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Lecture 15: MLE: Theory and Practice

Suppose  $X_1, ..., X_n$  independent and identically distributed random variables with  $p(x|\theta)$ , for some  $\theta \in \Theta$ . The Maximum Likelihood Estimator (MLE) is the random variable

$$\hat{\theta_n} = \arg \max_{\theta} \prod_{i=1}^n p(x_i|\theta)$$
$$= \arg \min_{\theta} -\sum_{i=1}^n \log p(x_i|\theta)$$

**Theorem 1** (Asymptotic Distribution of MLE) Let  $X_1, X_2, ..., X_n$  be iid random variables with  $p(x|\theta^*)$ , where  $\theta^* \in \Theta$  is a vector parameter. And let  $\hat{\theta_n} = \arg \max_{\theta} \prod_{i=1}^n p(x_i|\theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(x_i|\theta)$ . Define  $\log p(x|\theta) := \sum_{i=1}^n \log p(x_i|\theta)$ , and assume  $\frac{\partial \log p(x|\theta)}{\partial \theta_j}$  and  $\frac{\partial^2 \log p(x|\theta)}{\partial \theta_j \partial \theta_k}$  exist for all j,k. Then

$$\hat{\theta_n} \overset{asymp.}{\sim} N(\theta^*, \frac{1}{n}I^{-1}(\theta^*))$$

where  $I(\theta^*)$  is the Fisher- Information Matrix.

$$[I(\theta^*)]_{j,k} = -E[\frac{\partial^2 logp(x|\theta)}{\partial \theta_j \partial \theta_k}|_{\theta=\theta^*}]$$

 $\frac{\text{PROOF (scalar } \theta)}{\text{By the mean value theorem,}}$ 

$$\frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\hat{\theta}} = \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} + \frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta=\tilde{\theta}} (\hat{\theta} - \theta^*)$$

, where  $\tilde{\theta}$  is some value between  $\theta^*$  and  $\hat{\theta}$ . By definition,  $\frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\hat{\theta}} = 0$ , so

$$0 = \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} + \frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta=\tilde{\theta}} (\hat{\theta} - \theta^*)$$

Now consider  $\sqrt{n}(\hat{\theta} - \theta^*)$ . The reason for multiplying by  $\sqrt{n}$  is that in the case where  $X_1, X_2, ..., X_n$  be iid random variables with  $N(\theta^*, 1), \sqrt{n}(\hat{\theta} - \theta^*) \sim N(0, 1)$ . From equation above we have

$$\sqrt{n}(\hat{\theta} - \theta^*) = \frac{\frac{1}{\sqrt{n}} \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta = \theta^*}}{\frac{-1}{n} \frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta = \tilde{\theta}}}$$

Consider the numerator.

$$\frac{1}{\sqrt{n}}\frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} = \frac{1}{\sqrt{n}}\sum_{i=1}^n \frac{\partial logp(x_i|\theta)}{\partial \theta}|_{\theta=\theta^*}$$

By the Central Limit Theorem, we have

$$\frac{1}{\sqrt{n}} \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} \stackrel{distribution}{\longrightarrow} Normal$$

with mean

$$E[\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial logp(x_{i}|\theta)}{\partial \theta}|_{\theta=\theta^{*}}] = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}E[\frac{\partial logp(x_{i}|\theta)}{\partial \theta}|_{\theta=\theta^{*}}]$$

and

$$\begin{split} E[\frac{\partial logp(x_i|\theta)}{\partial \theta}|_{\theta=\theta^*}] &= \int \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} p(x|\theta^*) dx \\ &= \int \frac{1}{p(x|\theta^*)} \frac{\partial p(x|\theta)}{\partial \theta} p(x|\theta^*) dx \\ &= \int \frac{\partial p(x|\theta)}{\partial \theta} dx \\ &= \frac{\partial}{\partial \theta} \int p(x|\theta) d\theta = 0 \end{split}$$

and variance

$$E[(\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial logp(x_{i}|\theta)}{\partial \theta}|_{\theta=\theta^{*}})^{2}] = \frac{1}{n}\sum_{i=1}^{n}E[(\frac{\partial logp(x_{i}|\theta)}{\partial \theta})^{2}|_{\theta=\theta^{*}}]$$

