The Expectation Maximization Algorithm

İlker Bayram

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EM is an iterative procedure for obtaining maximum likeliood (ML) estimates. Suppose that X is distributed according to the pdf $f_X(\cdot;\theta)$, where θ is an unknown parameter of interest. Suppose also that we have n independent samples from f_X as, $x = (x_1, \ldots, x_n)$. Given x, recall that the ML estimate is the maximizer of the likelihood function $L(\cdot) = f_X(x;\cdot)$, and is given by,

$$\hat{\theta} = \arg\max_t \left\{ L(t) = f_X(x;t) := \prod_{i=1}^{n} f_X(x_i;t) \right\}.$$

When $L(t)$ has a simple expression, the ML estimate can be obtained analytically. However, in many scenarios of interest, this is not the case. EM is an iterative procedure for finding a local maximum of $L(\cdot)$.

Example : Suppose Z is a Bernoulli random variable with PMF

$$P_Z(z) = \begin{cases} \alpha_0, & \text{if } z = 1, \\ \alpha_1 = 1 - \alpha_0, & \text{if } z = 0, \end{cases}$$

where α_0 is an (unknown) constant. Given a realization of Z as z, suppose X is given as,

$$X = \begin{cases} w + \theta_0, & \text{if } z = 0, \\ w + \theta_1, & \text{if } z = 1, \end{cases}$$

where $w \sim \mathcal{N}(0,1)$ and θ_i are unknown. Note that the distribution of X is

$$f_X(x) = \alpha_0\, g(x;\theta_0) + \alpha_1\, g(x;\theta_1),$$

where

$$g(x;\theta) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(x-\theta)^2 \right).$$

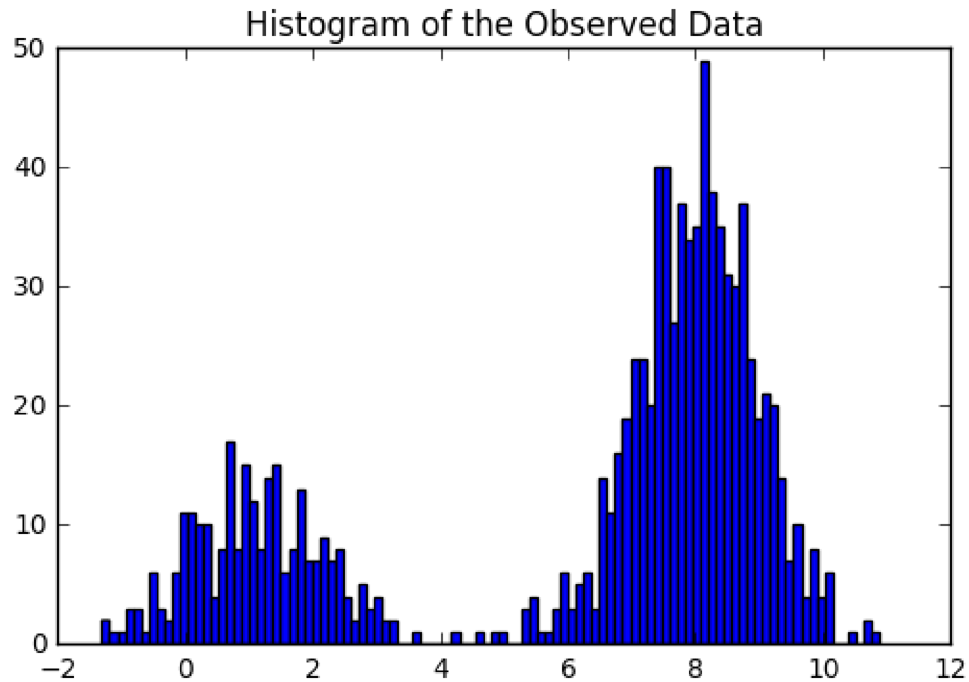
Suppose we are given independent realizations of X and asked to estimate α_i and θ_i. Notice that here, z_i's are unknown to us (constituting the hidden states, according to hidden Markov models terminology). Let us produce such a set of x_i's. In order to hide α_i's and θ_i's, we also select them randomly.

```
In [1]: import numpy
        n = 1000 #number of samples
        alp0 = numpy.random.uniform(0,1,1)
```

```
alp1 = 1 - alp0
theta = numpy.random.normal(0,5,2)
z = numpy.double( numpy.random.uniform(0,1,n) > alp0 )
x = z * numpy.random.normal(theta[0],1,n)
       + (1-z) * numpy.random.normal(theta[1],1,n)
```

