

# Biostatistics 602 - Statistical Inference Lecture 24 E-M Algorithm & Practice Examples

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## Interval Estimation

$\hat{\theta}(\mathbf{X})$  is usually represented as a point estimator

### Interval Estimator

Let  $[L(\mathbf{X}), U(\mathbf{X})]$ , where  $L(\mathbf{X})$  and  $U(\mathbf{X})$  are functions of sample  $\mathbf{X}$  and  $L(\mathbf{X}) \leq U(\mathbf{X})$ . Based on the observed sample  $\mathbf{x}$ , we can make an inference that

$$\theta \in [L(\mathbf{X}), U(\mathbf{X})]$$

Then we call  $[L(\mathbf{X}), U(\mathbf{X})]$  an interval estimator of  $\theta$ .

Three types of intervals

- Two-sided interval  $[L(\mathbf{X}), U(\mathbf{X})]$
- One-sided (with lower-bound) interval  $[L(\mathbf{X}), \infty)$
- One-sided (with upper-bound) interval  $(-\infty, U(\mathbf{X})]$

## Last Lecture

- What is an interval estimator?
- What is the coverage probability, confidence coefficient, and confidence interval?
- How can a  $1 - \alpha$  confidence interval typically be constructed?
- To obtain a lower-bounded (upper-tail) CI, whose acceptance region of a test should be inverted?
  - (a)  $H_0 : \theta = \theta_0$  vs  $H_0 : \theta > \theta_0$
  - (b)  $H_0 : \theta = \theta_0$  vs  $H_0 : \theta < \theta_0$

## Definitions

### Definition : Coverage Probability

Given an interval estimator  $[L(\mathbf{X}), U(\mathbf{X})]$  of  $\theta$ , its *coverage probability* is defined as

$$\Pr(\theta \in [L(\mathbf{X}), U(\mathbf{X})])$$

In other words, the probability of a random variable in interval  $[L(\mathbf{X}), U(\mathbf{X})]$  covers the parameter  $\theta$ .

### Definition: Confidence Coefficient

*Confidence coefficient* is defined as

$$\inf_{\theta \in \Omega} \Pr(\theta \in [L(\mathbf{X}), U(\mathbf{X})])$$

## Definitions

### Definition : Confidence Interval

Given an interval estimator  $[L(\mathbf{X}), U(\mathbf{X})]$  of  $\theta$ , if its confidence coefficient is  $1 - \alpha$ , we call it a  $(1 - \alpha)$  *confidence interval*

### Definition: Expected Length

Given an interval estimator  $[L(\mathbf{X}), U(\mathbf{X})]$  of  $\theta$ , its *expected length* is defined as

$$E[U(\mathbf{X}) - L(\mathbf{X})]$$

where  $\mathbf{X}$  are random samples from  $f_{\mathbf{X}}(\mathbf{x}|\theta)$ . In other words, it is the average length of the interval estimator.

## Typical strategies for finding MLEs

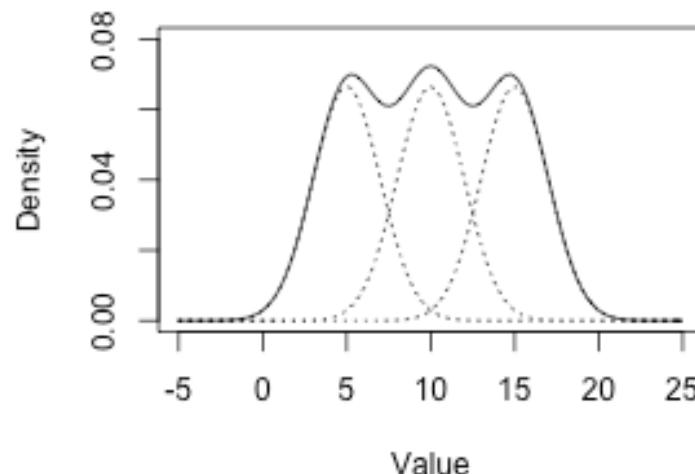
- 1 Write the joint (log-)likelihood function,  $L(\theta|\mathbf{x}) = f_{\mathbf{X}}(\mathbf{x}|\theta)$ .
- 2 Find candidates that makes first order derivative to be zero
- 3 Check second-order derivative to check local maximum.
  - (a) For one-dimensional parameter, negative second order derivative implies local maximum.
- 4 Check boundary points to see whether boundary gives global maximum.

