A prelude to the EM algorithm

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January 12, 2026

See here for a PDF version of this vignette.

Prerequisites

This document assumes basic familiarity with mixture models, likelihoods and Bayesian computations for the two-class problem.

Overview

The *expectation-maximization algorithm*, usually known as the "EM algorithm", is a widely used computational method for performing the maximum likelihood method in certain models. Its attractions include that it is often simple to code and it is "monotonic" (that is, every iteration increases the likelihood). It is also often quick to find a "reasonably good" solution, although if a very precise solution is required, then it can be slow. In this document we describe the EM algorithm for a particular problem — maximum likelihood estimation of the mixture proportions — where it has a particularly simple and intuitive form. We do not give any formal derivation or explain why it works, which will require further study. The idea is to motivate you to perfom this further study.

The problem

Consider again the medical screening example from [this vignette][mixture_model_01]. This example involves a test for a disease that is based on measuring the concentration (X) of a protein in the blood. In normal individuals, X has a Gamma distribution with mean 1 and shape 2 (so the scale parameter is 0.5, as scale = mean/shape). In diseased individuals the protein becomes elevated, and X has a Gamma distribution with mean 2 and shape 2 (so scale = 1).

Now consider the following question. Suppose we observe data $x_1, \ldots, x_n$ on n individuals randomly sampled from a population. How can we estimate the proportion of individuals in the population that are diseased?

Formulation via maximum likelihood

A natural approach to parameter estimation to use maximum likelihood. The first step in this approach is to write down the likelihood. To do this, note that the samples are independent from the following mixture model:

$$p(x \mid \pi) = \pi_1 \text{Gamma}(x; 0.5, 2) + \pi_2 \text{Gamma}(x; 1, 2),$$

where $\pi = (\pi_1, \pi_2)$, with π_1 giving the proportion of normal individuals and π_2 giving the proportion of diseased individuals. Note that $\pi_1 + \pi_2 = 1$ as these are the only possibilities, so there is only really one parameter to be estimated here.

The likelihood for π is:

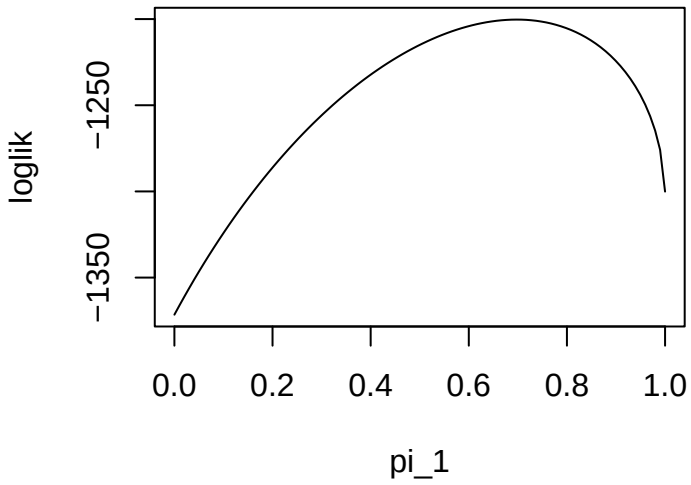
$$L(\pi) = \prod_{i=1}^{n} \{\pi_1 \text{Gamma}(x_i; 0.5, 2) + \pi_2 \text{Gamma}(x_i; 1, 2)\},$$

and so the log-likelihood is

$$l(\pi) = \sum_{i=1}^{n} \log\{\pi_1 \text{Gamma}(x_i; 0.5, 2) + \pi_2 \text{Gamma}(x_i; 1, 2)\}.$$