Note that

$$E\left[\frac{\partial^2 logp(x_i|\theta)}{\partial \theta^2}\right] = \int \left(\frac{1}{p(x|\theta)} \frac{\partial^2 p(x_i|\theta)}{\partial \theta^2} - \left(\frac{1}{p(x|\theta)} \frac{\partial p(x_i|\theta)}{\partial \theta}\right)^2\right) p(x|\theta) d\theta$$
$$= -E\left[\left(\frac{\partial logp(x_i|\theta)}{\partial \theta}\right)^2\right]$$

So the variance is

$$-\frac{1}{n}\sum_{i=1}^{n}E\left[\frac{\partial^{2}logp(x_{i}|\theta)}{\partial\theta^{2}}|_{\theta=\theta^{*}}\right] = I(\theta^{*})$$

Now consider the denominator.

$$\frac{1}{n} \frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta=\tilde{\theta}} = \frac{1}{n} \sum_{i=1}^n \frac{\partial^2 logp(x_i|\theta)}{\partial \theta^2}|_{\theta=\theta^*}$$
$$\stackrel{SLLN}{\to} E[\frac{\partial^2 logp(x_i|\theta)}{\partial \theta^2}|_{\theta=\theta^*}]$$
$$= -I(\theta^*)$$

So from the equation below,

$$\sqrt{n}(\hat{\theta} - \theta^*) = \frac{\frac{1}{\sqrt{n}} \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta = \theta^*}}{\frac{-1}{n} \frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta = \tilde{\theta}}}$$

the numerator

$$\frac{1}{\sqrt{n}} \frac{\partial logp(x|\theta)}{\partial \theta}|_{\theta=\theta^*} \stackrel{distribution}{\longrightarrow} N(0, I(\theta^*))$$

Lecture 15: MLE: Theory and Practice

and the denominator

$$-\frac{1}{n}\frac{\partial^2 logp(x|\theta)}{\partial \theta^2}|_{\theta=\tilde{\theta}} \stackrel{SLLN}{\to} I(\theta^*)$$

Hence, the whole term converges as follows

$$\begin{split} \sqrt{n}(\hat{\theta} - \theta^*) & \stackrel{distribution}{\to} & \frac{1}{I(\theta^*)}N(0, I(\theta^*)) \\ & \equiv & N(0, I^{-1}(\theta^*)) \end{split}$$

## 1 Invariance of the MLE

**Theorem 2** Let  $\tau = g(\theta^*)$  be a function of  $\theta^*$ , and let  $\hat{\theta_n}$  be the MLE of  $\theta^*$ . Then  $\hat{\tau_n} = g(\hat{\theta_n})$  is the MLE of  $\tau$ .

PROOF:

Let  $h = g^{-1}$  denote the inverse map of g. Define the induced log-likelihood function

$$L(x|\tau) = \max_{\theta \in h(\tau)} logp(x|\theta)$$

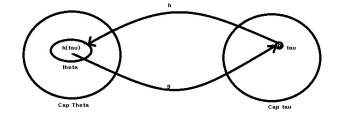


Figure 1: h is the inverse map of g

The MLE of  $\tau$  is

$$\begin{aligned} \hat{\tau_n} &= \arg \max_{\tau} L(x|\tau) \\ &= \arg \max_{\tau} \max_{\theta \in h(\tau)} logp(x|\theta) \\ &= g(\hat{\tau_n}) \end{aligned}$$

**Example 1**  $X_i \stackrel{i.i.d}{\sim} Poisson(\lambda)$ , i = 1,...,nFind the MLE of probability that  $x \sim Poisson(\lambda)$  is greater than  $\lambda$ . Define

$$\begin{split} \rho &= g(\lambda) &= P(X > \lambda) \\ &= \sum_{k = \lfloor \lambda + 1 \rfloor}^{\infty} e^{-\lambda} \frac{\lambda^k}{k!} \\ &= 1 - \sum_{k=0}^{\lfloor \lambda \rfloor} e^{-\lambda} \frac{\lambda^k}{k!} \end{split}$$