## Confidence set and confidence interval

There is no guarantee that the confidence set obtained from Theorem 9.2.2 is an interval, but quite often

- 1 To obtain  $(1 - \alpha)$  two-sided CI  $[L(\mathbf{X}), U(\mathbf{X})]$ , we invert the acceptance region of a level  $\alpha$  test for  $H_0 : \theta = \theta_0$  vs.  $H_1 : \theta \neq \theta_0$
- 2 To obtain a lower-bounded CI  $[L(\mathbf{X}), \infty)$ , then we invert the acceptance region of a test for  $H_0 : \theta = \theta_0$  vs.  $H_1 : \theta > \theta_0$ , where  $\Omega = \{\theta : \theta \geq \theta_0\}$ .
- 3 To obtain an upper-bounded CI  $(-\infty, U(\mathbf{X})]$ , then we invert the acceptance region of a test for  $H_0 : \theta = \theta_0$  vs.  $H_1 : \theta < \theta_0$ , where  $\Omega = \{\theta : \theta \leq \theta_0\}$ .

## Example: A mixture distribution



## A general mixture distribution

$$f(x|\pi, \phi, \eta) = \sum_{i=1}^k \pi_i f(x; \phi_i, \eta)$$

- $x$  observed data
- $\pi$  mixture proportion of each component
- $f$  the probability density function
- $\phi$  parameters specific to each component
- $\eta$  parameters shared among components
- $k$  number of mixture components

## Solution when $k = 1$

$$f(x|\theta) = \sum_{i=1}^k p_i f_i(x|\mu_i, \sigma_i^2)$$

- $\pi = \pi_1 = 1$
- $\mu = \mu_1 = \bar{x}$
- $\sigma^2 = \sigma_1^2 = \sum_{i=1}^n (x_i - \bar{x})^2 / n$

## MLE Problem for mixture of normals

### Problem

$$f(x|\theta = (\pi, \mu, \sigma^2)) = \sum_{i=1}^k p_i f_i(x|\mu_i, \sigma_i^2)$$

$$f_i(x|\mu_i, \sigma_i^2) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{(x - \mu_i)^2}{2\sigma_i^2}\right]$$

$$\sum_{i=1}^n \pi_i = 1$$

Find MLEs for  $\theta = (\pi, \mu, \sigma^2)$ .

## Incomplete data problem when $k > 1$

$$f(\mathbf{x}|\theta) = \prod_{i=1}^n \left[ \sum_{j=1}^k p_j f_i(x_i|\mu_j, \sigma_j^2) \right]$$

The MLE solution is not analytically tractable, because it involves multiple sums of exponential functions.

## Converting to a complete data problem

Let  $z_i \in \{1, \dots, k\}$  denote the source distribution where each  $x_i$  was sampled from.

$$f(\mathbf{x}|\mathbf{z}, \theta) = \prod_{i=1}^n \left[ \sum_{j=1}^k I(z_i = j) f_i(x_i | \mu_j, \sigma_j^2) \right] = \prod_{i=1}^n f_i(x_i | \mu_{z_i}, \sigma_{z_i}^2)$$

$$\hat{\pi}_i = \frac{\sum_{i=1}^n I(z_i = i)}{n}$$

$$\hat{\mu}_i = \frac{\sum_{i=1}^n I(z_i = i) x_i}{\sum_{i=1}^n I(z_i = i)}$$

$$\hat{\sigma}_i^2 = \frac{\sum_{i=1}^n I(z_i = i) (x_i - \hat{\mu}_i)^2}{\sum_{i=1}^n I(z_i = i)}$$

The MLE solution is analytically tractable, if  $\mathbf{z}$  is known.

