# Statistical Computing for Scientists and Engineers

Homework 2

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(a) Obtain analytic forms of: The posterior distribution of Eq. (3) and the marginal posterior distribution over  $\alpha$  and  $\beta:p(\alpha,\beta|y)$  by using Eq. (4), Eq.(5) and the hint provided.

Answer:

$$p(\theta, \alpha, \beta|y) \propto p(\alpha, \beta)p(\theta|\alpha, \beta)p(y|\theta, \alpha, \beta)$$

$$\propto (\alpha + \beta)^{-5/2} \prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta_j^{\alpha + y_j - 1} (a - \theta_j)^{\beta + n_j - y_j - 1}$$
(1)

$$p(\alpha, \beta|y) = \frac{p(\theta, \alpha, \beta|y)}{p(\theta|\alpha, \beta, y)}$$

$$\propto \frac{(\alpha + \beta)^{-5/2} \prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta_j^{\alpha + y_j - 1} (a - \theta_j)^{\beta + n_j - y_j - 1}}{\prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta + n_j)}{\Gamma(\alpha + y_j)\Gamma(\beta + n_j - y_j)} \theta_j^{\alpha + y_j - 1} (a - \theta_j)^{\beta + n_j - y_j - 1}}$$

$$\propto \frac{(\alpha + \beta)^{-5/2} \prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}}{\prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta + n_j)}{\Gamma(\alpha + y_j)\Gamma(\beta + n_j - y_j)}}$$
(2)

(b) Plot the marginal posterior density  $p(\alpha, \beta|y)$  as a function of the transformed variables  $\log\left(\frac{\alpha}{\beta}\right)$  and  $\log(\alpha+\beta) \in [(-1.3, -2.3); (1,5)]$ . Obtain the corresponding value of  $(\alpha, \beta)$ .

Answer: Let  $X = \log \frac{\alpha}{\beta}$ ,  $Y = \log(\alpha + \beta)$ . Then  $\beta = \frac{\exp(Y)}{1 + \exp(X)}$ ,  $\alpha = \exp(X)\beta$ . Using the python code that provided to us.

X = -1.79, Y = 2.99, then the corresponding value of  $(\alpha, \beta) = (2.85, 17.04)$ 

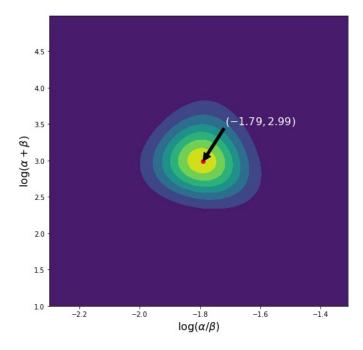


Figure 1: the marginal posterior density  $p(\alpha, \beta|y)$  as a function of the transformed variables  $\log\left(\frac{\alpha}{\beta}\right)$  and  $\log(\alpha+\beta)$ 

Jeffrey's prior and maximum entropy prior: Consider a random variable x described by a Possion distribution:

$$x \sim p(x; \theta) = \frac{\theta^x e^{-\theta}}{x!} \tag{3}$$

(a) Determine the Jeffrey prior  $\pi^J$  for  $\theta$ . Is the scale invariant prior  $\pi_0(\theta) = \frac{1}{\theta}$  preferable to  $\pi^J$ ? Why?

Answer:

$$p(x|\theta) = \frac{\theta^x e^{-\theta}}{x!} \tag{4}$$

Therefore,

$$I(\theta) = -E \left[ \frac{\partial^2}{\partial \theta^2} \ln p(x|\theta) \right] = \frac{\theta}{\theta^2} = \frac{1}{\theta}$$
 (5)

Therefore the Jeffreys' prior is given by:

$$\pi^{J} = [I(\theta)]^{1/2} = \theta^{-1/2} \tag{6}$$

The scale invariant prior  $\pi_0(\theta) = \frac{1}{\theta}$  is not preferable to  $\pi^J$  because they are not the same function.

(b) Find the maximum entropy prior for  $\theta$  for the reference measure  $\pi^J$  subject to the constraints  $E^{\pi}[\theta] = 1$ ,  $Var^{\pi}[\theta] = 1$ .

Answer: considering the reference measure as  $\pi_{ref} = \pi^J \propto \theta^{-1/2}$ .

