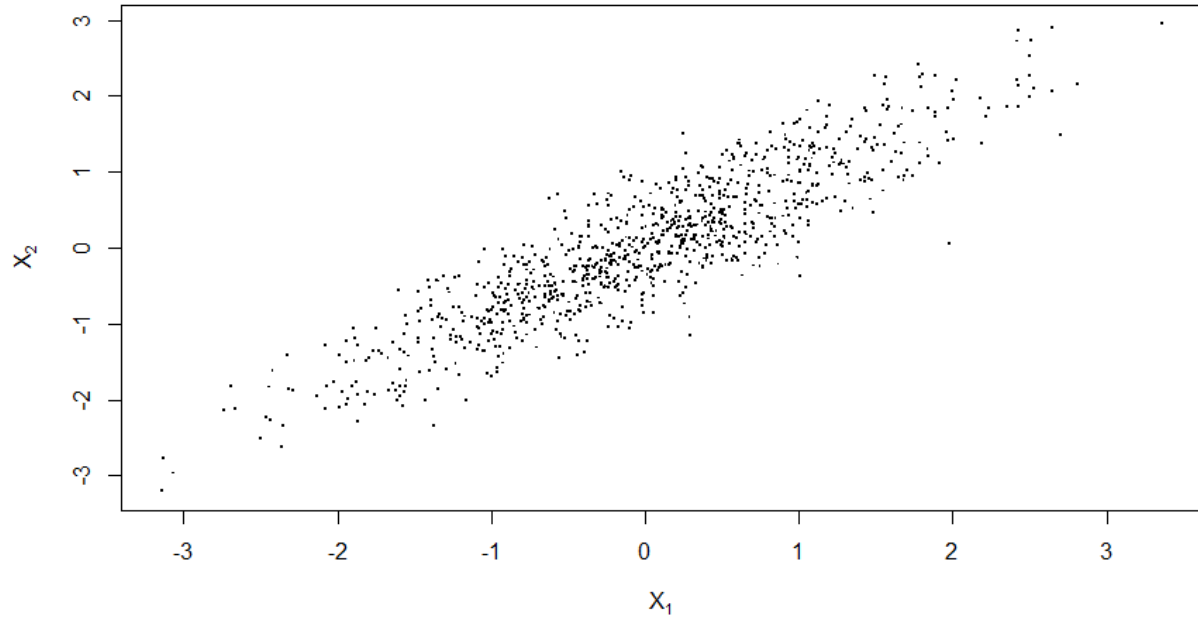


**Problem 1: Gibbs vs composition sampling vs random walk Metropolis-Hastings (RWMH).**

**1.1** The composition sampler for sampling from  $f_{12}$  that iterates:

- (1) Independent sampling of  $X_1$ :  $X_1 \sim N(0,1)$
- (2) Conditional sampling of  $X_2$ :  $X_2 \sim N(\rho X_1, [1 - \rho^2])$

Let  $n = 1000$  and  $\rho = 0.9$ , we derive the sequence  $(X_1^1, X_2^1), \dots, (X_1^n, X_2^n)$  of rvs produced by the composition sampler and plot the sequence in Fig. 1. It can be easily found that the two vectors  $X_1, X_2$  are not independent of each other.



**Fig. 1:** Scatter plot of the two vectors  $X_1, X_2$  produced by the composition sampler

**1.2** The “Metropolized” composition sampler for sampling from  $f_{12}$  that iterates:

- (1) A random walk Metropolis-Hastings sampling of  $X_1$ :

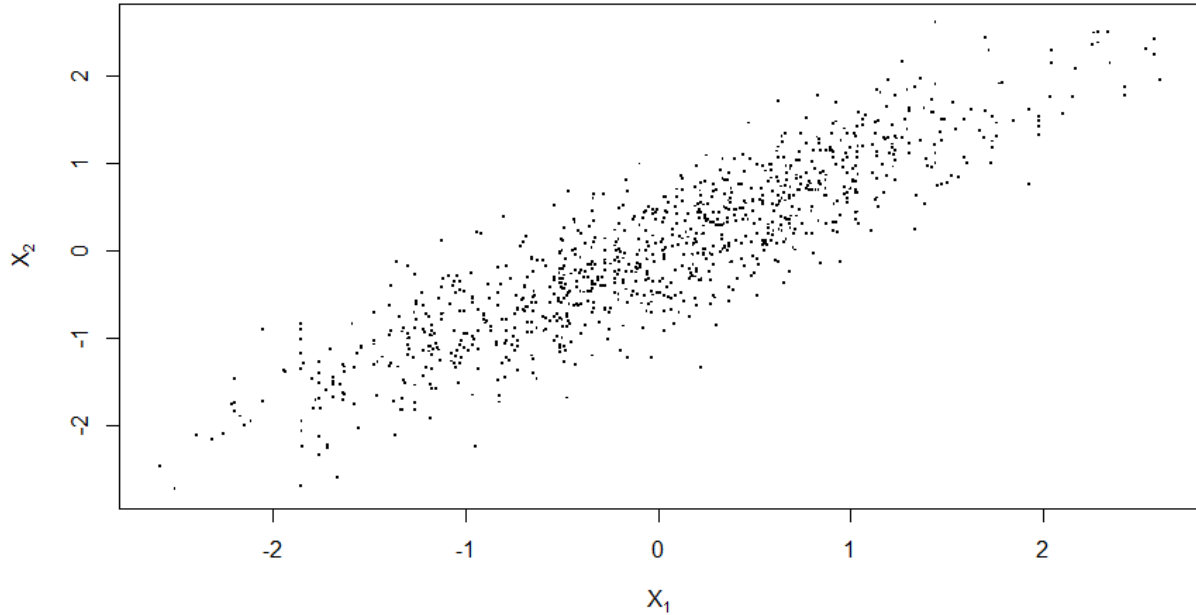
$$p(X_1) \propto \exp(-X_1^2/2)$$

Use  $N(X_1^t, 1)$  as the proposal, then propose  $X_1^* \sim N(X_1^t, 1)$

Accept  $X_1^{t+1} = X_1^*$  with probability  $\min\{1, r\}$  with  $r = \frac{p(X_1^*)}{p(X_1^t)}$ , otherwise  $X_1^{t+1} = X_1^t$ .

- (2) Conditional sampling of  $X_2$ :  $X_2 \sim N(\rho X_1, [1 - \rho^2])$

Let  $n = 1000$  and  $\rho = 0.9$ , we derive the sequence  $(X_1^1, X_2^1), \dots, (X_1^n, X_2^n)$  of rvs produced by the “Metropolized” composition sampler and plot the sequence in Fig. 2. It can be easily found that the two vectors  $X_1, X_2$  are not independent of each other, either.



**Fig. 2:** Scatter plot of the two vectors  $X_1, X_2$  produced by the “Metropolized” composition sampler

**1.3** A random walk Metropolis-Hastings algorithm for jointly sampling  $X_1, X_2$  is:

$$p(X_1, X_2) \propto \exp\left(-\frac{(X_1^2 + X_2^2 - 2\rho X_1 X_2)}{2(1 - \rho^2)}\right)$$

Perform a random walk Metropolis-Hastings algorithm using a normal proposal, i.e., if  $X_1^t, X_2^t$  are the current values for  $X_1, X_2$ , then

$$\begin{pmatrix} X_1^* \\ X_2^* \end{pmatrix} \sim N\left(\begin{bmatrix} X_1^t \\ X_2^t \end{bmatrix}, S\right)$$

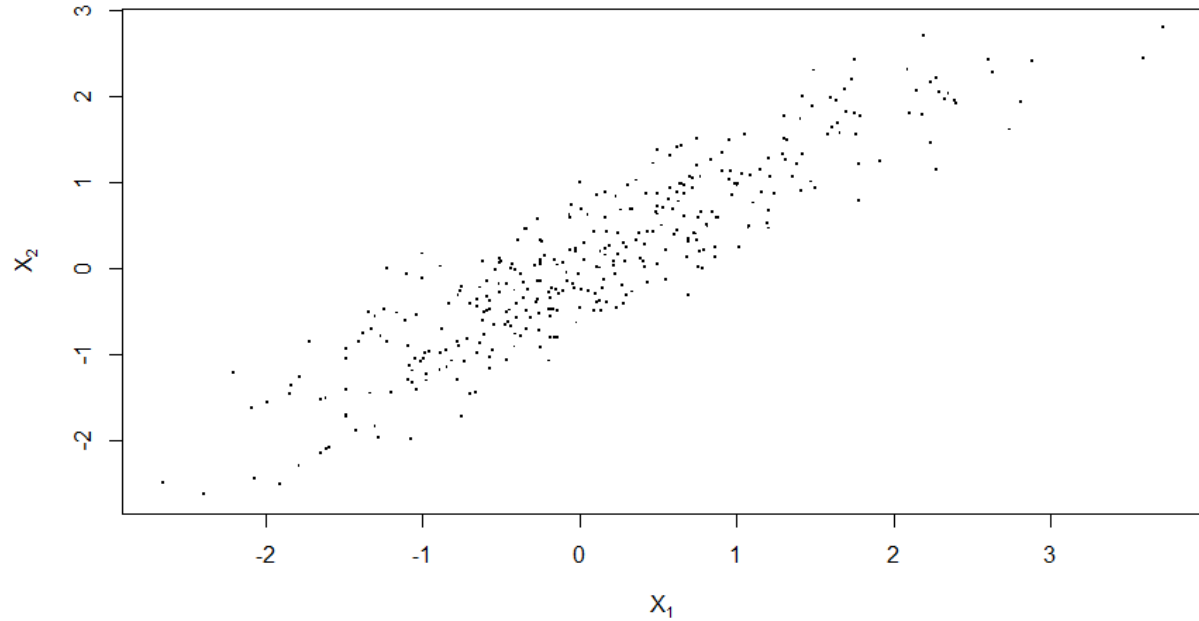
Where  $S$  is the tuning parameter.

Based on the lectures, we know the optimal random walk tuning parameter is  $2.4^2 \text{Var}(X)/d$  where  $\text{Var}(X)$  is the unknown covariance matrix. We can estimate  $\text{Var}(X)$  using the sample covariance matrix of draws. Therefore, the automatic adapting of the Metropolis-Hastings tuning parameter  $S$  is:

- (1) Start with  $S = \text{diag}(2)$
- (2) Run 50 iterations of the MCMC using  $2.4^2 S/d$
- (3) Set  $S$  to the sample covariance matrix of all previous draws

Accept  $\begin{pmatrix} X_1^{t+1} \\ X_2^{t+1} \end{pmatrix} = \begin{pmatrix} X_1^* \\ X_2^* \end{pmatrix}$  with probability  $\min\{1, r\}$  with  $r = \frac{p(X_1^*, X_2^*)}{p(X_1^t, X_2^t)}$ , otherwise  $\begin{pmatrix} X_1^{t+1} \\ X_2^{t+1} \end{pmatrix} = \begin{pmatrix} X_1^t \\ X_2^t \end{pmatrix}$ .

Let  $n = 1000$  and  $\rho = 0.9$ , we derive the sequence  $(X_1^1, X_2^1), \dots, (X_1^n, X_2^n)$  of rvs produced by the random walk Metropolis-Hastings algorithm for joint sampling  $X_1, X_2$  and plot the sequence in Fig. 3.



