

# Lecture 7 Point Estimation

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# Outline

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- 2 Method of Moments
- 3 Maximum Likelihood Estimations
- 4 Bayes Estimators



# Introduction

- Suppose  $X_1, X_2, \dots, X_n$  is a sample from  $f(x|\theta)$ , we want to find a statistic  $W(X_1, X_2, \dots, X_n)$  which is an estimator of  $\theta$ .

# Method of Moments

Let  $X_1, X_2, \dots, X_n$  be a sample from  $f(x|\theta_1, \dots, \theta_k)$ . Define

$$m_1 = \frac{1}{n} \sum_{i=1}^n X_i^1, \quad \mu_1 = EX^1$$

$$m_2 = \frac{1}{n} \sum_{i=1}^n X_i^2, \quad \mu_2 = EX^2$$

$$\vdots$$

$$m_k = \frac{1}{n} \sum_{i=1}^n X_i^k, \quad \mu_k = EX^k$$

Then we equate  $m_1 = \mu_1(\theta_1, \dots, \theta_k)$ ,  $m_2 = \mu_2(\theta_1, \dots, \theta_k)$ ,  $\dots$ ,  $m_k = \mu_k(\theta_1, \dots, \theta_k)$  to find  $\hat{\theta}_1, \dots, \hat{\theta}_k$ .

## Example 7.2.1 (Normal Method of Moments)

If  $X_1, X_2, \dots, X_n, \sim N(\theta, \sigma^2)$ . Then we have  $\mu_1 = \theta, \mu_2 = \sigma^2 + \theta^2$ .

Using method of moments, we equate

$$\bar{X} = \theta, \quad \frac{1}{n} \sum_{i=1}^n X_i^2 = \sigma^2 + \theta^2$$

$$\Rightarrow \hat{\theta} = \bar{X}, \quad \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X})^2$$

## Example 7.2.2 (Binomial Method of Moments)

Let  $X_1, X_2, \dots, X_n$  be i.i.d.  $\text{Bin}(k, p)$ , where both  $k$  and  $p$  are unknown. Equate the first two moments:

$$\begin{aligned}\bar{X} &= kp \\ \frac{1}{n} \sum_{i=1}^n X_i^2 &= kp(1-p) + k^2 p^2.\end{aligned}$$

After a little algebra, we have

$$\hat{k} = \frac{\bar{X}^2}{\bar{X} - (1/n) \sum (X_i - \bar{X})^2} \quad \text{and} \quad \hat{p} = \bar{X} / \hat{k}.$$

# Maximum Likelihood Estimations

Let  $X_1, X_2, \dots, X_n$  be i.i.d. from  $f(x|\theta_1, \dots, \theta_k)$ . Let

$L(\theta|x) = L(\theta_1, \dots, \theta_k|x_1, \dots, x_k) = \prod_{i=1}^n f(x_i|\theta_1, \dots, \theta_k)$  be the likelihood function.

## Definition 7.2.4

For each sample point  $x$ , let  $\hat{\theta}(x)$  be a parameter value at which  $L(\theta|x)$  attains its maximum as a function of  $\theta$ , with  $x$  held fixed. Then  $\hat{\theta}(x)$  is a maximum likelihood estimator of  $\theta$ .

**Remark** Sometime maximizing  $l(\theta|x) = \log(L(\theta|x))$  is much easier than maximizing  $L(\theta|x)$ .

- **Theorem 7.2.10 (Invariance Property of MLE)** If  $\hat{\theta}$  is the MLE of  $\theta$ , then for any function  $\tau(\theta)$ , the MLE of  $\tau(\theta)$  is  $\tau(\hat{\theta})$ .