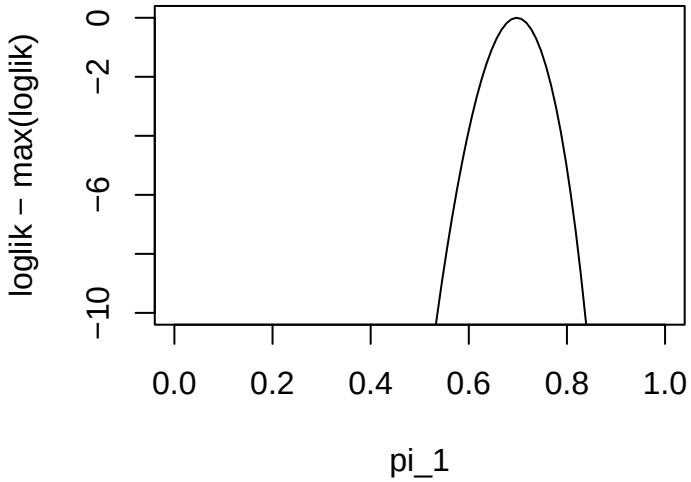
The following code simulates data from the model (with true value of $\pi_1 = 0.7$), then plots the log-likelihood.

```
n <- 1000
x <- rep(0,n)
shape <- c(2,2)
scale <- c(0.5,1)
for (i in 1:n) {
  if (runif(1) < 0.7)
    z <- 1
  else
    z <- 2
  x[i] <- rgamma(1,scale = scale[z],shape = shape[z])
}
mix_loglik <- function (pi1, x)
  sum(log(pi1*dgamma(x,scale = 0.5,shape = 2) +
          (1 - pi1)*dgamma(x,scale = 1,shape = 2)))
pi1_vec <- seq(0,1,length.out = 100)
loglik <- rep(0,100)
for (i in 1:length(pi1_vec))
  loglik[i] <- mix_loglik(pi1_vec[i],x)
plot(pi1_vec,loglik,type = "l",xlab = "pi_1")
```



In this second plot we "zoom in" on the log-likelihood near the maximum:

```
plot(pi1_vec,loglik - max(loglik),ylim = c(-10,0),type = "l",xlab = "pi_1")
```



We can see from these plots that the maximum likelihood estimate is near the true value of 0.7. However, we cannot actually find the maximum easily analytically (for example, try differentiating the log-likelihood and setting the derivative to zero). Therefore we need numerical methods. There are many numerical methods, and the EM algorithm is just one of many that could be used for this problem.

The EM algorithm

For this problem, the EM algorithm has an intuitive form which we now describe. (Note this is *not* a derivation of the EM algorithm — it is just an intuitive heuristic argument.)

For convenience, we introduce a latent variable Z_i for each individual i to indicate whether the individual is normal ($Z_i = 1$) or diseased ($Z_i = 2$). (Remember that the the Z_i are not observed.)

Now note that *if we knew* π, then we could easily compute the posterior probability that each individual is diseased given their test result, $X_i = x_i$. Specifically,

$$w_{ik} := \Pr(Z_i = k \mid X_i = x_i) = \frac{\pi_k L_{ik}}{\sum_{k'=1}^{2} \pi_{k'} L_{ik'}},$$

where $L_{ik} := p(x_i \mid Z_i = k)$. See Bayesian computations for the two-class problem for details on this calculation.

Furthermore, *if we knew these probabilities*, it would be natural to estimate the proportion of individuals in class k by the average of the w_{ik}; that is,

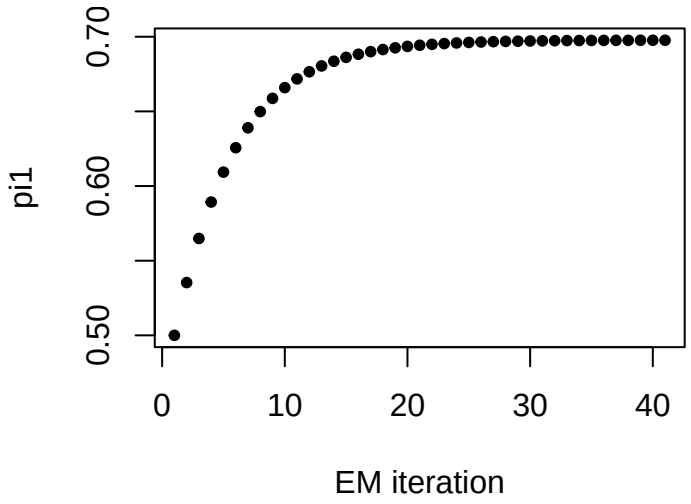
$$\pi_k \approx \frac{1}{n} \sum_{i=1}^{n} w_{ik}.$$