In the following, we pretend that we just observe x. Let us view the histogram of the data.

```
In [2]: import matplotlib.pyplot as plt
        plt.hist(x,100)
        plt.title("Histogram of the Observed Data")
        plt.show()
```



Unless the θ values are very close or one of α is close to unity, we should see two modes, possibly with different weights.

We will see in the following that if we knew z_i's, maximizing the likelihood function wrt α_i and θ_i is much easier. The idea in EM, to be detailed below, is to estimate, in an iterative manner, z_i's as well as the unknown parameters α_i, θ_i.

Let us now consider the hypothetical case where both x_i's and z_i's are known. Given z_i's let I_0 and I_1 denote the set of indices such that

$$z_i = \begin{cases} 0, & \text{if } i \in I_0, \\ 1, & \text{if } i \in I_1. \end{cases}$$

Note that $I_0 \cup I_1 = \{1, 2, \ldots, n\}$. The likelihood function in this case is denoted as $\tilde{L}(\alpha, \theta)$, and is given as,

$$\tilde{L}(a,t) = a_0^{|I_0|}\, a_1^{|I_1|}\, \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2} \sum_{i \in I_0} (x_i - t_0)^2 + \sum_{i \in I_1} (x_i - t_1)^2 \right),$$

where $|I_i|$ denotes the number of elements in I_i. Note that $|I_1| = n - |I_0|$. Using this as well as $\alpha_1 = 1 - \alpha_0$, we can write the log-likelihood function as,

$$\ln \tilde{L}(a,t) = |I_0|\, \ln(a_0) + (n - |I_0|)\, \ln(1 - a_0) - \frac{1}{2} \sum_{i \in I_0} (x_i - t_0)^2 - \frac{1}{2} \sum_{i \in I_1} (x_i - t_1)^2.$$

Setting the gradient of this function to zero, we obtain the following set of equations

$$\begin{aligned}
\frac{|I_0|}{\hat{\alpha}_0} - \frac{n - |I_0|}{1 - \hat{\alpha}_0} &= 0, \\
\sum_{i \in I_0} (\hat{\theta}_0 - x_i) &= 0, \\
\sum_{i \in I_1} (\hat{\theta}_1 - x_i) &= 0.
\end{aligned}$$

Solving for the unknowns, we obtain the maximizers

$$\begin{aligned}
\hat{\alpha}_0 &= \frac{|I_0|}{n}, \\
\hat{\theta}_0 &= \frac{1}{|I_0|} \sum_{i \in I_0} x_i, \\
\hat{\theta}_1 &= \frac{1}{n - |I_0|} \sum_{i \in I_1} x_i.
\end{aligned}$$

However, when knowledge about z is missing, the ML estimates of α_i and θ_i are not easy to obtain. The idea in EM is to estimate the the log likelihood with the full data (including z) using the current estimates of α_i, θ_i, and then use this estimated log-likelihood function to re-estimate (or, update the estimates of) α_i and θ_i. More precisely, suppose we have the observations x_i and our current estimates of the unknown parameters are $\hat{a}_i$, $\hat{t}_i$. Then, instead of $\ln \tilde{L}(a,t)$, consider the function

$$\begin{aligned}
Q(a,t;\hat{a},\hat{t}) &= \mathbb{E}_{\hat{a},\hat{t}} \left(\ln \tilde{L}(a,t) \right) \\
&= \sum_{z} \ln \tilde{L}(a,t)\, P_{Z|X}(z|x;\hat{a},\hat{t})
\end{aligned}$$

Notice that, here the expectation is computed using the PMF of z given x by taking the parameters α and θ as $\hat{a}$ and $\hat{t}$. Observe also that this gives a function $Q(a,t;\hat{a},\hat{t})$ that depends only on a_i and t_i. We maximize this function of a and t to update the desired parameters. That is our new estimates of α and θ are given as,

$$(\hat{a},\hat{t}) := \arg\max_{a,t} Q(a,t;\hat{a},\hat{t}).$$

Then we repeat the procedure over to further refine our estimates and continue ad infinitum. This is the expectation maximization algorithm.