Lecture 15: MLE: Theory and Practice

The MLE of  $\rho$  is

$$\hat{\rho_n} = 1 - \sum_{k=0}^{\lfloor \hat{\lambda_n} \rfloor} e^{-\hat{\lambda_n}} \frac{\hat{\lambda_n}^k}{k!}$$

where

$$\hat{\lambda} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

## 2 Numerical Methods for Obtaining the MLE

If  $X \sim p(x|\theta), \theta \in \Theta$ , then the MLE is the solution to the equations  $\frac{\partial logp(x|\theta)}{\partial \theta} = 0$ . Sometimes these equations have a simple closed form solution, and other times they do not and we must use computational methods to find  $\hat{\theta}$ .

**Example 2**  $X_i \stackrel{i.i.d}{\sim} Poisson(\lambda), \hat{\lambda_n} = \frac{1}{n} \sum X_i$ 

**Example 3**  $X \sim N(H\theta, I)$ , where H is  $n \times k$  and known and  $\theta$  is  $k \times 1$  and unknown.  $\hat{\theta} = (H^T H)^{-1} H^T X$ 

**Example 4**  $X_i \stackrel{i.i.d}{\sim} pN(\mu_0, \sigma_0^2) + (1-p)N(\mu_1, \sigma_1^2), i = 1, ..., n, \theta = [p \ \mu_0 \ \sigma_0^2 \ \mu_1 \ \sigma_1^2]^T$ 

$$p(x_i|\theta) = \frac{p}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{(x_i-\mu_0)^2}{2\sigma_0^2}} + \frac{1-p}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{(x_i-\mu_1)^2}{2\sigma_1^2}}$$

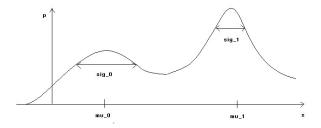


Figure 2: Mixed Gaussian Density

$$p(x|\theta) = \prod_{i=1}^{n} p(x_i|\theta), a \text{ product of sums of exponentials}$$

$$log \ p(x|\theta) = \sum of \ logs \ (sums \ of \ exponentials) \ \leftarrow Messy!$$

Sufficient Statistic:  $(X_1, X_2, ..., X_n)$ 

How to proceed?

$$\theta^{(t+1)} = \theta^{(t)} + \Delta \frac{\partial}{\partial \theta} \log p(x|\theta)|_{\theta = \theta^{(t)}}, \text{ where } \Delta \text{ is a step size.}$$

2. Expectation-Maximization Algorithm (EM algorithm)

## 3 The EM Algorithm

Suppose the log-likelihood function looks like this:

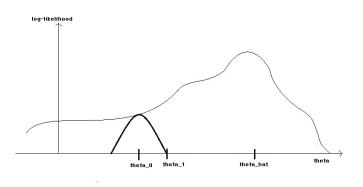


Figure 3: EM algorithm

We would like to find the maximum at the point  $\hat{\theta}$ . One way is to follow the gradient (uphill) from a random initial guess.

The EM algorithm operates a bit differently. It is an iterative method that constructs a surrogate function at an initial starting point  $\theta_0$  as shown above as the C2shed function. This function is designed to "touch" the log-likelihood at  $\theta_0$  and  $t_0$  be easy to maximize. The maximizer of the surrogate gives us a new point  $\theta_1$ which is guaranteed to have a likelihood value at least as large as  $\theta_0$ .

We then repeat this process at  $\theta_1$  and generate a sequence of values (with increasing likelihood:  $\theta_0, \theta_1, ...$ in this fashion). Unfortunately, unless the log-likelihood is concave (negative log-likelihood convex) and hence unimodal, there is no guarantee that any method, besides a global brute-force search, will converge to  $\hat{\theta}$ .