## Monte Carlo Optimization

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## Introduction

This section will cover topics to optimization problems, and solutions Monte Carlo methods provide. Topics covered include

- 1. Stochastic Search and Simulated Annealing
- 2. EM Algorithm and MC EM

## Light bulb example

This exercise is taken from Flury and Zoppe, 2000, see Exercises in EM.

Below is the setup for the first exercise.

## The First Exercise

Suppose there are two light bulb survival experiments. In the first, there are N bulbs whose exact lifetimes  $y_i$  for  $i \in \{1, ..., N\}$  are recorded. The lifetimes have an exponential distribution, such that  $y_i \sim Exp(\theta)$ . In the second experiment, there are M bulbs. After some time t > 0, a researcher walks into the room and only records how many lightbulbs are still burning out of M bulbs. Depending on whether the lightbulbs are still burning or out, the results from the second experiment are right- or -left-censored. There are indicators  $E_1, ..., E_M$  for each of the bulbs in the second experiment. If the bulb is still burning,  $E_i = 1$ , else  $E_i = 0$ .

Given this information, our task is to solve for an MLE estimator for  $\theta$ .

Our first step in solving this is finding the joint likelihood for the observed and unobserved data (i.e. complete-data likelihood).

Let  $X_1, ..., X_M$  be the (unobserved) lifetimes for the second experiment, and let  $Z = \sum_{i=1}^M E_i$  be the number of light bulbs still burning. Thus, the observed data from both the experiments combined is  $\mathcal{Y} = (Y_1, ..., Y_N, E_1, ..., E_M)$  and the unobserserved data is  $\mathcal{X} = (X_1, ..., X_M)$ .

The complete data log-likelihood is obtained by

$$L(\theta|X,Y) = \prod_{i=1}^{N} \frac{1}{\theta} e^{y_i/\theta} \times \prod_{i=1}^{M} \frac{1}{\theta} e^{x_i/\theta}$$
$$= \theta^{-N} e^{-N\bar{y}/\theta} \times \theta^{-M} e^{-\sum_{i=1}^{M} x_i/\theta}$$

And log-likelihood is obtained by

$$log(L(\theta)) = -N \times log(\theta) - N\bar{y}/\theta - M \times log(\theta) + \sum_{i=1}^{M} x_i/\theta$$
$$= -N(log(\theta) + \bar{y}/\theta) - M \times log(\theta) + \sum_{i=1}^{M} x_i/\theta$$

Or as written by Flury and Zoppe,

$$log^{c}(L(\theta|\mathcal{Y},\mathcal{X})) = -N(log(\theta) + \bar{Y}/\theta) - \sum_{i=1}^{M} (log(\theta) + X_{i}/\theta)$$

The next step, is to take the expectation of  $log(L(\theta))$  with respect to observed data.

$$\begin{split} E[log(L(\theta))|\mathcal{Y},\mathcal{X}] &= E[-N(log(\theta) + \bar{Y}/\theta) - \sum_{i=1}^{M} (log(\theta) + X_i/\theta)|\mathcal{Y},\mathcal{X}] \\ &= -N(log(\theta) + \bar{Y}/\theta) - E[\sum_{i=1}^{M} (log(\theta) + X_i/\theta)|\mathcal{Y},\mathcal{X}] \\ &= -N(log(\theta) + \bar{Y}/\theta) - M \times log(\theta) + E[\frac{1}{\theta} \sum_{i=1}^{M} X_i|\mathcal{Y},\mathcal{X}] \\ &= -N(log(\theta) + \bar{Y}/\theta) - M \times log(\theta) + \frac{1}{\theta} \sum_{i=1}^{M} E[X_i|\mathcal{Y},\mathcal{X}] \\ &= -N(log(\theta) + \bar{Y}/\theta) - M \times log(\theta) + \frac{1}{\theta} \sum_{i=1}^{M} E[X_i|\mathcal{Y},\mathcal{X}] \end{split}$$

which is linear for unobserved  $X_i$ . But

(2)

$$E[X_i|\mathcal{Y}] = E[X_i|E_i] = \begin{cases} t + \theta & \text{if } E_i = 1\\ \theta - t \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} & \text{if } E_i = 0 \end{cases}$$

For the first case,  $E_i = 1$ , so

$$E[x_i|x_i > t] = E[x_i + t]$$

$$= t + E[x_i]$$

$$= t + \theta$$

For the second case,  $E_i = 0$ , then

$$\int_0^t P(X_i > x | X_i < t) \ dx = \int_0^t \frac{P(x < X_i < t)}{P(X_i < t)} \ dx$$

For the denominator, we get

$$P(X_i < t) = \int_0^t \frac{1}{\theta} e^{-x_i/\theta} dx$$
$$= \frac{1}{\theta} (-\theta e^{-x_i/\theta})|_0^t$$
$$= 1 - e^{-t/\theta}$$

and for the numerator we obtain

$$\begin{split} P(x < X_i < t) &= \int_x^t \frac{1}{\theta} e^{-x_i/\theta} dx \\ &= \frac{1}{\theta} (-\theta e^{-x_i/\theta})|_0^t \\ &= e^{-x/\theta} - e^{-t/\theta} \end{split}$$