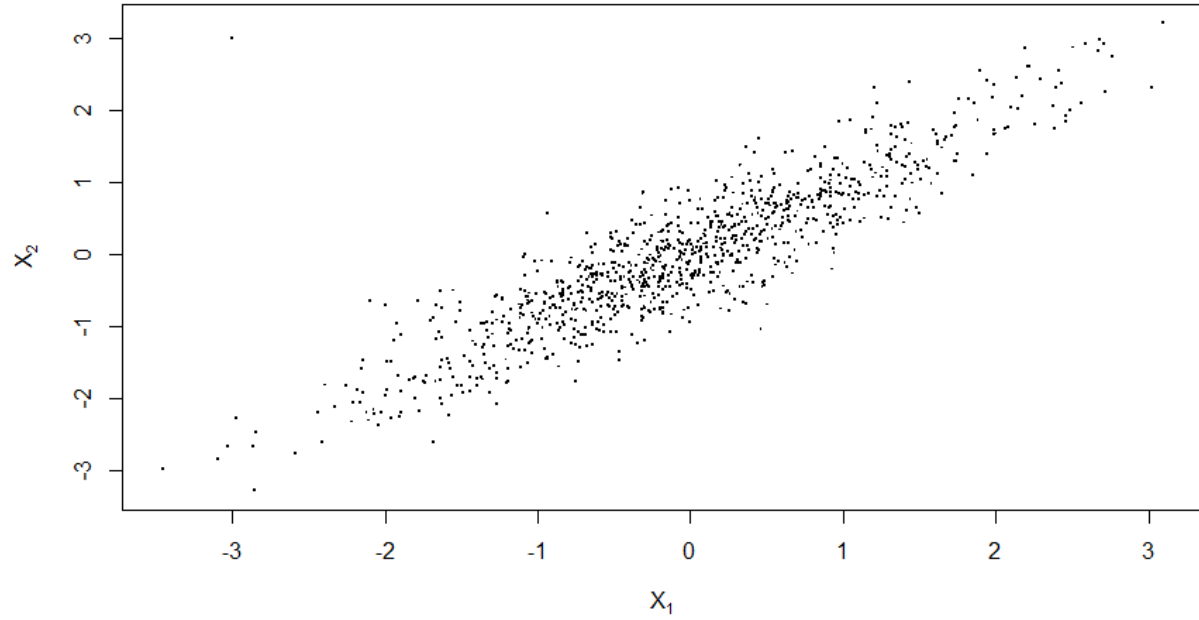
**Fig. 3:** Scatter plot of the two vectors  $X_1, X_2$  produced by the random walk Metropolis-Hastings algorithm for jointly sampling  $X_1, X_2$

#### 1.4 The Gibbs sampler for sampling from $f_{12}$ that iterates:

Beginning with an initial value  $(X_1^0, X_2^0)$ , an iteration of the Gibbs sampler involves:

- (1) Conditional sampling of  $X_1$ :  $X_1^{t+1} \sim N(\rho X_2^{t+1}, [1 - \rho^2])$
- (2) Conditional sampling of  $X_2$ :  $X_2^{t+1} \sim N(\rho X_1^t, [1 - \rho^2])$

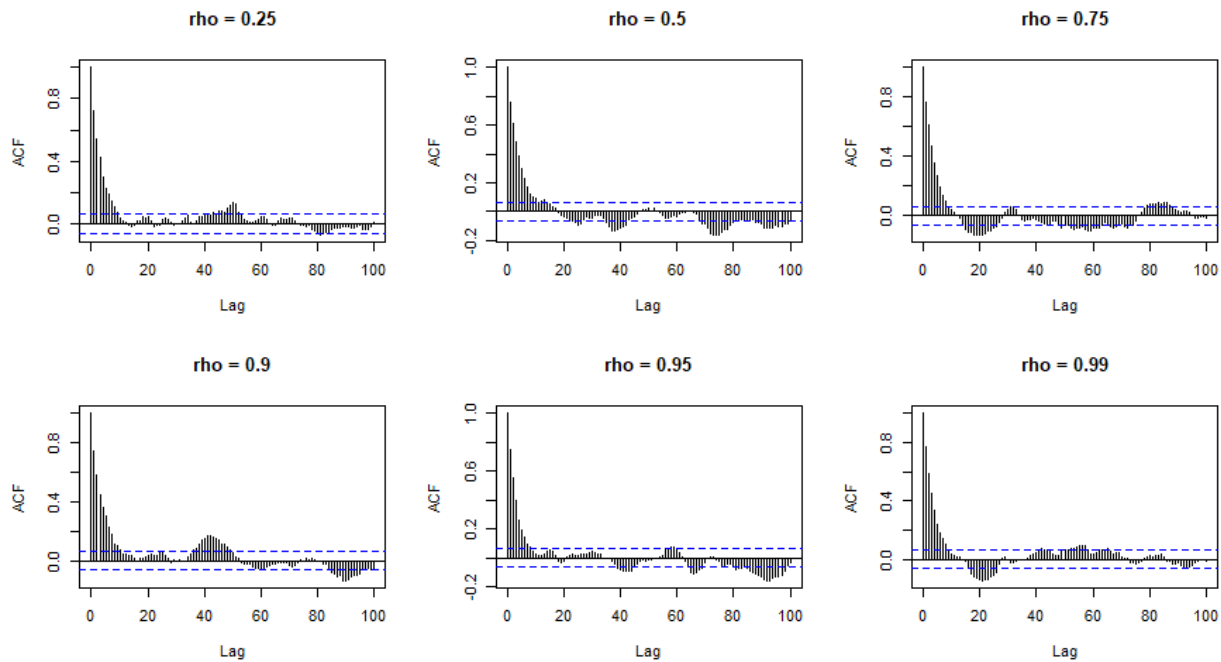
Let  $n = 1000$  and  $\rho = 0.9$ , we derive the sequence  $(X_1^1, X_2^1), \dots, (X_1^n, X_2^n)$  of rvs produced by the Gibbs sampler and plot the sequence in Fig. 4.



**Fig. 4:** Scatter plot of the two vectors  $X_1, X_2$  produced by the Gibbs sampler

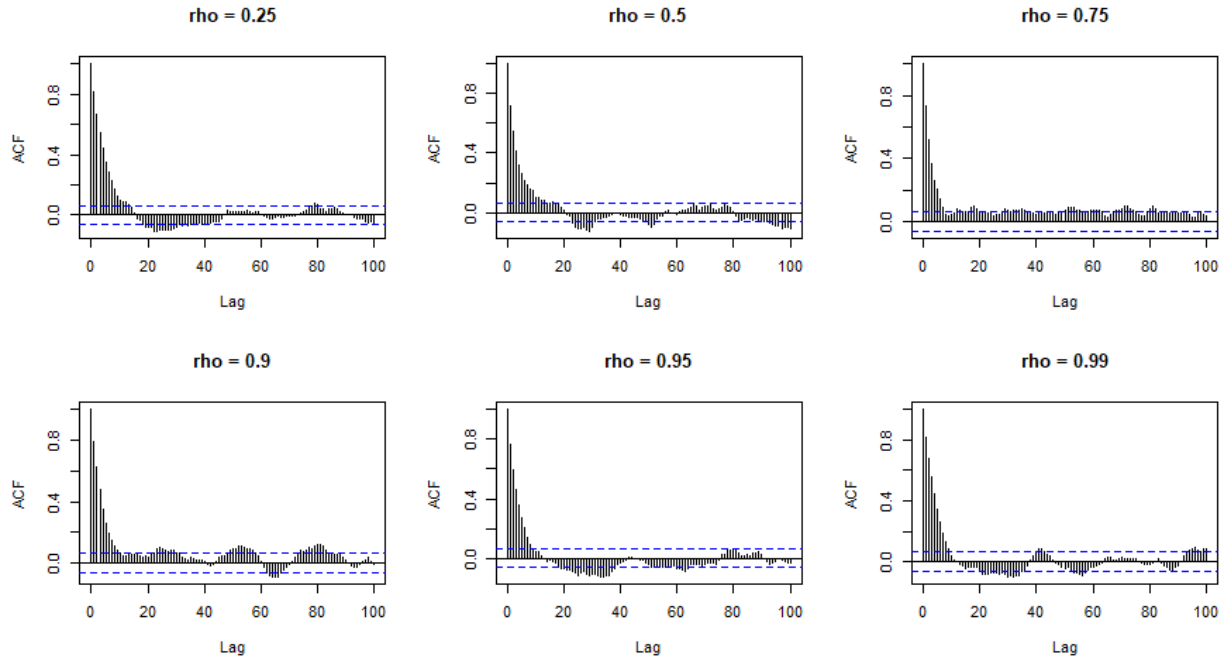
**1.5** Let  $n = 1000$  be the length of the Markov chain. For  $\rho = 0.25, 0.5, 0.75, 0.9, 0.95, 0.99$ , start the the three samplers (from 1.2, 1.3 and 1.4) at the origin, run them for  $n$  iterations. Visualize the autocorrelation in  $X_1^1, X_1^2, \dots, X_1^n$  in each chain, as shown in Fig. 5-7.

(1) The “Metropolized” composition sampler:



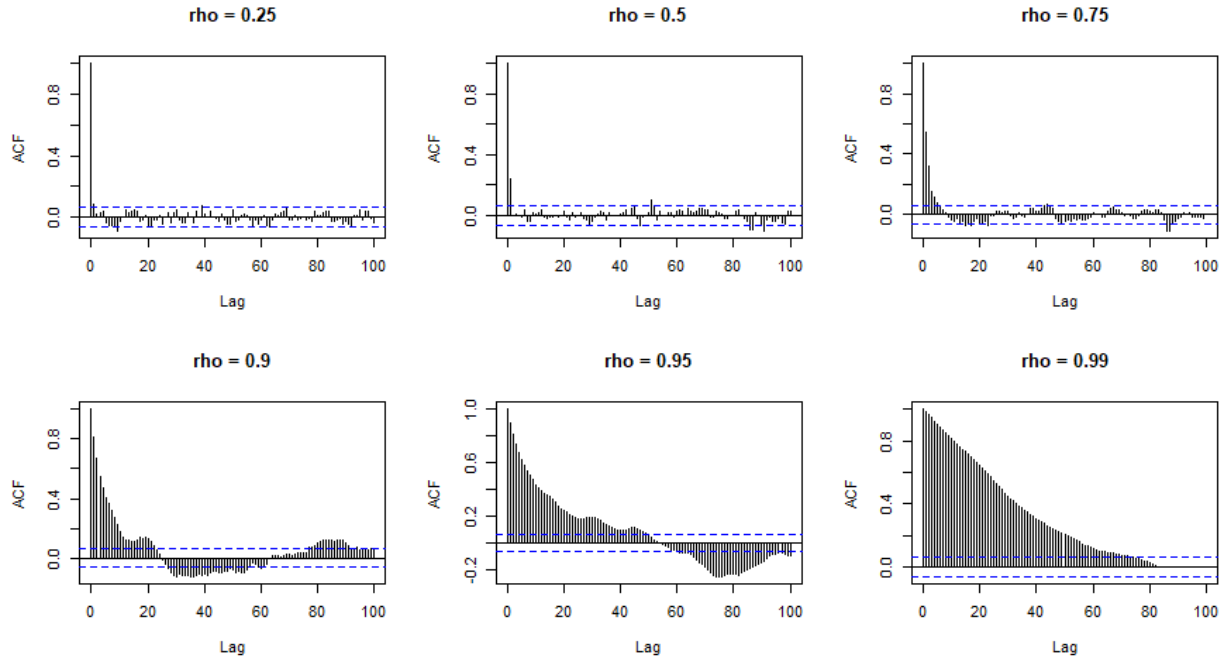
**Fig. 5:** Autocorrelation of the sequence  $X_1$  produced by the “Metropolized” composition sampler