## E-M Algorithm

E-M (Expectation-Maximization) algorithm is

- A procedure for typically solving for the MLE.
- Guaranteed to converge the MLE (!)
- Particularly suited to the "missing data" problems where analytic solution of MLE is not tractable

The algorithm was derived and used in various special cases by a number of authors, but it was not identified as a general algorithm until the seminal paper by Dempster, Laird, and Rubin in Journal of Royal Statistical Society Series B (1977).

## Overview of E-M Algorithm

### Basic Structure

- $\mathbf{y}$  is observed (or incomplete) data
- $\mathbf{z}$  is missing (or augmented) data
- $\mathbf{x} = (\mathbf{y}, \mathbf{z})$  is complete data

### Complete and incomplete data likelihood

- Complete data likelihood :  $f(\mathbf{x}|\theta) = f(\mathbf{y}, \mathbf{z}|\theta)$
- Incomplete data likelihood :  $g(\mathbf{y}|\theta) = \int f(\mathbf{y}, \mathbf{z}|\theta) dz$

We are interested in MLE for  $L(\theta|\mathbf{y}) = g(\mathbf{y}|\theta)$ .

## Maximizing incomplete data likelihood

$$L(\theta|\mathbf{y}, \mathbf{z}) = f(\mathbf{y}, \mathbf{z}|\theta)$$

$$L(\theta|\mathbf{y}) = g(\mathbf{y}|\theta)$$

$$k(\mathbf{z}|\theta, \mathbf{y}) = \frac{f(\mathbf{y}, \mathbf{z}|\theta)}{g(\mathbf{y}|\theta)}$$

$$\log L(\theta|\mathbf{y}) = \log L(\theta|\mathbf{y}, \mathbf{z}) - \log k(\mathbf{z}|\theta, \mathbf{y})$$

Because  $\mathbf{z}$  is missing data, we replace the right side with its expectation under  $k(\mathbf{z}|\theta', \mathbf{y})$ , creating the new identity

$$\log L(\theta|\mathbf{y}) = E [\log L(\theta|\mathbf{y}, \mathbf{Z})|\theta', \mathbf{y}] - E [\log k(\mathbf{Z}|\theta, \mathbf{y})|\theta', \mathbf{y}]$$

Iteratively maximizing the first term in the right-hand side results in E-M algorithm.

## Overview of E-M Algorithm (cont'd)

### Objective

- Maximize  $L(\theta|\mathbf{y})$  or  $l(\theta|\mathbf{y})$ .
- Let  $f(\mathbf{y}, \mathbf{z}|\theta)$  denotes the pdf of complete data. In E-M algorithm, rather than working with  $l(\theta|\mathbf{y})$  directly, we work with the surrogate function

$$Q(\theta|\theta^{(r)}) = E \left[ \log f(\mathbf{y}, \mathbf{Z}|\theta) | \mathbf{y}, \theta^{(r)} \right]$$

where  $\theta^{(r)}$  is the estimation of  $\theta$  in  $r$ -th iteration.

- $Q(\theta|\theta^{(r)})$  is the *expected log-likelihood of complete data*, conditioning on the observed data and  $\theta^{(r)}$ .

## Key Steps of E-M algorithm

### Expectation Step

- Compute  $Q(\theta|\theta^{(r)})$ .
- This typically involves in estimating the conditional distribution  $\mathbf{Z}|\mathbf{Y}$ , assuming  $\theta = \theta^{(r)}$ .
- After computing  $Q(\theta|\theta^{(r)})$ , move to the M-step

### Maximization Step

- Maximize  $Q(\theta|\theta^{(r)})$  with respect to  $\theta$ .
- The  $\arg \max_{\theta} Q(\theta|\theta^{(r)})$  will be the  $(r+1)$ -th  $\theta$  to be fed into the E-step.
- Repeat E-step until convergence

