x; heta
ight) = \log \sum_{u} p\left(x,y; heta
ight)$$

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$$egin{aligned} &-\log \mathbb{E}_{y \sim q(y|x)} \left \lfloor \overline{ q\left(y|x
ight)} 
ight 
floor \ & = \sum_{y} q\left(y|x
ight) \log rac{p\left(x,y; heta
ight)}{q\left(y|x
ight)} \end{aligned} = \sum_{y} q\left(y|x
ight) \log rac{p\left(x,y; heta
ight)}{q\left(y|x
ight)} \end{aligned}$$

where the inequality comes from **Jensen's inequality** . EM makes this bound tight for the current setting of  $\theta$  by setting q(y|x) to be  $p(y \mid x; \theta_0)$ .

Note: If you have taken 6.431x Probability–The Science of Uncertainty, you could review the video in Unit 8: Limit Theorems and Classical Statistics, Additional Theoretical Material, 2. Jensen's Inequality.

### Likelihood Function

1/1 point (graded)

What is the log-likelihood of the data  $l(\mathcal{D};\theta)$  given the initial setting of  $\theta$ ? Please round to the nearest tenth.

Note: You will want to write a script to calculate this, using the natural log (np.log) and np.float64 data types.

-24.51253233

**✓ Answer:** -24.5

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$$egin{align} P\left(\mathcal{D}; heta
ight) &= \prod_{i=0}^4 p\left(x; heta
ight) \ &= \prod_{i=0}^4 \pi_1 \mathcal{N}\left(x^{(i)};\mu_1,\sigma_1^2
ight) + \pi_2 \mathcal{N}\left(x^{(i)};\mu_2,\sigma_2^2
ight) \end{aligned}$$

Taking the log gives:

$$l\left(\mathcal{D}; heta
ight) = \sum_{i=0}^{4} \log\left(\pi_{1}\mathcal{N}\left(x^{(i)};\mu_{1},\sigma_{1}^{2}
ight) + \pi_{2}\mathcal{N}\left(x^{(i)};\mu_{2},\sigma_{2}^{2}
ight)
ight)$$

We then evaluate each Gaussian using the standard formulation:

$$\mathcal{N}\left(x;\mu,\sigma^{2}
ight)=rac{1}{\sqrt{2\pi\sigma^{2}}}e^{-rac{\left(x-\mu
ight)^{2}}{2\sigma^{2}}}$$

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#### **E-21Gh**

1/1 point (graded)

What is the formula for p  $(y=k\mid x, heta)$ ? Write in terms of  $\pi_k$ ,  $\pi_1$ ,  $\pi_2$ ,  $N_k$ ,  $N_1$ , and  $N_2$  (where  $N_k=\mathcal{N}$   $(x\mid \mu_k,\sigma_k^2)$ ).

$$rac{\pi_k \cdot N_k}{\pi_1 \cdot N_1 + \pi_2 \cdot N_2}$$

STANDARD NOTATION

#### **Solution:**

Following Bayes Rule we have:

$$p\left(y\mid x
ight) = rac{p\left(y
ight)p\left(x\mid y
ight)}{\sum_{y'}p\left(y'
ight)p\left(x|y'
ight)}$$

For this problem, this equates to:

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You have used 1 of 3 attempts

• Answers are displayed within the problem

### E-Step Weights

5/5 points (graded)

For each of the given data points say which Gaussian (1 or 2) they are given more weight towards in the first E-step using the given setting of  $\theta_0$ . This is, answer 2 if  $p(y=2\mid x,\theta_0)>p(y=1\mid x,\theta_0)$  and 1 otherwise.

 $x^{(0)}$  :

 $x^{(1)}:$ 

 $x^{(2)}$ :

 $x^{(3)}:$ 

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...

### M-Step

3/3 points (graded)

Fixing  $p\left(y=k\mid x,\theta_{0}\right)$ , we want to update  $\theta$  such that our lower bound is maximized.

What is the optimal  $\hat{\mu}_k$ ? Answer in terms of  $x^{(1)}$  ,  $x^{(2)}$  , and  $\gamma_{k1}$  ,  $\gamma_{k2}$  , which are defined to be  $\gamma_{ki}=p$   $(y=k\mid x^{(i)}; heta_0)$ 

(For ease of input, use subscripts instead superscripts, i.e. type <code>x\_i</code> for  $x^{(i)}$  . Type <code>gamma\_ki</code> for  $\gamma_{ki}$  .)