(2) A random walk Metropolis-Hastings algorithm for jointly sampling  $X_1, X_2$ :



**Fig. 6:** Autocorrelation of the sequence  $X_1$  produced by the random walk Metropolis-Hastings algorithm for jointly sampling  $X_1, X_2$

(3) The Gibbs sampler:



**Fig. 7:** Autocorrelation of the sequence  $X_1$  produced by the Gibbs sampler

**Table 1:** Effective sample sizes of the sequence  $X_1$  ( $n = 1000$ ) produced by different samplers

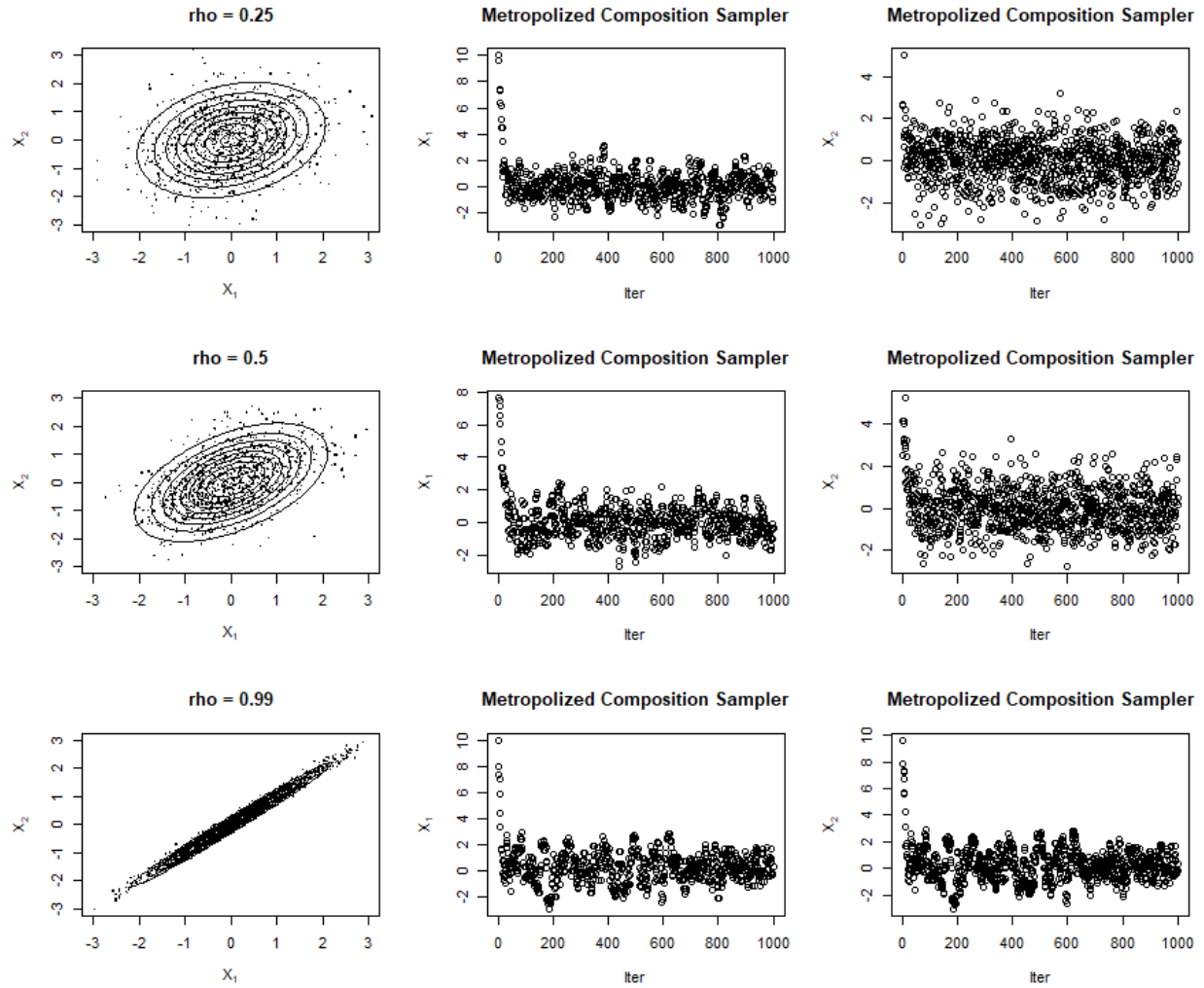
rho	“Metropolized” composition sampler	A random-walk Metropolis-Hastings	Gibbs sampler
0.25	739	319	1000
0.5	692	430	1000
0.75	711	338	1000
0.9	719	372	1000
0.95	692	328	1000
0.99	723	243	1000

Based on the results from Fig. 5-7 and Table 1, we can find that when sampling the sequences  $X_1, X_2$  in each chain, the Gibbs sampler performs better than the “Metropolized” composition sampler and the random-walk Metropolis-Hastings sampler for jointly sampling  $X_1, X_2$ , in terms of effective sample size. On the other hand, the  $\rho$  values hardly affect the effective sample sizes of the sequences  $X_1, X_2$  in each chain, but they can significantly influence the autocorrelation of the sequences  $X_1, X_2$  generated by the Gibbs sampler (i.e., larger  $\rho$  values correspond to stronger autocorrelation). In contrast, the autocorrelation of the sequences  $X_1, X_2$  produced by the other two samplers is less affected by the  $\rho$  values.

**1.6** Start the samplers far from the origin  $\begin{pmatrix} X_1^0 \\ X_2^0 \end{pmatrix} = \begin{pmatrix} -10 \\ 10 \end{pmatrix}$  for  $\rho = 0.25, 0.5, 0.99$ . Then we plot the

vector of states of  $X_2$  against that of states of  $X_1$  to visualize how the three samplers explore the support of the distribution and overlay it with the contours of the joint pdf. Also, we plot the states of each variable against the iteration number, as shown in Fig. 8-10 separately for three samplers.

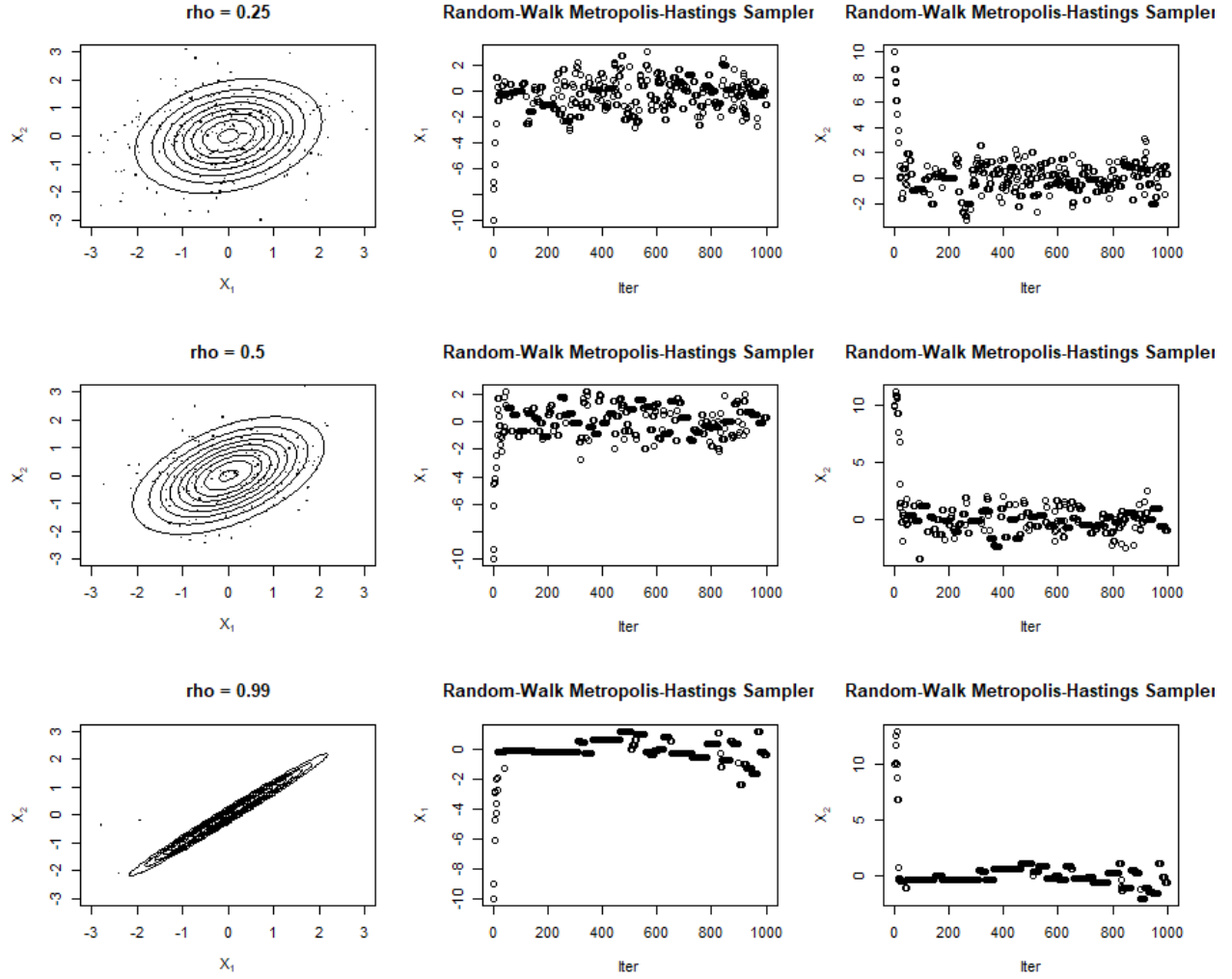
(1) The “Metropolized” composition sampler:



**Fig. 8:** Plots of the sequences  $X_1, X_2$  produced by the “Metropolized” composition sampler: (a) The three rows separately stand for the scenarios of  $\rho = 0.25, 0.5, 0.99$ ; (b) The first column refers to the support of the distribution and the contours of the joint pdf; (c) The second column refers to the states of  $X_1$  against the iteration number; (d) The third column refers to the states of  $X_2$  against the iteration number.

For the “Metropolized” composition sampler, most of the states of  $X_1, X_2$  are overlaid with the contour plots of  $X_1, X_2$ . When the starting point of  $X_1$  is far away from the origin, it just takes a few number of iterations to reach the high-probability density region of  $X_1$ . As  $\rho$  increases from 0.25 to 0.9, it takes a gradually increasing number of iterations to reach the high-probability density region of  $X_2$ .