## E-M algorithm for mixture of normals

### E-step

$$\begin{aligned} Q(\theta|\theta^{(r)}) &= E \left[ \log f(\mathbf{y}, \mathbf{Z}|\theta) | \mathbf{y}, \theta^{(r)} \right] \\ &= \sum_{\mathbf{z}} k(\mathbf{z}|\theta^{(r)}, \mathbf{y}) \log f(\mathbf{y}, \mathbf{z}|\theta) \\ &= \sum_{i=1}^n \sum_{z_i=1}^k k(z_i|\theta^{(r)}, y_i) \log f(y_i, z_i|\theta) \\ &= \sum_{i=1}^n \sum_{z_i=1}^k \frac{f(y_i, z_i|\theta^{(r)})}{g(y_i|\theta^{(r)})} \log f(y_i, z_i|\theta) \\ y_i, z_i|\theta &\sim \mathcal{N}(\mu_{z_i}, \sigma_{z_i}^2) \\ g(y_i|\theta) &= \sum_{j=1}^k \pi_j f(y_i, z_i = j|\theta) \end{aligned}$$

## E-M algorithm for mixture of normals (cont'd)

### M-step

$$\begin{aligned} Q(\theta|\theta^{(r)}) &= \sum_{i=1}^n \sum_{z_i=1}^k \frac{f(y_i, z_i|\theta^{(r)})}{g(y_i|\theta^{(r)})} \log f(y_i, z_i|\theta) \\ \pi_j^{(r+1)} &= \frac{1}{n} \sum_{i=1}^n k(z_i = j|y_i, \theta^{(r)}) = \frac{1}{n} \frac{f(y_i, z_i = j|\theta^{(r)})}{g(y_i|\theta^{(r)})} \\ \mu_j^{(r+1)} &= \frac{\sum_{i=1}^n x_i k(z_i = j|y_i, \theta^{(r)})}{k(z_i = j|y_i, \theta^{(r)})} = \frac{\sum_{i=1}^n x_i k(z_i = j|y_i, \theta^{(r)})}{n\pi_j^{(r+1)}} \\ \sigma_j^{2, (r+1)} &= \frac{\sum_{i=1}^n (x_i - \mu_j^{(r+1)})^2 k(z_i = j|y_i, \theta^{(r)})}{k(z_i = j|y_i, \theta^{(r)})} \\ &= \frac{\sum_{i=1}^n (x_i - \mu_j^{(r+1)})^2 k(z_i = j|y_i, \theta^{(r)})}{n\pi_j^{(r+1)}} \end{aligned}$$

## Does E-M iteration converge to MLE?

### Theorem 7.2.20 - Monotonic EM sequence

The sequence  $\{\hat{\theta}^{(r)}\}$  defined by the E-M procedure satisfies

$$L(\hat{\theta}^{(r+1)}|\mathbf{y}) \geq L(\hat{\theta}^{(r)}|\mathbf{y})$$

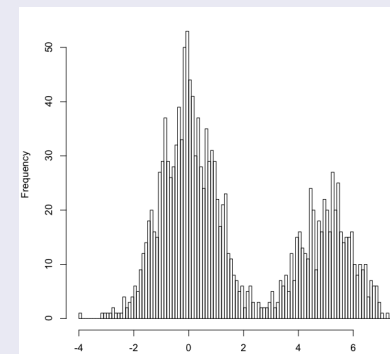
with equality holding if and only if successive iterations yield the same value of the maximized expected complete-data log likelihood, that is

$$E[\log L(\hat{\theta}^{(r+1)}|\mathbf{y}, \mathbf{Z})|\hat{\theta}^{(r)}, \mathbf{y}] = E[\log L(\hat{\theta}^{(r)}|\mathbf{y}, \mathbf{Z})|\hat{\theta}^{(r)}, \mathbf{y}]$$

Theorem 7.5.2 further guarantees that  $L(\hat{\theta}^{(r)}|\mathbf{y})$  converges monotonically to  $L(\hat{\theta}|\mathbf{y})$  for some stationary point  $\hat{\theta}$ .