For our problem, we can express $Q(a, t; \hat{a}, \hat{t})$ as follows.

$$\begin{aligned} Q(a, t; \hat{a}, \hat{t}) &= \sum_z \ln \tilde{L}(a, t)\, P_{Z|X}(z|x; \hat{a}, \hat{t}) \\ &= \sum_z \Bigg(|I_0| \ln(a_0) + (n - |I_0|) \ln(1 - a_0) \\ &\qquad -\frac{1}{2} \sum_{i \in I_0} (x_i - t_0)^2 - \frac{1}{2} \sum_{i \in I_1} (x_i - t_1)^2 \Bigg) P_{Z|X}(z|x; \hat{a}, \hat{t}) \end{aligned}$$

Observe also that, taking into account the fact that z_i can only take values from $\{0, 1\}$, we can write the term inside the parentheses as,

$$\left(n - \sum_i z_i \right) \ln(a_0) + \left(\sum_i z_i \right) \ln(1 - a_0) - \frac{1}{2} \sum_i (1 - z_i)\,(x_i - t_0)^2 - \frac{1}{2} \sum_i z_i\,(x_i - t_1)^2$$

Therefore, if we set $e_i = \mathbb{E}_{\hat{a}, \hat{t}}(z_i|x_i)$, then we can express $Q(a, t; \hat{a}, \hat{t})$, as

$$Q(a, t; \hat{a}, \hat{t}) = \left(n - \sum_i e_i \right) \ln(a_0) + \left(\sum_i e_i \right) \ln(1 - a_0) - \frac{1}{2} \sum_i (1 - e_i)\,(x_i - t_0)^2 - \frac{1}{2} \sum_i e_i\,(x_i - t_1)^2.$$

I leave it to you to verify that

$$\mathbb{E}_{\hat{a}, \hat{t}}(z_i|x_i) = \frac{(1 - \hat{a}_0)\, g(x_i; \hat{t}_1)}{\hat{a}_0\, g(x_i; \hat{t}_0) + (1 - \hat{a}_0)\, g(x_i; \hat{t}_1)}$$

Notice that this number can be computed since it depends solely on what is given (x_i) and the current estimates $\hat{a}_i$, $\hat{t}_i$. To simplify expressions, also let $s = \sum_i e_i$. Then, we can write

$$Q(a, t; \hat{a}, \hat{t}) = (n - s) \ln(a_0) + (s) \ln(1 - a_0) - \frac{1}{2} \sum_i (1 - e_i)\,(x_i - t_0)^2 - \frac{1}{2} \sum_i e_i\,(x_i - t_1)^2.$$

Setting the gradient of this function with respect to a, t to zero, we obtain the following set of equations that the maximizers $\bar{a}$, $\bar{t}$ should satisfy.