The maximum entropy prior under the constraints that the prior mean and variance of  $\theta$  are both 1:

Two constrains, therefore, K = 2.

$$E^{\pi}[\theta] = 1, g_1(\theta) = \theta.$$

$$Var^{\pi}[\theta] = 1 = E[(\theta - 1)^2], g_2(\theta) = (\theta - 1)^2.$$

$$\hat{\pi} = \frac{\pi_{ref}(\theta) \exp\left(\sum_{k=1}^{K} \lambda_k g_k(\theta)\right)}{\int \pi_{ref}(\theta) \exp\left(\sum_{k=1}^{K} \lambda_k g_k(\theta)\right)}$$
(7)

In this problem,

$$\hat{\pi} \propto \theta^{-1/2} \exp(\lambda_1 \theta + \lambda_2 (\theta - 1)^2) \tag{8}$$

(c) Find the maximum entropy prior for  $\theta$  for the reference measure  $\pi_0$  subject to the constraints  $E^{\pi}[\theta] = 1$ ,  $Var^{\pi}[\theta] = 1$ .

Answer: Considering the reference measure as  $\pi_{ref} = \pi_0 \propto \theta^{-1}$ .

The maximum entropy prior under the constraints that the prior mean and variance of  $\theta$  are both 1:

Two constrains, therefore, K = 2.

$$E^{\pi}[\theta] = 1, \ g_1(\theta) = \theta.$$

$$Var^{\pi}[\theta] = 1 = E[(\theta - 1)^2], g_2(\theta) = (\theta - 1)^2.$$

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(9)

In this problem,

$$\hat{\pi} \propto \theta^{-1} \exp(\lambda_1 \theta + \lambda_2 (\theta - 1)^2)$$
(10)

Laplace approximation: the data set  $X = (X_1, ..., X_n)$  presents the number of the wins of a football team in the past n home games. We can model this using

$$X_i \sim g(x_i|\theta) = \theta(\theta+1)x_i^{\theta-1}(1-x_i), x_i = (0,1)$$
 (11)

with parameter  $\theta > 0$ . Unfortunately, this model does not have any corresponding, useful, conjugate prior. But it is acceptable to impose a prior model on  $\theta$  with Gamma distribution.

(a) Derive the posterior PDF of  $\theta$ .

Answer:

$$p(\theta|x) = Gamma(\theta; a, b) \prod_{i=1}^{n} p(x_i|\theta)$$

$$= \frac{b^a \theta^{a-1} \exp\{-b\theta\}}{\Gamma(a)} \theta^n (\theta + 1)^n \prod_{i=1}^{n} x_i^{\theta - 1} (1 - x_i)$$
(12)

(b) Using Laplace approximation, find a normal distribution but approximates the posterior distribution using n = 20.

$$\sum_{x=i} \ln X_i = -4.59 \tag{13}$$

and a = b = 1 where a and b are the hyperparameters of the gamma distribution Gamma(a,b).

Answer:

n = 20; a = b = 1

$$p(\theta|x) = \frac{\exp\{-\theta\}}{\Gamma(1)} \theta^{20} (\theta+1)^{20} \prod_{i=1}^{20} x_i^{\theta-1} (1-x_i)$$
 (14)

$$\log p(\theta|x) = -\theta + 20\log(\theta(\theta+1)) + (\theta-1)\sum_{i=0}^{20}\log(x_i) + C$$
 (15)

the first derivative

$$\frac{d\log p(\theta|x)}{d\theta} = -1 + \frac{20}{\theta} + \frac{20}{\theta+1} + \sum_{i=1}^{20} \log(x_i) = 0$$
 (16)

$$\theta^{MAP} \approx 6.69 \tag{17}$$

the second derivative

$$A = -\frac{d^2 \log p(\theta|x)}{d\theta^2}\theta = \theta^{MAP} = 6.69 = -\frac{20}{\theta^2} - \frac{20}{(\theta+1)^2} \approx -(-0.785) = 0.785 = \frac{1}{\sigma^2}$$
(18)

Therefore,

$$p(\theta|x) \approx (2\pi)^{-10} |A|^{1/2} \exp\left\{-\frac{1}{2}(\theta - \theta^{MAP})^2 A\right\}$$

$$\approx (2\pi)^{-10} (0.785)^{1/2} \exp\left\{-\frac{1}{2}(\theta - 6.69)^2 0.785\right\}$$

$$\approx (2\pi)^{-10} (\frac{1}{\sigma^2})^{1/2} \exp\left\{-\frac{1}{2\sigma^2}(\theta - \theta^{MAP})^2\right\}$$
(19)

where  $\frac{1}{\sigma^2}=0.785, \theta^{MAP}=6.69$ 

Monte Carlo integration: Consider the following function,

$$f(x) = x^3 + 5x\cos x \tag{20}$$

(a) Calculate the integral  $I=\int_a^b f(x)dx$  with a=3 and b=4 using Monte Carlo integration with N=10000 samples. Compare this value with the exact solution.