## A working example (from BIOSTAT615/815 Fall 2012)

### Example Data (n=1,500)



### Running example of implemented software

```
user@host~/> ./mixEM ./mix.dat
Maximum log-likelihood = 3043.46, at pi = (0.667842,0.332158)
between N(-0.0299457,1.00791) and N(5.0128,0.913825)
```

## Practice Problem 1

### Problem

Let  $X_1, \dots, X_n$  be a random sample from a population with pdf

$$f(x|\theta) = \frac{1}{2\theta} \quad -\theta < x < \theta, \theta > 0$$

Find, if one exists, a best unbiased estimator of  $\theta$ .

### Strategy to solve the problem

- Can we use the Cramer-Rao bound? No, because the interchangeability condition does not hold
- Then, can we use complete sufficient statistics?
  - ① Find a complete sufficient statistic  $T$ .
  - ② For a trivial unbiased estimator of  $\theta$ , and compute  $\phi(T) = E[W|T]$  or
  - ③ Make a function  $\phi(T)$  such that  $E[\phi(T)] = \theta$ .

## Solution

First, we need to find a complete sufficient statistic.

$$f_X(x|\theta) = \frac{1}{2\theta} I(|x| < \theta)$$

$$f_{\mathbf{X}}(\mathbf{x}|\theta) = \frac{1}{(2\theta)^n} I(\max_i |x_i| < \theta)$$

Let  $T(\mathbf{X}) = \max_i |X_i|$ , then  $f_T(t|\theta) = \frac{nt^{n-1}}{\theta^n} I(0 < t < \theta)$

$$E[g(T)] = \int_0^\theta \frac{nt^{n-1}g(t)}{\theta^n} dt = 0$$

$$\int_0^\theta t^{n-1}g(t) dt = 0$$

$$\theta^{n-1}g(\theta) = 0$$

$$g(\theta) = 0$$

Therefore the family of  $T$  is complete.

## Solution

We need to make a  $\phi(T)$  such that  $E[\phi(T)] = \theta$ .

First, let's see what the expectation of  $T$  is

$$\begin{aligned} E[g(T)] &= \int_0^\theta t \frac{nt^{n-1}}{\theta^n} dt \\ &= \int_0^\theta \frac{nt^n}{\theta^n} dt \\ &= \frac{n}{n+1} \theta \end{aligned}$$

$\phi(T) = \frac{n+1}{n} T$  is an unbiased estimator and a function of a complete sufficient statistic.

Therefore,  $\phi(T)$  is the best unbiased estimator by Theorem 7.3.23.

## Solution for (a)

$$\begin{aligned} E[W] &= \sum_{\mathbf{x}} W(\mathbf{x}) \Pr(\mathbf{x}) \\ &= \sum_{\mathbf{x}} I\left(\sum_{i=1}^n X_i > X_{n+1}\right) \Pr(\mathbf{x}) \\ &= \sum_{\sum_{i=1}^n X_i > X_{n+1}} \Pr(\mathbf{x}) \\ &= \Pr\left(\sum_{i=1}^n X_i > X_{n+1}\right) = h(p) \end{aligned}$$

Therefore  $T$  is an unbiased estimator of  $h(p)$ .

## Practice Problem 2

### Problem

Let  $X_1, \dots, X_{n+1}$  be the iid Bernoulli( $p$ ), and define the function  $h(p)$  by

$$h(p) = \Pr\left(\sum_{i=1}^n X_i > X_{n+1} \mid p\right)$$

the probability that the first  $n$  observations exceed the  $(n+1)$ st.

1 Show that

$$W(X_1, \dots, X_{n+1}) = I\left(\sum_{i=1}^n X_i > X_{n+1}\right)$$

is an unbiased estimator of  $h(p)$ .