$$\frac{n - s}{\bar{a}_0} - \frac{s}{\bar{a}_0} = 0, \tag{1}$$

$$\sum_{i=1}^{n} (1 - e_i)\,(\bar{t}_0 - x_i) = 0, \tag{2}$$

$$\sum_{i=1}^{n} e_i\,(\bar{t}_1 - x_i) = 0. \tag{3}$$

Solving for the unknowns, we find the maximizers as

$$\bar{a}_0 = \frac{n-s}{n}, \tag{4}$$

$$\bar{t}_0 = \frac{1}{n-s} \sum_i^n (1-e_i)\, x_i, \tag{5}$$

$$\bar{t}_1 = \frac{1}{s} \sum_i^n e_i\, x_i, \tag{6}$$

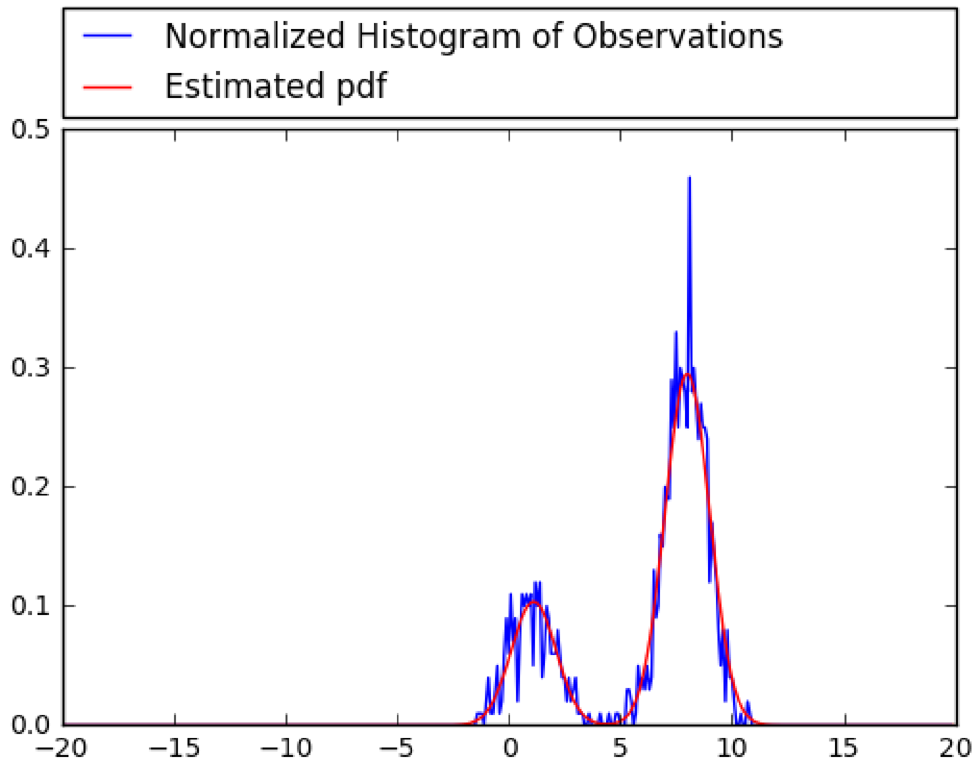
$$\tag{7}$$

We update $\hat{a} := \bar{a}$, $\hat{t} := \bar{t}$ and repeat the procedure over.
Let us now experiment numerically.

```
In [3]: # the Gaussian pdf
        def g( x , m ):
            return ( 1 / numpy.sqrt( 2 * numpy.pi ) )
                    * numpy.exp( -0.5 * ( x - m )**2 )

        # the Gaussian mixture pdf
        def f( x , t , a):
            return a * g( x , t[0] ) + ( 1 - a ) * g( x , t[1] )

        # initialize
        a = 0.5
        t = [ -1 , 1 ]

        for iter in range(0,1000):

            # the expectation step
            e = ( 1 - a ) * g( x, t[1] ) / f( x , t , a )
            s = sum(e)

            # maximization step
            a = ( n - s ) / n # update the weight parameter
            t[0] = sum( ( 1 - e ) * x ) / ( n - s )
            t[1] = sum( e * x ) / s
```

That's it. We now have our estimates of α and θ. Let's sketch the resulting Gaussian mixture pdf to see how well it matches the normalized histogram.

```
In [4]: u = numpy.arange( -20 , 20 , 0.1 )
        h , u = numpy.histogram( x , u , density = True )
        plt.plot( u[0:-1] , h , label = "Normalized Histogram of Observations" )
        plt.plot( u , f( u , t , a ) , 'r-' , label = "Estimated pdf" )
        plt.legend( bbox_to_anchor  = (0. , 1.02 , 1. , .102) ,
                loc = 3 ,  mode = "expand" , borderaxespad = 0.)
        plt.show()
```


Normalized Histogram of Observations
Estimated pdf
0.5
0.4
0.3
0.2
0.1
0.0
−20
−15
−10
−5
0
5
10
15
20