Answer:

$$I_{exact} = \int_{a}^{b} f(x)dx$$

$$= \int_{a}^{b} (x^{3} + 5x \cos x)dx$$

$$= \left[\frac{x^{4}}{4} + 5x \sin x + 5 \cos x\right] \Big|_{a}^{b}$$

$$= \left[\frac{x^{4}}{4} + 5x \sin x + 5 \cos x\right] \Big|_{3}^{4}$$

$$\approx 28.178894351627594$$
(21)

Using Monte Carlo integration with N=10,000 samples. using the python's function numpy.random.uniform(3,4,10000).

The integral I from Monte Carlo integration

$$I_{MC} = 28.192521342751455 \approx I_{exact}$$
 (22)

the error is about 0.05%.

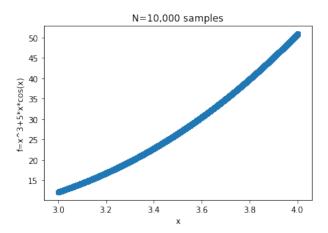


Figure 2: Monte Carlo integration for P4a with N= 10,000

(b) Check the relation between the number of samples N and solution accuracy by plotting the error for N = [10, 1000].

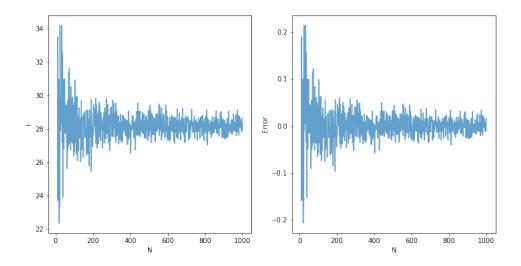


Figure 3: a. Integral I for N=[10,1000] b. Error for N=[10,1000]

#### Answer:

From the plot, we find that when N is small, the error is very large, but when N increases, the error becomes smaller.

(c) For N=100,1000,10000 and 100000 repeat the MC integration for m = 10000 times. Plot the histogram of the results of MC integration for each N. Use the law of large numbers to justify the trend in the histograms. Answer:

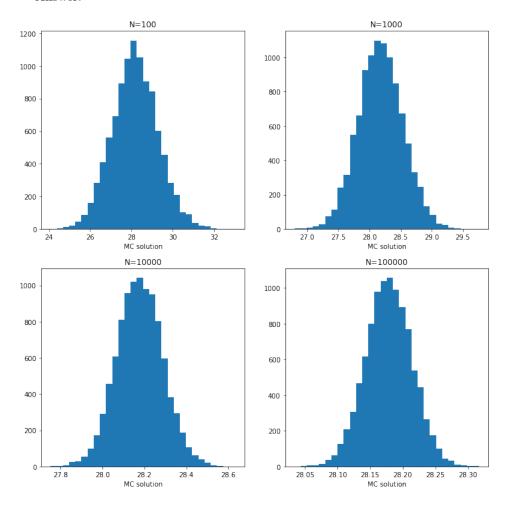


Figure 4: Histogram of the results of MC for each N

Using the law of large numbers to justify the trend in the histogram.  $Var[\bar{X_N}] = \frac{\sigma^2}{N}$ , therefore when N increases,  $Var[\bar{X_N}] = \frac{\sigma^2}{N}$  decreases, the histogram becomes more like a Gaussian distribution.

Bayesian Information Criterion (BIC): suppose we toss a biased coin where probability of heads (x = 1) is  $\theta_1$ . However, we only know about the outcome through an unreliable friend of ours, Joey, who can be trusted with a probability  $\theta_2$ . Let us call this report y. This means that we can write down  $p(y|x, \theta_2)$  as

(a) What is the joint probability distribution  $p(x, y | \theta_1, \theta_2)$ ? Write your name in a table.