(gamma\_k1\*x\_1+gamma\_k2\*x\_2)/(gamma\_k1+gamma\_k2)



**Answer:** (gamma\_k1 \* x\_1 + gamma\_k2 \* x\_2) / (gamma\_k1 + gamma\_k2)

$$\frac{\gamma_{k1}\cdot x_1+\gamma_{k2}\cdot x_2}{\gamma_{k1}+\gamma_{k2}}$$

What is the optimal  $\hat{\sigma}_k^2$ ? Answer in terms of  $x^{(1)}$ ,  $x^{(2)}$ ,  $\gamma_{k1}$  and  $\gamma_{k2}$ , which are defined as above to be  $\gamma_{ki}=p\,(y=k\mid x^{(i)};\theta_0)$ , and  $\hat{\mu}_k$ .

(Type hatmu\_k for  $\hat{\mu}_k$ . As above, for ease of input, use subscripts instead superscripts, i.e. type x\_i for  $x^{(i)}$ . Type gamma\_ki for  $\gamma_{ki}$ .)

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What is the optimal  $\hat\pi_k$ ? Answer in terms of  $\gamma_{k1}$  and  $\gamma_{k2}$ , which are defined as above to be  $\gamma_{ki}=p\,(y=k\mid x^{(i)}; heta_0)$ ,

(As above, type gamma\_ki for  $\gamma_{ki}$ .)

Note: that you must account for the constraint that  $\pi_1 + \pi_2 = 1$  where  $\pi_1, \pi_2 > 0$ .

Note: If you know that some aspect of your formula equals an exact constant, simplify and use this number, i.e.  $\gamma_{11} + \gamma_{21} = 1.$ 

(gamma\_k1+gamma\_k2)/2

✓ Answer: (gamma\_k1 + gamma\_k2) / 2

 $\underline{\gamma_{k1}} + \underline{\gamma_{k2}}$ 

STANDARD NOTATION

#### **Solution:**

The function we are optimizing is now:

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Taking  $\frac{\partial}{\partial \mu_k}$  and setting to 0 gives:

$$egin{aligned} rac{\partial}{\partial \mu_k} \sum_i \sum_k \gamma_{ki} \log \left( \pi_k \mathcal{N} \left( x^{(i)}; \mu_k, \sigma_k^2 
ight) 
ight) &= \sum_i \gamma_{ki} rac{\partial}{\partial \mu_k} \log \left( \pi_k \mathcal{N} \left( x^{(i)}; \mu_k, \sigma_k^2 
ight) 
ight) \ &= \sum_i \gamma_{ki} rac{\partial}{\partial \mu_k} (\log \left( rac{1}{\sqrt{2\pi\sigma_k^2}} 
ight) - rac{\left( x^{(i)} - \mu_k 
ight)^2}{2\sigma_k^2} 
ight) \ &= \sum_i \gamma_{ki} rac{x^{(i)} - \mu_k}{\sigma_k^2} = 0 \end{aligned}$$

Separating out  $\mu_k$  gives:

$$\mu_k = rac{\sum_i \gamma_{ki} x^{(i)}}{\sum_i \gamma_{ki}}$$

We can interpret this as a weighted average of the data points, normalized by the "total mass" assigned to Gaussian k. The weight is the probability that point  $x^{(i)}$  "belongs" to Gaussian k.

Solving for  $\sigma_k^2$  is similar:

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$$egin{align} egin{align} eg$$

Separating out  $\sigma_k^2$  gives:

$$\sigma_k^2 = rac{\sum_i \gamma_{ki} {(x^{(i)} - \mu_k)}^2}{\sum_i \gamma_{ki}}$$

Finally we solve for  $\pi_k$  while including a lagrange multiplier for the constraint that  $\sum_k \pi_k = 1$ .

$$egin{aligned} rac{\partial}{\partial \pi_k} \sum_i \sum_k \gamma_{ki} \log \left( \pi_k \mathcal{N} \left( x^{(i)}; \mu_k, \sigma_k^2 
ight) 
ight) + \lambda \left( \sum_k \pi_k - 1 
ight) \ &= \sum_i \gamma_{ki} rac{\partial}{\partial \pi_k} \log \left( \pi_k 
ight) + rac{\partial}{\partial \pi_k} \lambda \left( \sum_k \pi_k - 1 
ight) \ &= rac{\sum_i \gamma_{ki}}{\pi_k} + \lambda = 0 \end{aligned}$$