**Remark**  $X_1, \dots, X_n$  in most cases do not have to be **identically distributed**.

# Bayes Estimators

Let  $\mathbf{X} \sim f(\mathbf{x}|\theta)$ ,  $\theta \sim \pi(\theta)$ , where  $\pi(\theta)$  is the prior distribution of  $\theta$ . Then after observing  $\mathbf{X} = \mathbf{x}$ , the posterior distribution of  $\theta$  is

$$\pi(\theta|\mathbf{x}) = \frac{f(\mathbf{x}|\theta)\pi(\theta)}{m(\mathbf{x})}$$

where  $m(\mathbf{x})$  is the marginal distribution of  $\mathbf{X}$ ,

$$m(\mathbf{x}) = \int f(\mathbf{x}|\theta)\pi(\theta)d\theta.$$



## Example 7.2.14

Let  $X_1, X_2, \dots, X_n$  be i.i.d. Bernoulli( $p$ ). Then  $Y = \sum_{i=1}^n X_i$  is Bin( $n, p$ ).

We assume the prior distribution on  $p$  is Beta( $\alpha, \beta$ ). Then

$$\begin{aligned} f(y, p) &= \left[ \binom{n}{y} p^y (1-p)^{n-y} \right] \left[ \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1} (1-p)^{\beta-1} \right] \\ &= \binom{n}{y} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{y+\alpha-1} (1-p)^{n-y+\beta-1} \\ f(y) &= \int_0^1 f(y, p) dp = \binom{n}{y} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \cdot \frac{\Gamma(y + \alpha)\Gamma(n - y + \beta)}{\Gamma(n + \alpha + \beta)} \end{aligned}$$

Therefore  $f(p|y) = \frac{\Gamma(n+\alpha+\beta)}{\Gamma(y+\alpha)\Gamma(n-y+\beta)} p^{y+\alpha-1} (1-p)^{n-y+\beta-1}$ , which is Beta( $y + \alpha, n - y + \beta$ ). Bayes estimator of  $p$  is the mean of  $f(p|y)$ , which is

$$\hat{p}_B = \frac{y + \alpha}{\alpha + \beta + n}.$$

### Definition 7.2.6 (Conjugate Family)

Let  $\mathcal{F}$  denote the class of pdf or pmf  $f(x|\theta)$  (indexed by  $\theta$ ). A class  $\Pi$  of prior distribution is a conjugate family of  $\mathcal{F}$  if the posterior distribution is in the class  $\Pi$  for all  $f \in \mathcal{F}$ , all prior in  $\Pi$ , and all  $x \in \mathcal{X}$

$$P(\theta) = \pi(\theta|\mathbf{y}) = \frac{f(\mathbf{y}|\theta)\pi(\theta)}{\int_{\theta} f(\mathbf{y}|\theta)\pi(\theta)d\theta} \quad (12.3')$$

- Estimating the normalising constant
- Markov chain Monte Carlo (MCMC): Monte Carlo integration and Markov chain sampling

we estimated unknown parameters using the methods:

- Maximum likelihood : Newton - Raphson(NR)
- MCMC
- NR比MCMC收敛的快。
- 对于多峰分布，NR只能找到一个，而MCMC可以找到多个。
- NW对于固定的似然初始值，它的路径是一样的；而MCMC即使初始值相同，它的路径也是随机的。

- **Target density**  $P(\theta)$  is not always achievable because it may have a complex, or even unknown, form.
- Markov chains provide a method of drawing samples from target densities (regardless of their complexity).
- Using these conditional steps, we build up a chain of samples  $(\theta^1, \dots, \theta^M)$  after specifying a starting value  $\theta^0$

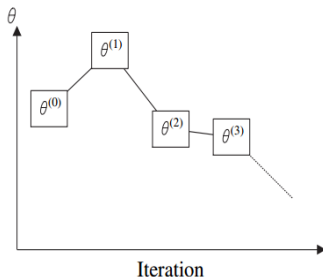


Figure 13.3 A simple example of a Markov chain.