2 Find the best unbiased estimator of  $h(p)$ .

## Solution for (b)

$T = \frac{1}{n+1} \sum_{i=1}^{n+1} X_i$  is complete sufficient statistic for  $p$ .

$$\begin{aligned} \phi(T) &= E[W|T] = \Pr(W = 1|T) \\ &= \Pr\left(\sum_{i=1}^n X_i > X_{n+1} | T\right) \end{aligned}$$

- If  $T = 0$ , then  $\sum_{i=1}^n X_i = X_{n+1}$
- If  $T = 1$ , then
  - $\Pr(\sum_{i=1}^n X_i = 1 > X_{n+1} = 0) = n/(n+1)$
  - $\Pr(\sum_{i=1}^n X_i = 0 < X_{n+1} = 1) = 1/(n+1)$
- If  $T = 2$  then
  - $\Pr(\sum_{i=1}^n X_i = 2 > X_{n+1} = 0) = \binom{n}{2} / \binom{n+1}{2} = (n-1)/(n+1)$
  - $\Pr(\sum_{i=1}^n X_i = 1 = X_{n+1} = 1) = 2/(n+1)$
- If  $T > 2$ , then  $\sum_{i=1}^n X_i \geq 2 > 1 \geq X_{n+1}$

## Solution for (b) (cont'd)

Therefore, the best unbiased estimator is

$$\begin{aligned} \phi(T) &= \Pr\left(\sum_{i=1}^n X_i > X_{n+1} | T\right) \\ &= \begin{cases} 0 & T = 0 \\ n/(n+1) & T = 1 \\ (n-1)/(n+1) & T = 2 \\ 1 & T \geq 3 \end{cases} \end{aligned}$$

## (a) Posterior distribution of $\theta$

$$\begin{aligned} f(\mathbf{x}, \theta) &= \pi(\theta)f(\mathbf{x}|\theta)\pi(\theta) \\ &= \frac{1}{\Gamma(\alpha)\beta^\alpha} \theta^{\alpha-1} e^{-\theta/\beta} \prod_{i=1}^n [\theta \exp(-\theta x_i)] \\ &= \frac{1}{\Gamma(\alpha)\beta^\alpha} \theta^{\alpha-1} e^{-\theta/\beta} \theta^n \exp\left(-\theta \sum_{i=1}^n x_i\right) \\ &= \frac{1}{\Gamma(\alpha)\beta^\alpha} \theta^{\alpha+n-1} \exp\left[-\theta \left(1/\beta + \sum_{i=1}^n x_i\right)\right] \\ &\propto \text{Gamma}\left(\alpha + n - 1, \frac{1}{\beta^{-1} + \sum_{i=1}^n x_i}\right) \\ \pi(\theta|\mathbf{x}) &= \text{Gamma}\left(\alpha + n - 1, \frac{1}{\beta^{-1} + \sum_{i=1}^n x_i}\right) \end{aligned}$$

## Practice Problem 3

### Problem

Suppose  $X_1, \dots, X_n$  are iid samples from  $f(x|\theta) = \theta \exp(-\theta x)$ . Suppose the prior distribution of  $\theta$  is

$$\pi(\theta) = \frac{1}{\Gamma(\alpha)\beta^\alpha} \theta^{\alpha-1} e^{-\theta/\beta}$$

where  $\alpha, \beta$  are known.

- (a) Derive the posterior distribution of  $\theta$ .
- (b) If we use the loss function  $L(\theta, a) = (a - \theta)^2$ , what is the Bayes rule estimator for  $\theta$ ?

## (b) Bayes' rule estimator with squared error loss

Bayes' rule estimator with squared error loss is posterior mean. Note that the mean of  $\text{Gamma}(\alpha, \beta)$  is  $\alpha\beta$ .

$$\begin{aligned} \pi(\theta|\mathbf{x}) &= \text{Gamma}\left(\alpha + n - 1, \frac{1}{\beta^{-1} + \sum_{i=1}^n x_i}\right) \\ E[\theta|\mathbf{x}] &= E[\pi(\theta|\mathbf{x})] \\ &= \frac{\alpha + n - 1}{\beta^{-1} + \sum_{i=1}^n x_i} \end{aligned}$$



# Summary

## Today

- E-M Algorithm
- Practice Problems for the Final Exam

## Next Lectures

- Bayesian Tests
- Bayesian Intervals
- More practice problems