Altogether, we obtain

$$\begin{split} \int_{0}^{t} P(X_{i} > x | X_{i} < t) \ dx &= \int_{0}^{t} \frac{P(x < X_{i} < t)}{P(X_{i} < t)} \ dx \\ &= \int_{0}^{t} \frac{e^{-x/\theta} - e^{-t/\theta}}{(1 - e^{-t/\theta})} \ dx \\ &= \frac{1}{(1 - e^{-t/\theta})} \int_{0}^{t} (e^{-x/\theta} - e^{-t/\theta}) \ dx \\ &= \frac{1}{(1 - e^{-t/\theta})} (\int_{0}^{t} e^{-x/\theta} - \int_{0}^{t} e^{-t/\theta} \ dx) \\ &= \frac{1}{(1 - e^{-t/\theta})} (\theta(1 - e^{-t/\theta}) - x \times e^{-t/\theta}|_{0}^{t}) \\ &= \theta - t \times \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} \end{split}$$

In order to calculate EM esimates for  $\theta$ , we will plug in the expected values

$$E[X_i|\mathcal{Y}] = E[X_i|E_i] = \begin{cases} t + \theta & \text{if } E_i = 1\\ \theta - t \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} & \text{if } E_i = 0 \end{cases}$$

into the log-likelihood

$$\begin{split} \log(L(\theta)) &= -N(\log(\theta) + \bar{y}/\theta) - M \times \log(\theta) + \sum_{i=1}^{M} x_i/\theta \\ &= -N \times \log(\theta) - N\bar{y}/\theta - M \times \log(\theta) + \sum_{i=1}^{M} x_i/\theta \\ &= -(N+M) \times \log(\theta) - N\bar{y}/\theta + \sum_{i=1}^{M} x_i/\theta \\ &= -(N+M) \times \log(\theta) - \frac{1}{\theta} (N\bar{y} + \sum_{i=1}^{M} x_i) \\ &= -(N+M)\log(\theta) - \frac{1}{\theta} [N\bar{Y} + Z(t+\theta) + (M-Z)(\theta - t \times \frac{e^{-t/\theta}}{1 - e^{-t/\theta}})] \end{split}$$

As we iterate through estimates of  $\theta$ , we will use conditioned estimates of  $\theta$  given previous estimates of  $\theta$ . Such that the jth step consists of replacing  $X_i$  in (1) by its expected value (2), using the current numerical parameter value  $\theta^{(j-1)}$ .

(3) 
$$\log(L(\theta)) = -(N+M)\log(\theta) - \frac{1}{\theta}[N\bar{Y} + Z(t+\theta^{(j-1)}) + (M-Z)(\theta^{(j-1)} - tp^{(j-1)})]$$

where

$$p^{(j)} = \frac{e^{-t/\theta^{(j)}}}{1 - e^{-t/\theta^{(j)}}}$$

Once we take the derivative of the log-likelihood and set it to zero, we will come up with an estimate for  $\theta$ 

$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}x} ln(L(\theta)) &= 0 \\ 0 &= -\frac{(N+M)}{\theta} + \frac{1}{\theta^2} \big[ N\bar{Y} + Z(t+\theta) + (M-Z) \big( \theta - t \times \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} \big) \big] \\ \frac{(N+M)}{\theta} &= \frac{1}{\theta^2} \big[ N\bar{Y} + Z(t+\theta) + (M-Z) \big( \theta - t \times \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} \big) \big] \\ \theta &= \big[ N\bar{Y} + Z(t+\theta) + (M-Z) \big( \theta - t \times \frac{e^{-t/\theta}}{1 - e^{-t/\theta}} \big) \big] \ / \ (N+M) \end{split}$$

Thus, for each jth M-step, we will calculate

$$\begin{split} \theta^{(j)} &= f(\theta^{(j-1)}) \\ \theta &= \left[ N\bar{Y} + Z(t+\theta^{(j-1)}) + (M-Z) \left( \theta^{(j-1)} - t \times \frac{e^{-t/\theta^{(j-1)}}}{1 - e^{-t/\theta^{(j-1)}}} \right) \right] \; / \; (N+M) \end{split}$$

```
set.seed(5678)
theta = 5
rate = 1/theta
t = 5
N = 100
M = 50
y = rexp(n = N, rate = rate)
x = rexp(n = M, rate = rate)
x = sort(x)
E = as.integer(x > t)
N.ybar = sum(y)
Z = sum(E)
t = 5
theta.j = 0.1
theta.jp1 = 0.5
for(i in 1:10){
  theta.j = theta.jp1
  p = (exp(-t/theta.j)/(1-exp(-t/theta.j)))
 theta.jp1 = (N.ybar + Z*(t + theta.j) + (M-Z)*(theta.j - t*p)) / (N+M)
  print(theta.jp1)
}
## [1] 4.624345
## [1] 5.366158
## [1] 5.445061
## [1] 5.45323
## [1] 5.454073
## [1] 5.45416
## [1] 5.454169
## [1] 5.45417
## [1] 5.45417
## [1] 5.45417
## compare against MLE from observed data
mean(y)
```

## [1] 6.036602

## note, results will vary if you remove seed