Answer:

$$\begin{array}{ccc} & y{=}0 & y{=}1 \\ x{=}0 & (1-\theta_1)\theta_2 & (1-\theta_1)(1-\theta_2) \\ x{=}1 & \theta_1(1-\theta_2) & \theta_1\theta_2 \end{array}$$

(b) Consider we have the outcomes

$$x = (1, 1, 0, 1, 1, 0, 0)$$
  

$$x = (1, 0, 0, 0, 1, 0, 1)$$
(23)

Find the maximum likelihood estimate for  $\theta_1$  and  $\theta_2$ .

$$p(\theta_1, \theta_2 | X, Y) = \theta_1^4 (1 - \theta_1)^3 \theta_2^4 (1 - \theta_2)^3$$
(24)

$$\log p(\theta_1, \theta_2 | X, Y) = 4\log \theta_1 + 3\log(1 - \theta_1) + 4\log \theta_2 + 3\log(1 - \theta_2)$$
 (25)

$$\frac{\log p}{d\theta_2} = \frac{4}{\theta_2} - \frac{3}{1 - \theta_2} = 0; \theta_2 = \frac{4}{7}$$
 (26)

$$\frac{\log p}{d\theta_1} = \frac{4}{\theta_1} - \frac{3}{1 - \theta_1} = 0; \theta_1 = \frac{4}{7} \tag{27}$$

(c)We denote this model with  $M_2$ , where index 2 stands for the number of parameters in the model. Find  $p(D|\hat{\theta_1}, \hat{\theta_2}, M_2)$  where  $\hat{\theta}$  denotes the MLE solution for parameter  $\theta$ .

Answer:

From b,  $\theta_1 = \frac{4}{7}$  and  $\theta_2 = \frac{4}{7}$ 

$$y=0 \quad y=1$$

$$x=0 \quad \frac{12}{49} \quad \frac{9}{49}$$

$$x=1 \quad \frac{12}{49} \quad \frac{16}{49}$$

$$p(X,Y|\theta_1,\theta_2,M_2) = (\frac{4}{7})^8 (\frac{3}{7})^6 \approx 7.044 \times 10^{-5}$$
(28)

(d) If we also denote a model with 4 parameters  $\bar{\theta}=(\theta_{0,0},\theta_{0,1},\theta_{1,0},\theta_{1,1})$  that represents  $p(x,y|\bar{\theta})=\theta_{x,y}$ . Find the MLE of  $\bar{\theta}$ .

Answer:

$$\begin{array}{ccc} & y{=}0 & y{=}1 \\ x{=}0 & \theta_{0,0} & \theta_{0,1} \\ x{=}1 & \theta_{1,0} & \theta_{1,1} \end{array}$$

$$p(\bar{\theta}|X,Y) = \theta_{0,0}^2 \theta_{0,1} \theta_{1,0}^2 \theta_{1,1}^2$$
  

$$\theta_{0,1} = 1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}$$
(29)

$$p(\bar{\theta}|X,Y) = \theta_{0,0}^2 (1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}) \theta_{1,0}^2 \theta_{1,1}^2$$
(30)

$$\log p = 2\log \theta_{0,0} + \log(1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}) + 2\log \theta_{1,0} + 2\log \theta_{1,1}$$
 (31)

$$\frac{d\log p}{d\theta_{0,0}} = \frac{2}{\theta_{0,0}} - \frac{1}{1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}} = 0 \tag{32}$$

$$\frac{d\log p}{d\theta_{1,0}} = \frac{2}{\theta_{1,0}} - \frac{1}{1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}} = 0 \tag{33}$$

$$\frac{d\log p}{d\theta_{1,1}} = \frac{2}{\theta_{1,1}} - \frac{1}{1 - \theta_{0,0} - \theta_{1,0} - \theta_{1,1}} = 0 \tag{34}$$

$$\theta_{0,0} = \frac{2}{7}$$

$$\theta_{0,1} = \frac{1}{7}$$

$$\theta_{1,0} = \frac{2}{7}$$

$$\theta_{1,1} = \frac{2}{7}$$
(35)

(e) Find  $p = (D|\hat{\theta}, M_4)$  where  $\hat{\theta}$  denotes the MLE solution for parameters  $\bar{\theta}$ . Answer:

$$\begin{array}{ccc} & y{=}0 & y{=}1 \\ x{=}0 & \frac{2}{7} & \frac{1}{7} \\ x{=}1 & \frac{2}{7} & \frac{2}{7} \end{array}$$

$$p(X, Y | \theta_{0,0}, \theta_{0,1}, \theta_{1,0}, \theta_{1,1}, M_2) = (\frac{2}{7})^6 (\frac{1}{7}) \approx 7.771 \times 10^{-5}$$
 (36)

(f) Find the Bayesian Information Criterion for  $M_2$  and  $M_4$ . Which model is preferred by this criterion?