So we have the following challenge: if we knew w we could estimate π, but we need to know π to compute w. This suggests, at least intuitively, an iterative procedure: iterate (1) computing w and (2) estimating π. Here is code implementing this idea:

```
simple_em <- function (x, pi1_init, niter) {
  n <- length(x)
  pi1 <- rep(0,niter + 1)
  pi1[1] <- pi1_init
  L <- matrix(0,n,2)
  L[,1] <- dgamma(x,scale = 0.5,shape = 2)
  L[,2] <- dgamma(x,scale = 1,shape = 2)
  w <- matrix(nrow = n,ncol = 2)
  for (iter in 1:niter) {
    w[,1] <- pi1[iter] * L[,1]
    w[,2] <- (1 - pi1[iter]) * L[,2]
    for (i in 1:n)
      w[i,] <- w[i,]/(w[i,1] + w[i,2])
    pi1[iter + 1] <- mean(w[,1])
  }
  return(pi1)
}
```

Note that the iterative procedure needs a *starting point*—an initial estimate of *pi*. Let's see what happens when we start at $\pi_1 = 0.5$ and run it for 40 iterations:

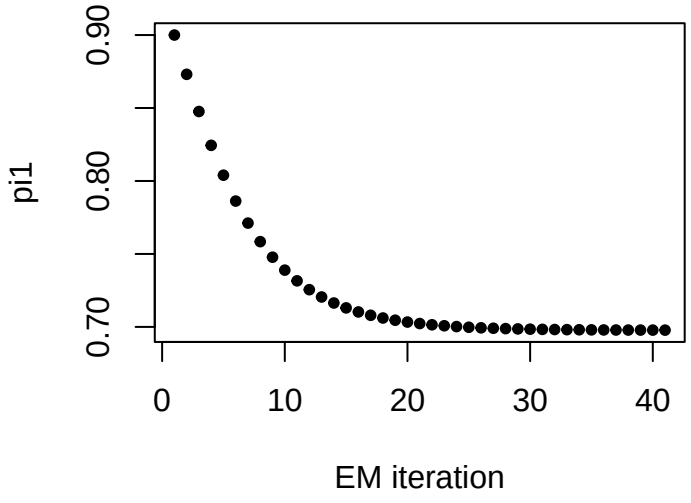
```
pi1_iter <- simple_em(x,pi1_init = 0.5,niter = 40)
plot(pi1_iter,xlab = "EM iteration",ylab = "pi1",pch = 20)
```




```
pi1_iter[41]
# [1] 0.6976
```

Let's try another starting point:

```
pi1_iter = simple_em(x,pi1_init = 0.9,niter = 40)
plot(pi1_iter,xlab = "EM iteration",ylab = "pi1",pch = 20)
```

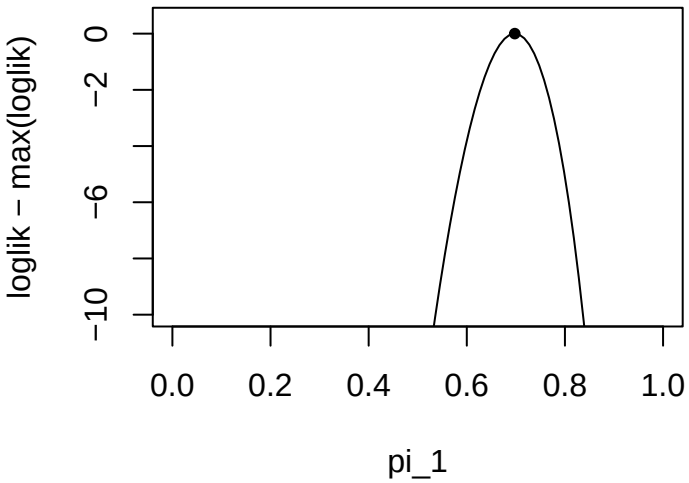



```
pi1_iter[41]
# [1] 0.6978
```

We see it converges to the same value.

Check whether this value is close to the maximum likelihood estimate:

```
plot(pi1_vec,loglik - max(loglik),ylim = c(-10,0.5),type = "l",xlab = "pi_1")
points(pi1_iter[41],mix_loglik(pi1_iter[41],x) - max(loglik),pch = 20)
```


loglik − max(loglik)
−10
−6
−2
0
0.0
0.2
0.4
0.6
0.8
1.0
pi_1