(2) A random walk Metropolis-Hastings algorithm for jointly sampling  $X_1, X_2$ :

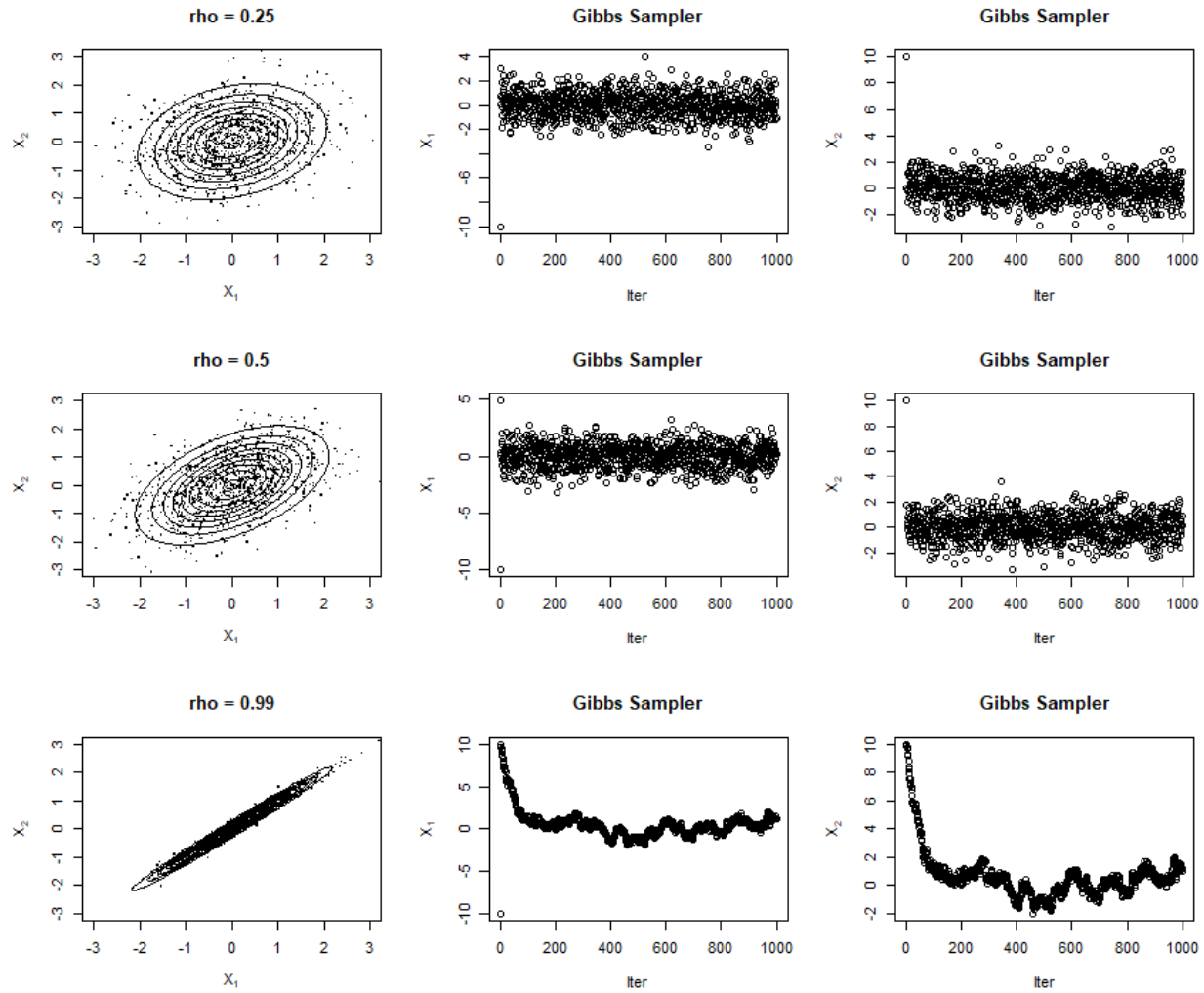


**Fig. 9:** Plots of the sequences  $X_1, X_2$  produced by the random-walk Metropolis-Hastings sampler: (a) The three rows separately stand for the scenarios of  $\rho = 0.25, 0.5, 0.99$ ; (b) The first column refers to the support of the distribution and the contours of the joint pdf; (c) The second column refers to the states of  $X_1$  against the iteration number; (d) The third column refers to the states of  $X_2$  against the iteration number.

For the random-walk Metropolis-Hastings sampler, it exhibits almost the same patterns as the “Metropolized” composition sampler, in terms of sampling  $X_1, X_2$ . The main difference is that the effective sample size of the random-walk Metropolis-Hastings sampler is significantly less than that of the “Metropolized” composition sampler.



(3) *The Gibbs sampler:*



**Fig. 10:** Plots of the sequences  $X_1, X_2$  produced by the Gibbs sampler: (a) The three rows stand for the scenarios of  $\rho = 0.25, 0.5, 0.99$ , respectively; (b) The first column refers to the support of the distribution and the contours of the joint pdf; (c) The second column refers to the states of  $X_1$  against the iteration number; (d) The third column refers to the states of  $X_2$  against the iteration number.

For the Gibbs sampler, similarly, most of the states of  $X_1, X_2$  are overlaid with the contour plots of  $X_1, X_2$ . However, when the starting point of  $X_1, X_2$  is far away from the origin, it takes a larger number of iterations to reach the high-probability density region of  $X_1, X_2$ , particularly when  $\rho$  increases from 0.25 to 0.9.

**Problem 2: Effective Sample Size in an AR(1) model.**

Problem 2:

(2.1)

$$\text{Var}(\bar{Y}_n) = \text{Var}\left(\frac{1}{n}(Y_1 + Y_2 + \dots + Y_n)\right)$$

$$= \frac{1}{n^2} \text{Var}\left(\sum_{i=1}^n Y_i\right)$$

$$= \frac{1}{n^2} \left[ \sum_{i=1}^n \text{Var}(Y_i) + \sum_{i \neq j} \text{Cov}(Y_i, Y_j) \right]$$

$$= \frac{1}{n^2} \left[ n\sigma^2 + \sigma^2 \sum_{i \neq j} \rho^{|i-j|} \right] \quad i, j \in \{1, 2, \dots, n\}$$

$$= \frac{1}{n^2} \left[ n\sigma^2 + \sigma^2 \frac{2n\rho(1-\rho) - 2\rho(1-\rho^n)}{(1-\rho)^2} \right]$$

$$= \frac{\sigma^2}{n^2} \cdot \frac{n(1-\rho^2) - 2\rho(1-\rho^n)}{(1-\rho)^2}$$

(2.2)

$$\text{Effective sample size is } \sigma^2 / \text{Var}(\bar{Y}_n) = \frac{n^2(1-\rho)^2}{n(1-\rho^2) - 2\rho(1-\rho^n)}$$

Here, we set  $n=100$ .when  $\rho=0$ , effective sample size is 100when  $\rho=0.25$ , effective sample size is 60when  $\rho=0.5$ , effective sample size is 34when  $\rho=0.75$ , effective sample size is 15when  $\rho=0.9$ , effective sample size is 6when  $\rho=0.95$ , effective sample size is 3when  $\rho=0.99$ , effective sample size is 1

(2.3)

Since  $\bar{Y}_n \sim N(\mu, \text{Var}(\bar{Y}_n))$ 

$$\text{Let } X = \frac{\bar{Y}_n - \mu}{\sqrt{\text{Var}(\bar{Y}_n)}} \sim N(0, 1)$$

Therefore, the exact 95% CI for  $X$  is  $[-1.96, 1.96]$ .

$$\text{So, } -1.96 \leq \frac{\bar{Y}_n - \mu}{\sqrt{\text{Var}(\bar{Y}_n)}} \leq 1.96$$



So the exact 95% CI for  $\mu$  is

$$\bar{Y}_n - 1.96 \sqrt{\text{Var}(\bar{Y}_n)} \leq \mu \leq \bar{Y}_n + 1.96 \sqrt{\text{Var}(\bar{Y}_n)}$$

$$\bar{Y}_n - 1.96 \sigma \sqrt{\frac{n(1-p^2) - 2p(1-p^n)}{n^2(1-p)^2}} \leq \mu \leq \bar{Y}_n + 1.96 \sigma \sqrt{\frac{n(1-p^2) - 2p(1-p^n)}{n^2(1-p)^2}}$$

So the exact 95% CI for  $\mu$  is

$$\left[ \bar{Y}_n - 1.96 \sigma \sqrt{\frac{n(1-p^2) - 2p(1-p^n)}{n^2(1-p)^2}}, \bar{Y}_n + 1.96 \sigma \sqrt{\frac{n(1-p^2) - 2p(1-p^n)}{n^2(1-p)^2}} \right]$$

where  $\bar{Y}_n = \frac{1}{n} \sum_{i=1}^n Y_i$

(2.4) When  $n$  is held fixed and  $p \rightarrow 1$ ,

$$\begin{aligned} \lim_{p \rightarrow 1} \frac{n(1-p^2) - 2p(1-p^n)}{n^2(1-p)^2} &= \lim_{p \rightarrow 1} \frac{-2np - 2 + 2(n+1)p^n}{2n^2(p-1)} = \lim_{p \rightarrow 1} \frac{-2n + 2n(n+1)p^{n-1}}{2n^2} \\ &= \lim_{p \rightarrow 1} \frac{-2n + 2n^2 + 2n}{2n^2} \\ &= 1 \end{aligned}$$

So when  $n$  is held fixed and  $p \rightarrow 1$ ,

the exact 95% CI for  $\mu$  is approaching  $[\bar{Y}_n - 1.96\sigma, \bar{Y}_n + 1.96\sigma]$   
 where  $\bar{Y}_n = \frac{1}{n} \sum_{i=1}^n Y_i$ .

(2.5) Here, when the rvs are positively correlated, we do not use

conventional CIs. Instead, we have to consider the effect of correlations between the rvs. The main reason lies in that the data of the rvs are not independent of each other, instead, they are highly correlated.

2.6 Here, we simulate a time series of length  $n$  from a Gaussian  $AR(1)$  process. Specifically, we separately set  $n = 10^2, 10^3, 10^4$  and  $\rho = 0, 0.25, 0.5, 0.75, 0.9, 0.95, 0.99$  to calculate and compare the effective sample size based on three different calculation methods, as presented in Table 2.

**Table 2:** Comparison of effective sample size by different calculation methods and  $n$  values

rho	0	0.25	0.5	0.75	0.9	0.95	0.99
Method	$n = 100$						
(i)	100	60	34	15	6	3	1
(ii)	35	28	22	14	10	8	7
(iii)	101	57	70	22	11	3	5
Method	$n = 1000$						
(i)	1,000	600	334	143	53	26	6
(ii)	333	258	222	140	99	77	61
(iii)	1,001	540	360	149	44	22	11
Method	$n = 10000$						
(i)	10,000	6,000	3,334	1,429	527	257	51
(ii)	3,317	2,762	2,100	1,423	942	753	609
(iii)	10,001	5,722	3,328	1,416	545	267	46

**Note:** (i) means the formula: effective sample size =  $\sigma^2 / \text{Var}(\bar{Y}_n)$ ;

(ii) refers to the “theoretical” formula: effective sample size =  $n / (1 + 2 \sum_{k=1}^{\infty} \rho_k)$  where  $\rho_k$  is the lag- $k$  autocorrelation;

(iii) denotes that effective sample size is equal to the number of independent samples based on estimates from lecture slides.