Giving 
$$\pi_k = -rac{\sum_i \gamma_{ki}}{\lambda}.$$

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Combining the two gives:

$$\lambda = -\sum_i \sum_k \gamma_{ki}$$

which we recognize as N, the total number of points. Thus  $\hat{\pi}_k$  is  $\frac{\sum_i \gamma_{ki}}{N}$ .

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You have used 2 of 3 attempts

• Answers are displayed within the problem

## Training 1

1/1 point (graded)

In the first M-step, which Gaussian will shift to the left more (relatively)?

Gaussian 1

Gaussian 2 🗸

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Intuitively, Gaussian 2 is influenced most by the points  $x^{(0)}$ ,  $x^{(1)}$ , and so it will move to the left. Gaussian 1 will be more influenced by the points at  $x^{(2)}$ ,  $x^{(3)}$  and  $x^{(4)}$  and so it will not move very much to the left. If we computed the actual values, we would see that the updated means for the two Gaussians are approximately  $\mu_1=5.1317$  and  $\mu_2=1.4710$ .

Submit

You have used 1 of 1 attempt

• Answers are displayed within the problem

## Training 2

1/1 point (graded)

In the first M-step, which Gaussian's variance will increase more (relatively)?

Gaussian 1

Gaussian 2 🗸

#### **Solution:**

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You have used 1 of 1 attempt

• Answers are displayed within the problem

## Training 3

1/1 point (graded)

After convergence, which variance will be larger?





#### **Solution:**

Gaussian 1 will be centered around the cluster of 3 points on the right, while Gaussian 2 will be centered around the 2 points on the left. Gaussian 1 will have larger variance because of the larger spread of the right cluster.

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You have used 1 of 1 attempt

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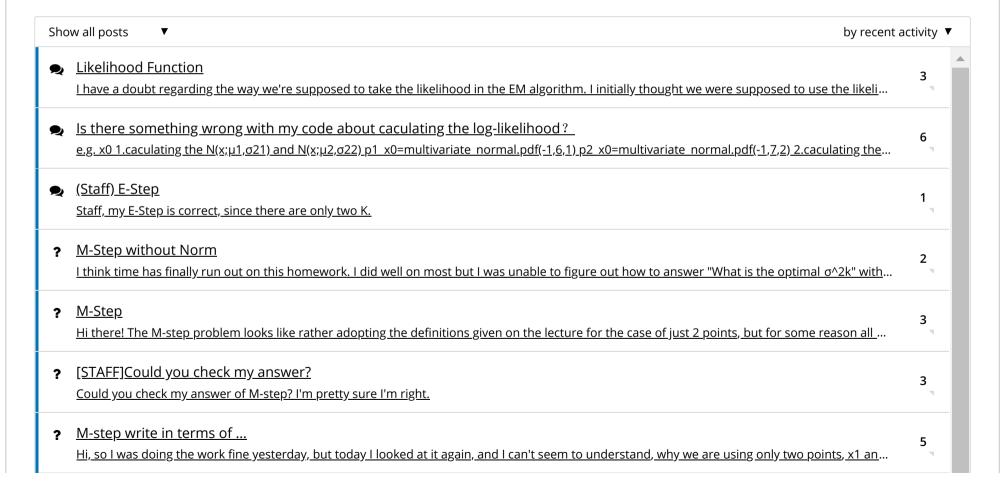
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### Discussion

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**Topic:** Unit 4 Unsupervised Learning (2 weeks): Homework 5 / 3. EM Algorithm

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**☑** E-Step, how to enter a sum from 1 to k? 5 E-Step, how to enter a sum from 1 to k? **Likelihood Function** 6 ● E-Step Weights: results surprised me! 2 By running my script for the calculation I got the correct answers. But they were very different from my initial naive guess by inspection! Another ... **☑** E-step - symbols and notation 5 I think I know how to calculate  $p(y=k|x,\theta)$  but I don't see how to do this with the symbols given. Any pointers? [Training 3] How to debug this part?

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