Markov property:

$$P(\theta^i = a | \theta^{i-1}, \theta^{i-2}, \dots, \theta^0) = P(\theta^i = a | \theta^{i-1})$$

An algorithm for creating a Markov chain for a target probability density  $P(\theta)$  is:

- 1 Choose an initial value  $\theta^0$ . The restriction on the initial value is that it needs to be within the distribution of  $P(\cdot)$ , so that  $P(\theta) > 0$
- 2 Create a new sample using  $\theta^1 \sim \pi(\theta^1 | \theta^0, \mathbf{y})$
- 3 Repeat step 2 M times, each time increasing both indices by 1.

**Transitional density:**  $\pi(\theta^{i+1} | \theta^i)$ , Normal distribution.

# The Metropolis – Hastings sampler

- The Metropolis – Hastings sampler works by randomly **proposing a new value**  $\theta^*$
- If this proposed value is **accepted** (according to a criterion below),  $\theta^{i+1} = \theta^*$
- If this proposed value is **rejected** (according to a criterion below),  $\theta^{i+1} = \theta^i$
- Another proposal is made and the chain progresses by assessing this new proposal

- $\theta^* = \theta^i + Q$ ,  $Q$  is called the **proposal density**,  $N(0,1)$  or  $U[-1,1]$
- The acceptance criterion is:

$$\theta^{i+1} = \begin{cases} \theta^* & \text{if } U < \alpha \\ \theta^i & \text{otherwise} \end{cases}$$

where  $U \sim U[-1, 1]$  and

$$\alpha = \min\left\{\frac{\pi(\theta^*|\mathbf{y})}{\pi(\theta^i|\mathbf{y})} \cdot \frac{Q(\theta^i|\theta^*)}{Q(\theta^*|\theta^i)}, 1\right\}$$

where  $P(\theta|\mathbf{y})$  is the probability of  $\theta$  given the data  $\mathbf{y}$  (the likelihood)

If the proposal density is symmetric ( $Q(a|b) = Q(b|a)$ ), then

$$\alpha = \min\left\{\frac{\pi(\theta^*|\mathbf{y})}{\pi(\theta^i|\mathbf{y})}, 1\right\}$$

### 例1: The Metropolis - Hastings sampler

设  $Y_1, Y_2, \dots, Y_n \sim^{iid} N(\mu, \sigma^2)$ ,  $(\mu, \sigma^2)$  的先验分布为  $\pi(\mu, \sigma^2) \propto \frac{1}{\sigma^2}$ 。计算  $E(\mu|Y = y)$  和  $E(\sigma^2|Y = y)$ 。

解:  $(\mu, \sigma^2)$  后验分布为

$$\pi(\mu, \sigma^2 | Y = y) \propto \left(\frac{1}{\sigma^2}\right)^{\frac{n}{2}+1} \exp\left\{-\frac{\sum_{i=1}^n (y_i - \mu)^2}{2\sigma^2}\right\}$$

- 《统计模拟及其R实现》P203
- 为了比较方法, 假设  $Y_1, Y_2, \dots, Y_n \sim^{iid} N(2, 4^2)$



# The Gibbs sampler

- The Gibbs sampler is another way of generating a Markov chain.
- It splits the parameters into a number of components and then updates each one in turn.
- For the beetle mortality example, a Gibbs sampler to update the two unknown parameters would be:
  - 1 Assign an initial value to the two unknowns:  $\beta_1^0$  and  $\beta_2^0$
  - 2 (a) Generate  $\beta_2^1 \sim \pi(\beta_2 | \mathbf{y}, \beta_1^0)$   
 (b) Generate  $\beta_1^1 \sim \pi(\beta_1 | \mathbf{y}, \beta_2^0)$
  - 3 Repeat the step 2  $M$  times, each time increasing the sample indices by 1.