Answer: From the Bayesian Information Criterion for  $M_2$  and  $M_4$ , For  $M_2,k=2,N=7,L=p(X,Y|\theta_1,\theta_2,M_2)=(\frac{4}{7})^8(\frac{3}{7})^6\approx 7.044\times 10^{-5}$ 

$$BIC = k \log(N) - 2\log(L) \approx 23.01 \tag{37}$$

For  $M_4,k=3$  (there is a constrain for the four parameters, therefore only three parameters are free parameters, and k should be 3),  $N=7, L=p(X,Y|\theta_{0,0},\theta_{0,1},\theta_{1,0},\theta_{1,1},M_2)=(\frac{2}{7})^6(\frac{1}{7})\approx 7.771\times 10^{-5}$ 

$$BIC = k \log(N) - 2\log(L) \approx 24.76 \tag{38}$$

Since  $BIC_{M_4} > BIC_{M_2}$ ,  $M_2$  is more preferred by this criterion.

Maximum Likelihood Estimation (MLE) and Maximum A Posterior (MAP): Consider a random variable x described by

(a) Derive the maximum likelihood estimate (MLE) ( $\lambda_{MLE}$ )

Answer: The likelihood is given by

$$p(x|\lambda) = \prod_{i=1}^{n} \lambda \exp\{-\lambda x_i\}$$
(39)

The log likelihood:

$$ln p = n ln \lambda - \lambda \sum x_i$$
(40)

Now set set derivative w.r.t  $\lambda$  to 0:

$$\frac{d\ln p}{d\lambda} = \frac{n}{\lambda} + \sum x_i = 0 \tag{41}$$

Therefore,

$$\lambda_{MLE} = \frac{1}{\bar{x}} \cdot \left( \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \right) \tag{42}$$

(b)Obtain an analytic form of the posterior distribution of Eq.(11) and Derive the maximum a posterior estimator (MAP)  $\lambda_{MAP}$  as a function of  $\alpha, \beta$ .

Answer: Let us consider the data  $X = x_1, x_2, ..., x_n$ . The posterior distribution  $p(\lambda|X)$  is given by:

$$p(\lambda|X) = \frac{p(\lambda|X)p(\lambda)}{\int p(\lambda|X)p(\lambda)}$$

$$\propto p(\lambda|X)p(\lambda)$$

$$\lambda^{n} \exp\left\{-\lambda \sum_{i=1}^{N} x_{i}\right\} Gamma(\alpha, \beta)$$

$$\lambda^{n} \exp\left\{-\lambda \sum_{i=1}^{N} x_{i}\right\} \lambda^{\alpha-1} \exp\{-\beta\lambda\}$$

$$e^{-\lambda(\sum_{i=1}^{N} x_{i} + \beta)} \lambda^{n+\alpha-1}$$

$$(43)$$

$$p(\lambda|X) \propto Gamma(\alpha + n, \sum_{i=1}^{N} x_i + \beta)$$
 (44)

The log posterior:

$$\log p(\lambda|X) \propto -\lambda \left(\sum_{i=1}^{N} x_i + \beta\right) + (n + \alpha - 1)\log \lambda \tag{45}$$

$$0 = \frac{d\log p(\lambda|X)}{d\lambda} = -(\sum_{i=1}^{N} x_i + \beta) + \frac{n+\alpha-1}{\lambda}$$
(46)

$$\lambda_{MAP} = \frac{n + \alpha - 1}{\sum_{i=1}^{N} x_i + \beta} \tag{47}$$

(c) Generate N=20 samples drawn from an exponential distribution with parameter  $\lambda=0.2$ . Fix  $\beta=100$  and vary  $\alpha$  over the range(1,40) using a step-size of 1.

Compute the corresponding MLE and MAP estimates for  $\lambda$ 

For each  $\alpha$ , compute the mean squared  $error^2$  of both estimates compared against the true value and then plot the mean squared error as a function of  $\alpha$ .

Now, fix  $\alpha = 30$ ,  $\theta = 100$  and vary N over the range(1,500) using a step-size of 1. Plot the mean squared error for each N of the corresponding estimates and explain under what condition is the MAP estimator better.

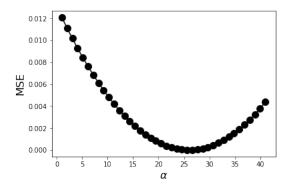


Figure 5: MSE as a function of  $\alpha$ 

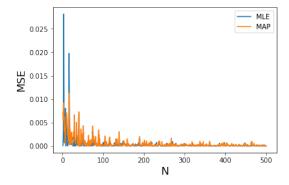


Figure 6: MSE as a function of N

From Figure 6, when N is small, then the MAP estimator would be better than the MLE estimator.