Table 2 suggests that as  $\rho$  increases from 0 to 0.99, the effective sample size calculated whether method (i), (ii), or (iii) all decrease in general, particularly for those produced by method (i) and (iii). On the other hand, when  $0 < \rho < 0.75$ , the effective sample size calculated by method (i) and (iii) is significantly larger than that computed by method (ii); When  $0.75 < \rho < 1$ , the effective sample size calculated by method (ii) is larger than that computed by method (i) and (iii). In addition, the values of  $n$  just change the effective sample size, but hardly affect the ratio of effective sample size to the total samples.

**Problem 3: Bayesian model selection in logistic regression.**

The full specification of a *Logistic Regression* model can be summarized as follows:

$$y_i = \text{Binomial}(u_i)$$

$$\ln \frac{u_i}{1 - u_i} = \beta_{\gamma_0} + \beta_{\gamma_1}x_1 + \beta_{\gamma_2}x_2 + \beta_{\gamma_3}x_3 + \beta_{\gamma_4}x_4$$

Here, we define 16 *Logistic Regression* models with different variable selection from  $M_0$  (intercept-only model) to  $M_{15}$  (intercept and  $X_1, X_2, X_3, X_4$  included), and put a flat prior over over the model space consisting of the 16 models with  $P(M_\gamma) = 1/16$ . So, the log-posterior is:

$$\log P(M_\gamma | Y) = \log \frac{P(Y | M_\gamma) P(M_\gamma)}{P(Y)} = \log P(Y | M_\gamma) + \log P(M_\gamma) - \log P(Y)$$

Here, we let  $M_\gamma$  be the model indexed by  $\gamma$  and  $\gamma$  is a vector of 4 switches that determine the variable selection of the model. As a result,  $\gamma$  varies from (0,0,0,0) to (1,1,1,1).  $\beta_\gamma$  denotes the vector of coefficients  $\beta_{\gamma_0}, \beta_{\gamma_1}, \dots$  in model  $M_\gamma$  and the dimension of  $\beta_\gamma$  ranges from 1 to 5 depending on how many variables are selected for the Logistic Regression model. Also, we put independent normal priors on  $\beta_\gamma$ , i.e.,  $\beta_\gamma \sim N(0, \sigma^2 I_d)$ , where  $d = 1 + \sum_j \gamma_j$ . In terms of the Random-Walk Metropolis-Hastings (RWMH) algorithm, we use the proposal pdf as follows:

$$(\beta_\gamma^*) \sim N(\beta_\gamma^t, \text{scale}^2 I_d) \text{ where } d = 1 + \sum_j \gamma_j$$

**3.1 Scenario 1:  $\sigma = 2$  and  $\gamma = (1, 1, 1, 1)$ :** To estimate the model posterior probabilities, we first assume  $\sigma = 2$  and  $\gamma = (1, 1, 1, 1)$  as an example to demonstrate the implementation of the log-posterior. Specifically, we conduct MCMC simulations to generate  $k$  (i.e.,  $k = 1$ ) chains, initialize it at the MLE for a given model, and then estimate the mean and variance of  $\beta_\gamma$ , as well as the values of the log-posterior at each of the MCMC samples.

**Step 1:** Calculate the MLE and the log-posterior at the MLE for the  $M_{15}$  Logistic Regression model (intercept and  $X_1, X_2, X_3, X_4$  included) as follows:

*Coefficients:*  $\beta_{15} = [0.6328, 0.7390, 1.1137, 0.4781, 0.6944]$  for intercept and  $X_1, X_2, X_3, X_4$

The *log-posterior probability* is -46.9689 at the MLE

```
## ----- calculate log-posterior -----
lupost_factory <- function(x, y, beta, sigma = 2) {
  eta <- as.numeric(x %*% beta)
  logp <- ifelse(eta < 0, eta - log1p(exp(eta)), - log1p(exp(- eta)))
  logq <- ifelse(eta < 0, - log1p(exp(eta)), - eta - log1p(exp(- eta)))
  logl <- sum(logp[y == 1]) + sum(logq[y == 0]) # binomial(u), just keep y
  ## log: makes multiply become sum
  return(logl + log(1/16) - sum(beta^2) / (2 * sigma^2)) # log-posterior
}

i = 16
out <- glm(y~., data = logit[model_index[i,]==1], family = binomial, x = TRUE)
summary(out)
lupost <- lupost_factory(out$x, out$y, out$coefficients, sigma = 2)
print(lupost)
```

**Step 2:** Use the Random Walk Metropolis-Hastings (RWMH) sampling method to perform the MCMC simulations with the MLE as an initial value and  $n = 1000$ . The proposal pdf  $g$  is  $\beta_{15} \sim N(0, \text{diag}(\text{scale}^2))$  where we let the value of scale be 0.2 to guarantee a larger acceptance probability of  $\beta_{15}$ .

```
## ----random walk metropolis hastings algorithm-----
#sigma = 2
metropolis_hastings_normal = function(x,y,beta, n_points, scale) {
  #initialize
  s = diag(length(beta)) * scale^2 #
  current = beta
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  #index = sample.int(length(y),b,len)
  for (i in 2:n_points) {
    proposed = mvrnorm(1,current,2.4^2*s/length(beta))
    logr = lupost_factory(x,y,proposed,sigma=2)-lupost_factory(x,y,current,sigma=2)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma=2)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
    # if (i%%50 == 0) s = var(theta[1:i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}

# coef_sampling
model_sampler = metropolis_hastings_normal(out$x, out$y, out$coefficients, n<-1000, scale<-0.2)

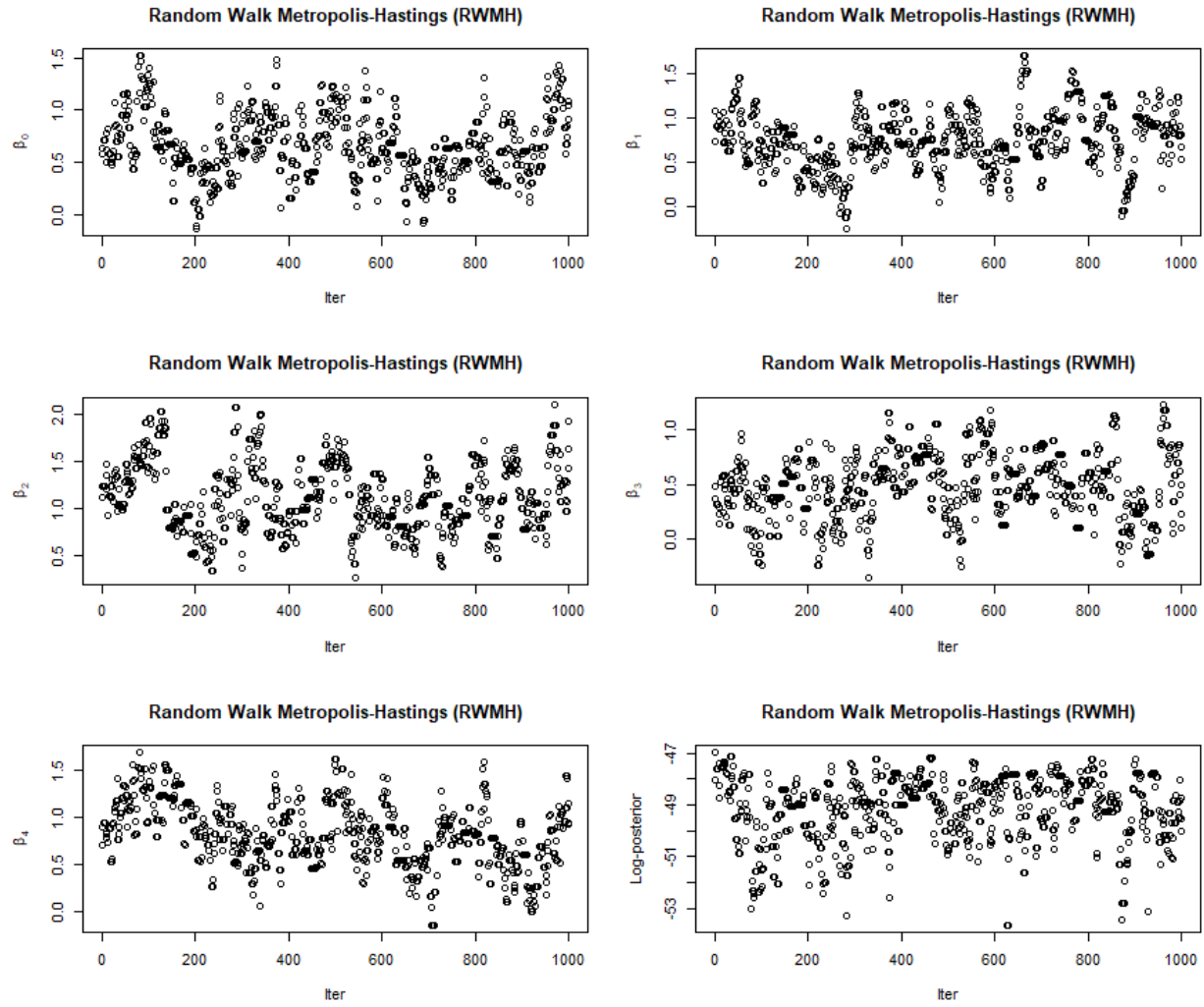
print(model_sampler$acceptance)
print(model_sampler$means)
print(model_sampler$standard_error)
```

**Step 3:** Visualize the plots of the sequences  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler and the corresponding log-posterior probability for each iteration, as shown in Fig. 11 and 12. Also, some statistical indicators are calculated as follows:

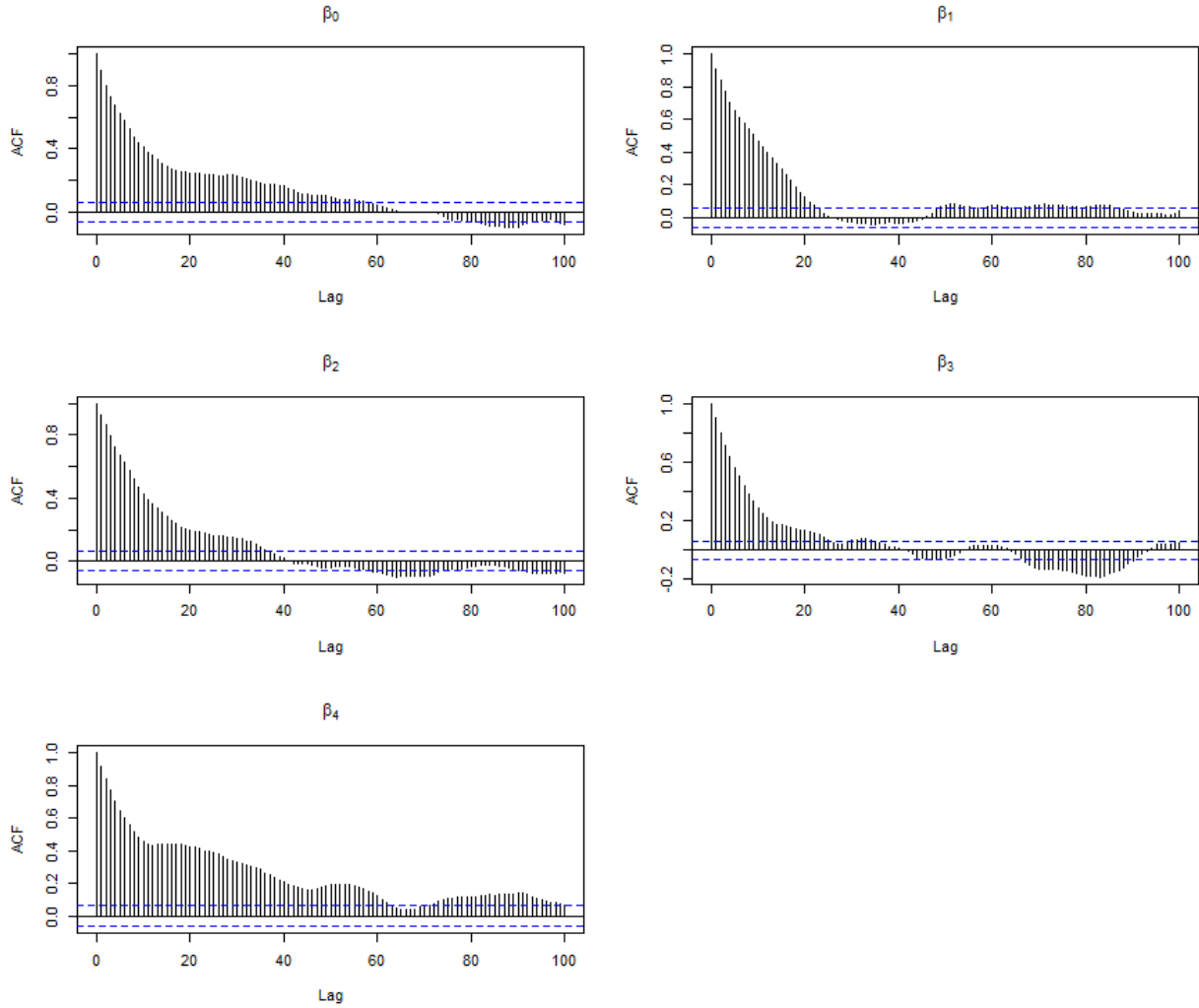
Acceptance probability: 0.482 when scale = 0.2.

MCMC estimates of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$ : [0.6568,0.7466,1.1150,0.4803,0.8190]

MCMC variance estimates of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$ : [0.0863,0.1060,0.1291,0.0867,0.1143]



**Fig. 11:** Plots of the sequences  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler, as well as the corresponding log-posterior probability for each iteration.



**Fig. 12:** Plots of autocorrelation of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler

**3.2 Scenario 2:  $\sigma \sim Ca^+(0, 1)$  and  $\gamma = (1, 1, 1, 1)$ :** Here, we assume  $\sigma \sim Ca^+(0, 1)$  and  $\gamma = (1, 1, 1, 1)$  to model the log-posterior probabilities and the other 15 scenarios for the *Logistic Regression* model allowing a general  $\sigma \sim Ca^+(0, 1)$  are implemented and shown in Problem 3.5. For this specific scenario 2, we conduct MCMC simulations to generate  $k$  (i.e.,  $k = 1$ ) chains, initialize it at the MLE for a given model, and then estimate the mean and variance of  $\beta_\gamma$ , as well as the values of the log-posterior at each of the MCMC samples.

**Step 1:** Calculate the MLE for the  $M_{15}$  Logistic Regression model (intercept and  $X_1, X_2, X_3, X_4$  included) as follows:

*Coefficients:*  $\beta_{15} = [0.6328, 0.7390, 1.1137, 0.4781, 0.6944]$  for intercept and  $X_1, X_2, X_3, X_4$



**Step 2:** Use the Random Walk Metropolis-Hastings (RWMH) sampling method to perform the MCMC simulations with the MLE as an initial value and  $n = 1000$ . Also, we sample  $\sigma$  from  $Ca^+(0,1)$  to calculate the log-posterior probabilities at each of the MCMC samples. The proposal pdf  $g$  is  $\beta_{15} \sim N(0, \text{diag}(\text{scale}^2))$  where we let the value of scale be 0.2 to guarantee a larger acceptance probability of  $\beta_{15}$ .

```
# sigma comes from half-cauchy
metropolis_hastings_cauchy = function(x,y,beta, n_points, scale) {
  #initialize
  current = beta
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta,2), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  for (i in 2:n_points) {
    sigma = abs(rcauchy(1, 0, 1))
    S = diag(length(beta)) * scale^2
    proposed = mvrnorm(1,current,2.4^2*S/length(beta))
    logr = lupost_factory(x,y,proposed,sigma)-lupost_factory(x,y,current,sigma)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}

# coef_sampling
model_sampler = metropolis_hastings_cauchy(out$x, out$y, out$coefficients, n<-1000, scale<-0.2)

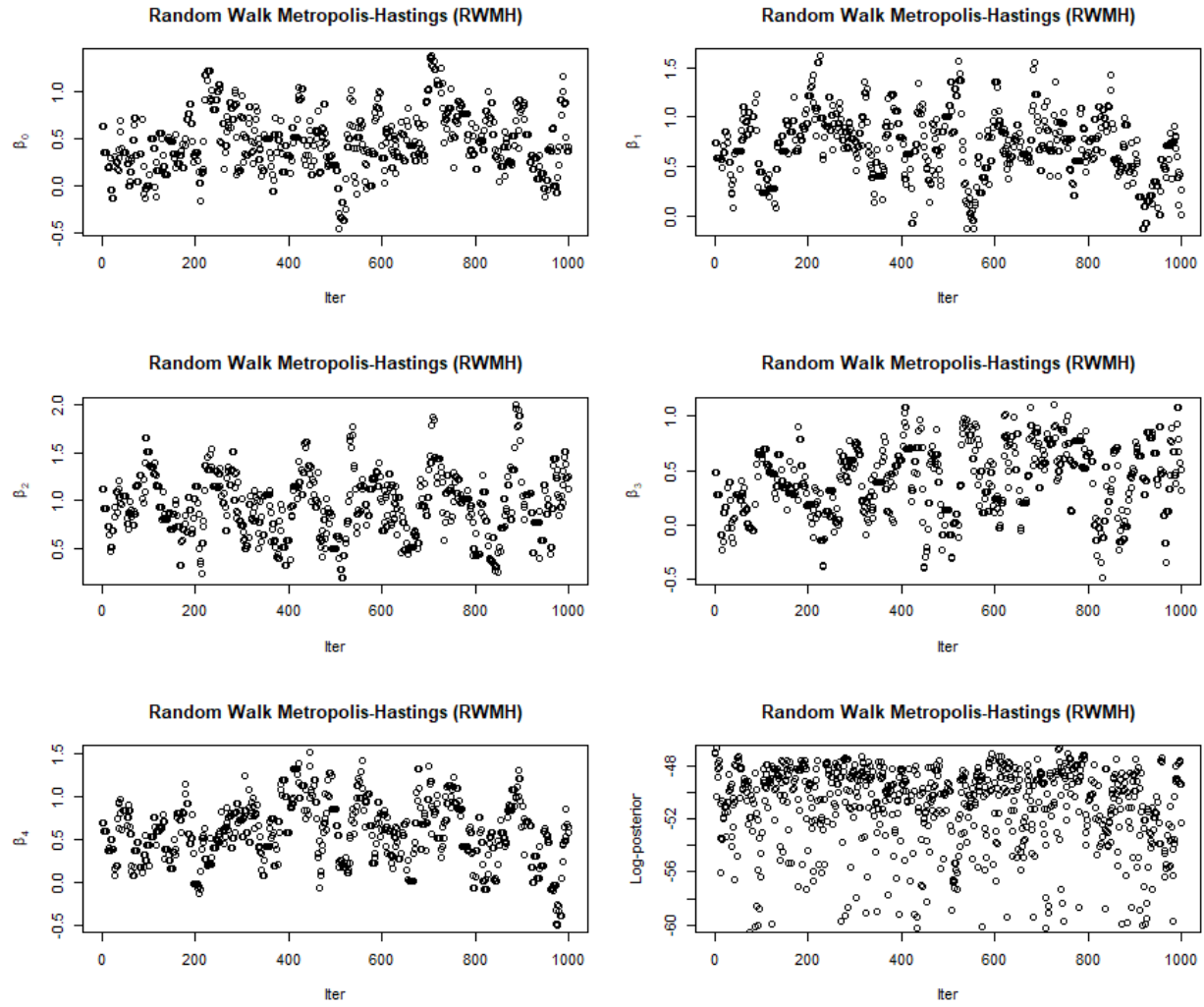
print(model_sampler$acceptance)
print(model_sampler$means)
print(model_sampler$standard_error)
```

**Step 3:** Visualize the plots of the sequences  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler and the corresponding log-posterior probability for each iteration, as shown in Fig. 13 and 14. Also, some statistical indicators are calculated as follows:

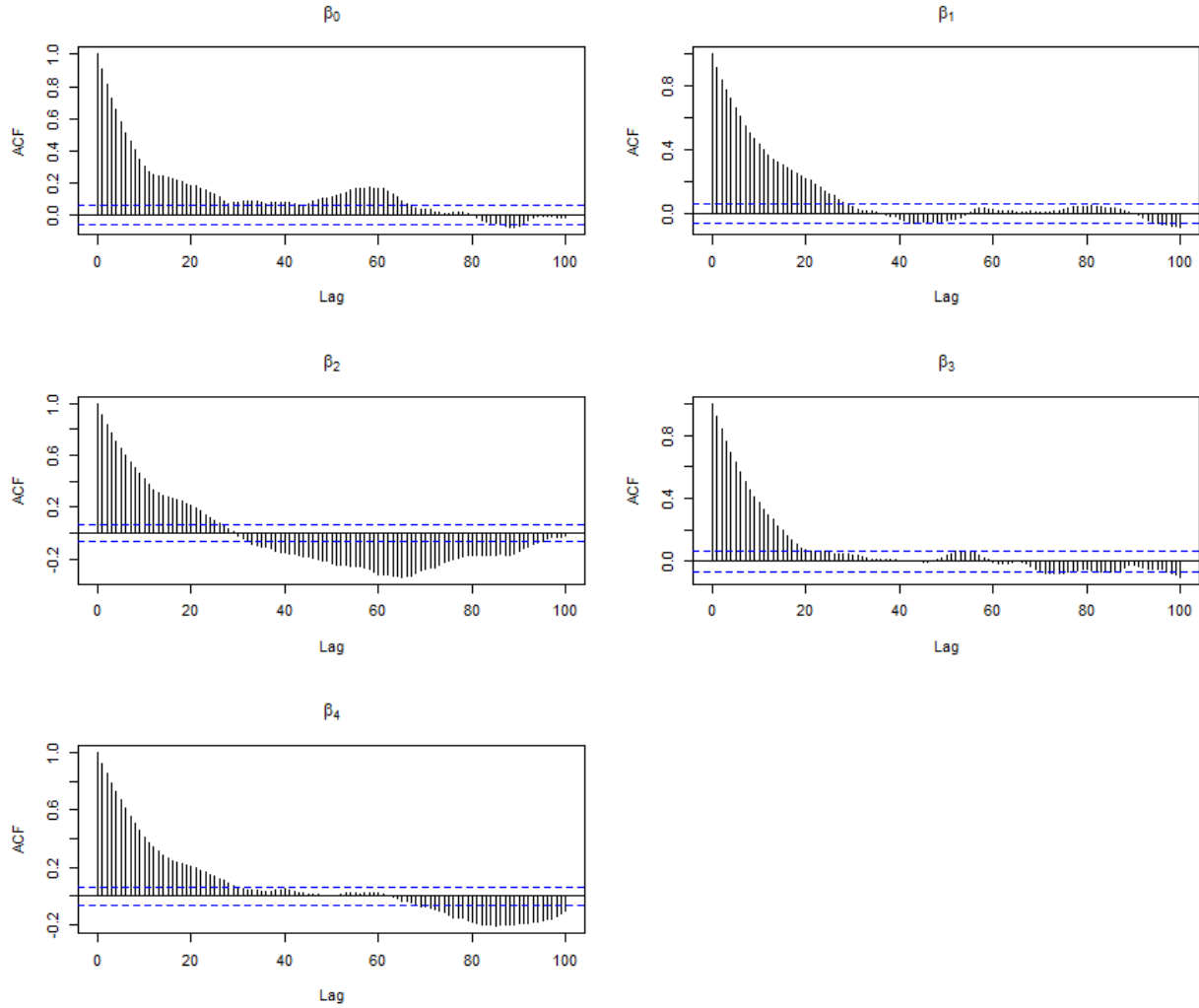
Acceptance probability: 0.453 when scale = 0.2.

MCMC estimates of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$ : [0.4622,0.7085,0.9415,0.4170,0.5764]

MCMC variance estimates of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$ : [0.0995,0.1088,0.1096,0.0999,0.1248]



**Fig. 13:** Plots of the sequences  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler, as well as the corresponding log-posterior probability for each iteration.



**Fig. 14:** Plots of autocorrelation of  $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$  produced by the RWMH sampler

**3.3 Reparameterize the log-posterior for implementation:** Since, RWMH generally does not “like” constrained parameters, for instance,  $\sigma \sim \text{Ca}^+(0,1)$  where  $\sigma$  is always positive, we replace the constrained  $\sigma$  with an unconstrained parameter  $\tau = \ln(\sigma)$  to reparameterize the log-posterior for each of the MCMC samples.

**3.4 Tune RWMH:** Here, we set different scales (corresponding to the covariance matrix of the proposal pdf) to check the effect of the scale on the acceptance rate of the RWMH algorithm. We vary the scale from 0.1, 0.2, 0.3, 0.4, 0.5, 1, 2, to 3 and return the corresponding acceptance rate, as shown in Table 3.

**Table 3:** The effect of scale of the proposal pdf on the acceptance rate of RWMH

scale	0.1	0.2	0.3	0.4	0.5	1	2	3
Acceptance rate	0.713	0.518	0.316	0.206	0.120	0.013	0.001	0

Note: The results are based on the scenario 1 where  $\sigma = 2$ .

As presented in Table 3, we can easily find that as the scale of the proposal pdf increases from 0.1 to 3, the acceptance rate gradually decreases until 0 when the scale is larger than 1. Therefore, across all 16 variable subsets (and two models, with known and unknown  $\sigma$ ), we can let the scale be 0.2 to guarantee adequate acceptance rate while maintaining a large sampling range for  $\beta_\gamma$ , no exception for the full model (with  $\gamma = (1,1,1,1)$  and unknown  $\sigma$ ).

### 3.5 Model/Variable selection:

- *Random-Walk Metropolis-Hastings (RWMH) Algorithm for sampling from a proposal pdf  $g$  that is multivariate normal distribution*

**Step 1: RWMH Algorithm.** We have known the optimal random walk tuning parameter is  $2.4^2 \text{Var}(X)/d$  where  $\text{Var}(X)$  is the covariance matrix. Here,  $\text{Var}(X) = \text{scale}^2$  and we set  $\text{scale} = 0.1$ . Therefore, the implementation of the RWMH algorithm is shown below:

- (1) Start with  $\text{Var}(X) = \text{diag}(d) * \text{scale}^2$  where  $d = 1 + \sum_j \gamma_j$
- (2) Run  $n = 1000$  iterations of the MCMC using  $\frac{2.4^2 \text{Var}(X)}{d}$ :  $(\beta_\gamma^*) \sim N\left(\beta_\gamma^t, \frac{2.4^2 \text{Var}(X)}{d}\right)$
- (3) Accept  $(\beta_\gamma^{t+1}) = (\beta_\gamma^*)$  with probability  $\min\{1, r\}$  with  $r = \frac{\log P(M_\gamma: \beta_\gamma^*|Y)}{\log P(M_\gamma: \beta_\gamma^t|Y)}$ , otherwise  $(\beta_\gamma^{t+1}) = (\beta_\gamma^t)$ .

**Step 2:** Perform MCMC simulations for 16 models under two cases:  $\sigma = 2$  and  $\sigma \sim \text{Ca}^+(0,1)$ .

**Step 3:** Present the statistical results of MCMC estimates for the 16 models in Table 4 and 5 with rows corresponding to different values of  $\gamma$  and columns referring to the MCMC estimates of mean and variance of  $\beta_\gamma$ , mean and credible interval (CI) of  $P(y|M_\gamma)$ , and the estimated Bayesian factor of  $M_\gamma$  vs  $M_0$ :  $BF(M_\gamma: M_0)$ .

- (1)  $\sigma = 2$

```

## ----random walk metropolis hastings algorithm-----
#sigma = 2
metropolis_hastings_normal = function(x,y,beta, n_points, scale) {
  #initialize
  S = diag(length(beta)) * scale^2 #
  current = beta
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  #index = sample.int(length(y),blen)
  for (i in 2:n_points) {
    proposed = mvrnorm(1,current,2.4^2*S/length(beta))
    logr = lupost_factory(x,y,proposed,sigma=2)-lupost_factory(x,y,current,sigma=2)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma=2)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
    # if (i%%50 == 0) S = var(theta[1:i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}

```

**Table 4:** MCMC estimates for the 16 Logistic Regression models

Model $M_Y$	Coefficients $\beta_Y$		Likelihood $\ln P(y M_Y)$		$BF(M_Y: M_0)$
	Estimate	Variance	Estimate	CI	
(0,0,0,0)	[0.2154,0,0,0]	[0.0433,0,0,0]	-69.35	[-71.61,-68.81]	1
(0,0,0,1)	[0.2471,0,0,0.12202]	[0.0506,0,0,0.0960]	-58.68	[-60.82,-57.72]	4.3045e4
(0,0,1,0)	[0.2063,0,0,0.8265,0]	[0.0417,0,0,0.0576,0]	-63.41	[-65.66,-62.50]	3.7993e2
(0,0,1,1)	[0.2937,0,0,0.5803,1.1183]	[0.0611,0,0,0.0747,0.0908]	-56.99	[-59.36,-55.69]	2.3328e5
(0,1,0,0)	[0.4824,0,1.4769,0,0]	[0.0625,0,0.1107,0,0]	-53.18	[-56.28,-52.17]	1.0533e7
(0,1,0,1)	[0.5261,0,1.2458,0,0.9477]	[0.0760,0,0.1085,0,0.0981]	-49.25	[-52.02,-47.94]	5.3619e8
(0,1,1,0)	[0.5697,0,1.4649,0.8255,0]	[0.0674,0,0.1055,0.1458,0]	-51.05	[-54.56,-49.55]	8.8632e7
(0,1,1,1)	[0.6212,0,1.3246,0.6784, 0.9376]	[0.0593,0,0.1365,0.1157, 0.1116]	-47.97	[-51.20,-46.35]	1.9285e9
(1,0,0,0)	[0.3086,1.5316,0,0,0]	[0.0537,0.1507,0,0,0]	-55.17	[-58.41,-54.05]	1.4398e6
(1,0,0,1)	[0.3648,1.2513,0,0,0.8172]	[0.0538,0.1069,0,0,0.1232]	-52.21	[-55.87,-50.96]	2.7785e7
(1,0,1,0)	[0.3267,1.3549,0,0.4552,0]	[0.0656,0.1250,0,0.0861,0]	-54.22	[-56.96,-52.78]	3.7229e6
(1,0,1,1)	[0.3490,1.0380,0,0.3894, 0.8049]	[0.0559,0.1344,0,0.0903, 0.1629]	-52.03	[-55.46,-50.27]	3.3264e7
(1,1,0,0)	[0.5808,1.1003,1.1791,0,0]	[0.0717,0.0998,0.1162,0,0]	-47.81	[-50.59,-46.57]	2.2631e9
(1,1,0,1)	[0.6039,0.8048,1.1341,0, 0.7721]	[0.0886,0.1188,0.1187,0, 0.1512]	-46.69	[-49.43,-45.09]	6.9361e9
(1,1,1,0)	[0.6759,0.9033,1.3236, 0.5219,0]	[0.0887,0.1340,0.1465, 0.1095,0]	-47.51	[-51.80,-45.70]	3.0549e9
(1,1,1,1)	[0.7153,0.8049,1.1465, 0.4571,0.7817]	[0.1066,0.1159,0.1326, 0.1659,0.1392]	-46.39	[-50.22,-44.26]	9.3627e9

$$(2) \sigma \sim Ca^+(0,1)$$

```
# sigma comes from half-cauchy
metropolis_hastings_cauchy = function(x,y,beta, n_points, scale) {
  #initialize
  current = beta
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta,2), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  for (i in 2:n_points) {
    sigma = abs(rcauchy(1, 0, 1))
    s = diag(length(beta)) * scale^2
    proposed = mvrnorm(1,current,2.4^2*s/length(beta))
    logr = lupost_factory(x,y,proposed,sigma)-lupost_factory(x,y,current,sigma)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}
```