上面举例比较简单，复杂的见《统计模拟及其R实现》P199 例8.4

## 例1续: The Gibbs sampler

设  $Y_1, Y_2, \dots, Y_n \sim^{iid} N(\mu, \sigma^2)$ ,  $(\mu, \sigma^2)$  的先验分布为  $\pi(\mu, \sigma^2) \propto \frac{1}{\sigma^2}$ 。计算  $E(\mu|Y = y)$  和  $E(\sigma^2|Y = y)$ 。

解:  $(\mu, \sigma^2)$  后验分布为

$$\pi(\mu, \sigma^2|Y = y) \propto \left(\frac{1}{\sigma^2}\right)^{\frac{n}{2}+1} \exp\left\{-\frac{\sum_{i=1}^n (y_i - \mu)^2}{2\sigma^2}\right\}$$

则:

$$\pi(\mu|\sigma^2, y) \propto \exp\left\{-\frac{\sum_{i=1}^n (y_i - \mu)^2}{2\sigma^2}\right\} \propto N(\bar{y}, \frac{\sigma^2}{n}) \quad (1)$$

$$\pi(\sigma^2|\mu, y) \propto \left(\frac{1}{\sigma^2}\right) \exp\left\{-\frac{\sum_{i=1}^n (y_i - \mu)^2}{2\sigma^2}\right\} \propto IG\left(\frac{n}{2}, \frac{\sum_{i=1}^n (y_i - \mu)^2}{2}\right) \quad (2)$$

# 考虑Logit模型

例：考虑54个老人智力得分。

Table 7.8 *Symptoms of senility ( $s=1$  if symptoms are present and  $s=0$  otherwise) and WAIS scores ( $x$ ) for  $N=54$  people.*

$x$	$s$	$x$	$s$	$x$	$s$	$x$	$s$	$x$	$s$
9	1	7	1	7	0	17	0	13	0
13	1	5	1	16	0	14	0	13	0
6	1	14	1	9	0	19	0	9	0
8	1	13	0	9	0	9	0	15	0
10	1	16	0	11	0	11	0	10	0
4	1	10	0	13	0	14	0	11	0
14	1	12	0	15	0	10	0	12	0
8	1	11	0	13	0	16	0	4	0
11	1	14	0	10	0	10	0	14	0
7	1	15	0	11	0	16	0	20	0
9	1	18	0	6	0	14	0		

注：中科大张伟平《计算统计讲义》

考虑Logit模型:

$$Y_i \sim \text{Bin}(1, \pi_i), \quad \log \frac{\pi_i}{1 - \pi_i} = \beta_0 + \beta_1 x_i, \quad i = 1, 2, \dots, 54$$

则似然函数为:

$$\begin{aligned} f(\mathbf{y} | \beta_0, \beta_1) &= \prod_{i=1}^n \left( \frac{e^{\beta_0 + \beta_1 x_i}}{1 + e^{\beta_0 + \beta_1 x_i}} \right)^{y_i} \left( \frac{1}{1 + e^{\beta_0 + \beta_1 x_i}} \right)^{1 - y_i} \\ &= \exp \left\{ \sum_{i=1}^n [(\beta_0 + \beta_1 x_i) y_i - \log(1 + e^{\beta_0 + \beta_1 x_i})] \right\} \end{aligned}$$

考虑 $\beta_0, \beta_1$ 的先验分布为独立的正态分布:

$$\beta_j \sim N(\mu_j, \sigma_j^2)$$

从而后验分布为:

$$\begin{aligned}
 f(\beta_0, \beta_1 | \mathbf{y}) &\propto f(\mathbf{y} | \beta_0, \beta_1) \pi(\beta_0, \beta_1) \\
 &\propto \exp \left\{ \sum_{i=1}^n [(\beta_0 + \beta_1 x_i) y_i - \log(1 + e^{\beta_0 + \beta_1 x_i})] \right. \\
 &\quad \left. - \frac{(\beta_0 - \mu_0)^2}{\sigma_0^2} - \frac{(\beta_1 - \mu_1)^2}{\sigma_1^2} \right\}
 \end{aligned}$$

# Diagnostics of chain convergence

- Assumption: the sample densities for the unknown parameters were good estimates of the target densities.
- If this assumption is incorrect, then inferences could be invalid.
- We can only make valid inference when a chain has **converged** to the target density.
  - Chain history
  - Chain autocorrelation
  - Multiple chains

# Chain history

A chain that has converged should show a **reasonable degree of randomness** between iterations, signifying that the Markov chain has found an area of high likelihood and is integrating over the target density (known as mixing).

- $\text{logit}(\pi_i) = \beta_1 + \beta_2 x_1$
- $\text{logit}(\pi_i) = \beta_1 + \beta_2 (x_1 - \bar{x})$

**Note:** By centring the dose covariate we have greatly **improved the convergence** because centring **reduces the correlation between the parameter estimates**  $\beta_1$  and  $\beta_2$

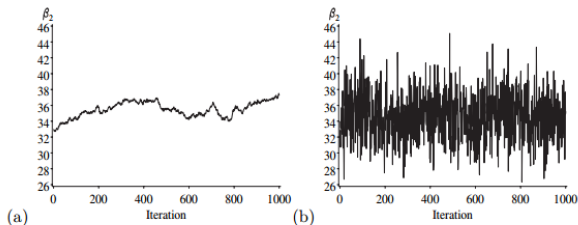


Figure 13.11 Example of a chain showing (a) poor convergence and (b) reasonable convergence (first 1,000 iterations using Gibbs sampling). Estimate for  $\beta_2$  using the logit link using two different parameterizations.





(b)

## 13.5.2 Chain autocorrelation

- Autocorrelation is a useful diagnostic because it summarizes the dependence between neighbouring samples.
- Ideally we would like neighbouring samples to be completely independent, as this would be the most efficient chain possible.
- In practice we usually accept some autocorrelation, but large values (greater than 0.4) can be problematic.
- **Autocorrelation function (ACF)**

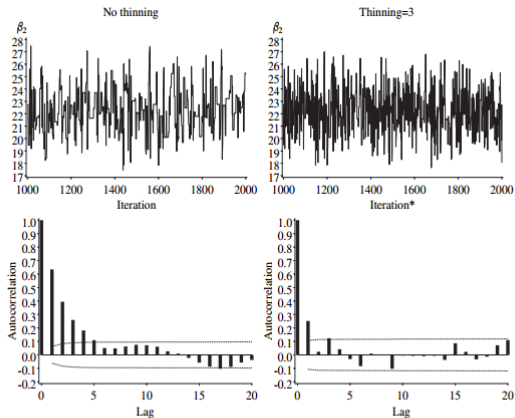


Figure 13.13 *Reduction in autocorrelation of Metropolis–Hastings samples after thinning. Chain history (top row) and ACF (bottom row) for the estimate of  $\beta_2$  from the beetle mortality example using the extreme value model and a centered dose.*

# Multiple chains

## Advantage:

- Using multiple chains is a good way to assess convergence.
- If we start multiple chains at widely varying starting values and each chain converges to the same solution, this would increase our confidence in this solution.
- This method is particularly good for assessing the influence of initial values.

**Drawback:** It may be difficult to generate suitably varied starting values, particularly for **complex problems** with **many unknown parameters** and **multi-dimensional likelihoods**.

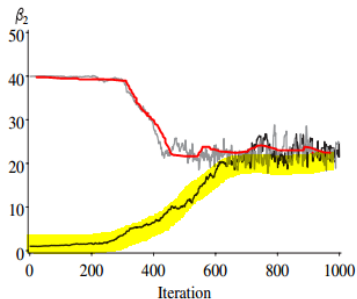


Figure 13.14 *Two chains with different starting values. Estimates of  $\beta_2$  using Metropolis–Hastings sampling for the extreme value model using the beetle mortality data.*