**Table 5:** MCMC estimates for the 16 Logistic Regression models

Model $M_Y$	Coefficients $\beta_Y$		Likelihood $\ln P(y M_Y)$		$BF(M_Y; M_0)$
	Estimate	Variance	Estimate	CI	
(0,0,0,0)	[0.1919,0,0,0]	[0.0461,0,0,0]	-69.38	[-71.59,-68.81]	1
(0,0,0,1)	[0.2006,0,0,0.9396]	[0.0501,0,0,0.1183]	-59.50	[-68.46,-57.73]	1.9536e4
(0,0,1,0)	[0.2048,0,0,0.6879,0]	[0.0482,0,0,0.0682,0]	-63.72	[-67.47,-62.53]	2.8715e2
(0,0,1,1)	[0.2422,0,0,0.4260,0.9228]	[0.0606,0,0,0.0820,0.1433]	-57.92	[-64.09,-55.65]	9.4845e4
(0,1,0,0)	[0.3403,0,1.0826,0,0]	[0.0660,0,0.1424,0,0]	-54.51	[-62.01,-52.18]	2.8705e6
(0,1,0,1)	[0.4388,0,1.0395,0,0.8299]	[0.0934,0,0.1322,0,0.1106]	-50.16	[-56.12,-47.95]	2.2240e8
(0,1,1,0)	[0.3853,0,1.1193,0.5458,0]	[0.0711,0,0.1128,0.1345,0]	-52.02	[-58.75,-49.68]	3.4622e7
(0,1,1,1)	[0.4334,0,1.0024,0.4453,0.7046]	[0.0946,0,0.1421,0.1202,0.1391]	-49.50	[-55.74,-46.53]	4.3030e8
(1,0,0,0)	[0.2665,1.2798,0,0,0]	[0.0774,0.1368,0,0,0]	-55.65	[-59.74,-54.06]	9.1804e5
(1,0,0,1)	[0.2752,0.9845,0,0,0.6820]	[0.0746,0.1015,0,0,0.0963]	-52.85	[-57.61,-51.00]	1.5097e7
(1,0,1,0)	[0.2607,1.0528,0,0.3963,0]	[0.0794,0.1210,0,0.0887,0]	-55.08	[-61.28,-52.76]	1.6223e6
(1,0,1,1)	[0.3212,0.9640,0,0.3635,0.7200]	[0.0525,0.1324,0,0.0887,0.1061]	-52.06	[-55.84,-50.18]	3.3264e7
(1,1,0,0)	[0.4539,0.9080,0.9567,0,0]	[0.1049,0.1435,0.1514,0,0]	-49.12	[-53.90,-46.67]	6.2923e8
(1,1,0,1)	[0.4635,0.7260,0.9536,0,0.6514]	[0.1108,0.1464,0.1454,0,0.1265]	-47.57	[-52.30,-45.24]	2.9646e9
(1,1,1,0)	[0.3611,0.7434,0.8036,0.4515,0]	[0.0834,0.1462,0.1025,0.0956,0]	-48.85	[-55.93,-45.85]	8.2426e8
(1,1,1,1)	[0.4236,0.7067,0.9181,0.4272,0.5393]	[0.0800,0.1199,0.1127,0.0802,0.1192]	-46.66	[-51.98,-44.28]	7.3650e9

- *RWMH Algorithm for importance sampling from a proposal pdf  $g$  that is multivariate normal with mean equal to the posterior mode and covariance matrix taken to be the sample covariance matrix from the MCMC samples from the posterior (after tuning)*

**Step 1: RWMH for importance sampling.** We have known the optimal random walk tuning parameter is  $2.4^2 \text{Var}(X)/d$  where  $\text{Var}(X)$  is the unknown covariance matrix. We can estimate

$Var(X)$  using the sample covaraiance matrix of draws. Therefore, the implementation of the RWMH algorithm for importance sampling is shown below:

- (1) Start with  $Var(X) = diag(d)$  where  $d = 1 + \sum_j \gamma_j$
- (2) Run 50 iterations of the MCMC using  $\frac{2.4^2 Var(X)}{d}$ :  $(\beta_\gamma^*) \sim N\left(\beta_\gamma^t, \frac{2.4^2 Var(X)}{d}\right)$
- (3) Set  $Var(X)$  to the sample covariance matrix of all previous draws
- (4) Accept  $(\beta_\gamma^{t+1}) = (\beta_\gamma^*)$  with probability  $\min\{1, r\}$  with  $r = \frac{\log P(M_\gamma: \beta_\gamma^* | Y)}{\log P(M_\gamma: \beta_\gamma^t | Y)}$ , otherwise  $(\beta_\gamma^{t+1}) = (\beta_\gamma^t)$ .

**Step 2:** Perform MCMC simulations for 16 models under two cases:  $\sigma = 2$  and  $\sigma \sim Ca^+(0, 1)$ .

**Step 3:** Present the statistical results of MCMC estimates for the 16 models in Table 6 and 7 with rows corresponding to different values of  $\gamma$  and columns referring to the MCMC estimates of mean and variance of  $\beta_\gamma$ , mean and credible interval (CI) of  $P(y|M_\gamma)$ , and the estimated Bayesian factor of  $M_\gamma$  vs  $M_0$ :  $BF(M_\gamma: M_0)$ .

(1)  $\sigma = 2$

```
## -----RWMH Importance Sampling-----
# sigma = 2
RWMH_importance_sampling_normal = function(x,y,beta, n_points) {
  #initialize
  current = beta
  S = diag(length(beta))
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta,sigma=2), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  for (i in 2:n_points) {
    proposed = mvrnorm(1,coef[which.max(lupost),],2.4^2*S/length(beta))
    logr = lupost_factory(x,y,proposed,sigma=2)-lupost_factory(x,y,current,sigma=2)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma=2)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
    if (i%%50 == 0) S = var(coef[1:i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}
```

**Table 6:** MCMC estimates for the 16 Logistic Regression models

Model $M_\gamma$	Coefficients $\beta_\gamma$		Likelihood $\ln P(y M_\gamma)$		$BF(M_\gamma: M_0)$
	Estimate	Variance	Estimate	CI	
(0,0,0,0)	[0.1892,0,0,0,0]	[0.0323,0,0,0,0]	-69.21	[-70.91,-68.81]	1
(0,0,0,1)	[0.2555,0,0,0,1.2122]	[0,0,0,0,0]	-57.70	[-57.70,-57.70]	9.9708e4
(0,0,1,0)	[0.2270,0,0,0.7968,0]	[0.0189,0,0,0.0153,0]	-62.80	[-64.02,-62.49]	6.0789e2
(0,0,1,1)	[0.2716,0,0,0.5704,1.0762]	[0,0,0,0,0]	-55.56	[-55.56,-55.56]	8.4746e5
(0,1,0,0)	[0.5039,0,1.4490,0,0]	[0.0387,0,0.0769,0,0]	-52.79	[-54.58,-52.15]	1.3524e7
(0,1,0,1)	[0.5531,0,1.2797,0,0.9368]	[0,0,0,0,0]	-47.86	[-47.86,-47.86]	1.8715e9
(0,1,1,0)	[0.5464,0,1.3983,0.6846,0]	[0,0,0,0,0]	-49.48	[-49.48,-49.48]	3.7037e8

(0,1,1,1)	[0.5990,0.12936,0.6042,0.8794]	[0,0,0,0,0]	-46.17	[-46.17,-46.17]	1.0143e10
(1,0,0,0)	[0.3152,1.4634,0,0,0]	[0,0,0,0,0]	-54.03	[-54.03,-54.03]	3.9137e6
(1,0,0,1)	[0.3635,1.1525,0,0,0.8294]	[0,0,0,0,0]	-50.85	[-50.85,-50.85]	9.4112e7
(1,0,1,0)	[0.3119,1.3016,0,0.4541,0]	[0,0,0,0,0]	-52.65	[-52.65,-52.65]	1.5557e7
(1,0,1,1)	[0.3652,1.0603,0,0.4021,0.7744]	[0,0,0,0,0]	-50.02	[-50.02,-50.02]	2.1583e8
(1,1,0,0)	[0.5582,1.0823,1.1421,0,0]	[0.0003,0.0674,0.0208,0,0]	-46.83	[-47.98,-46.50]	5.2422e9
(1,1,0,1)	[0.6043,0.8305,1.0877,0,0.7049]	[0,0,0,0,0]	-44.79	[-44.79,-44.79]	4.0315e10
(1,1,1,0)	[0.5784,0.9363,1.1591,0.4673,0]	[0,0,0,0,0]	-45.42	[-45.42,-45.42]	2.1472e10
(1,1,1,1)	[0.6330,0.7453,1.1005,0.4734,0.6975]	[0.0199,0.0200,0.0855,0.0295,0.0501]	-44.58	[-46.76,-43.87]	4.9736e10

(2)  $\sigma \sim Ca^+(0,1)$

```
# sigma comes from half cauchy
RWMH_importance_sampling_cauchy = function(x,y,beta, n_points) {
  #initialize
  current = beta
  s = diag(length(beta))
  coef = matrix(current, nrow=n_points, ncol=length(beta), byrow=TRUE)
  lupost = matrix(lupost_factory(x,y,beta,sigma=2), nrow=n_points, ncol=1, byrow=TRUE)
  likelihood = matrix(likelihood_factory(x,y,beta), nrow=n_points, ncol=1, byrow=TRUE)
  nn = 0
  for (i in 2:n_points) {
    sigma = abs(rcauchy(1, 0, 1))
    proposed = mvrnorm(1,coef[which.max(lupost),],2.4^2*s/length(beta))
    logr = lupost_factory(x,y,proposed,sigma)-lupost_factory(x,y,current,sigma)
    if (log(runif(1)) < logr) {current = proposed; nn = nn + 1}
    coef[i,] = current
    lupost[i] = lupost_factory(x,y,coef[i,],sigma)
    likelihood[i] = likelihood_factory(x,y,coef[i,])
    if (i%%50 == 0) s = var(coef[1:i,])
  }
  sampler = list(coefficient=coef, log_posterior=lupost, acceptance=nn/n_points,
    coef_means = colMeans(coef), # MCMC estimate
    coef_variance = colMeans(coef^2)-colMeans(coef)^2,
    likelihood_est = mean(likelihood),
    likelihood_CI = c(sort(likelihood)[round(n_points*0.025)],sort(likelihood)[round(n_points*0.975)]))
  return(sampler)
}
```

**Table 7:** MCMC estimates for the 16 Logistic Regression models

Model $M_Y$	Coefficients $\beta_Y$		Likelihood $\ln P(y M_Y)$		$BF(M_Y: M_0)$
	Estimate	Variance	Estimate	CI	
(0,0,0,0)	[0.1792,0,0,0,0]	[0.0340,0,0,0,0]	-69.24	[-71.10,-68.81]	1
(0,0,0,1)	[0.2555,0,0,0,1.2122]	[0,0,0,0,0]	-57.70	[-57.70,-57.70]	1.0274e5
(0,0,1,0)	[0.1927,0,0,0.7130,0]	[0.0288,0,0,0.0595,0]	-63.39	[-66.29,-62.50]	3.4723e2
(0,0,1,1)	[0.2716,0,0,0.5704,1.0762]	[0,0,0,0,0]	-55.56	[-55.56,-55.56]	8.7327e5
(0,1,0,0)	[0.5087,0,1.4370,0,0]	[0,0,0,0,0]	-52.14	[-52.14,-52.14]	2.6695e7
(0,1,0,1)	[0.5143,0,1.2557,0,0.9479]	[0.0176,0,0.0067,0,0.0014]	-48.00	[-48.62,-47.86]	1.6765e9
(0,1,1,0)	[0.4547,0,1.2433,0.6206,0]	[0.0836,0,0.1288,0.0921,0]	-51.38	[-60.16,-49.49]	5.7082e7
(0,1,1,1)	[0.5231,0,1.2564,0.6084,0.7646]	[0.0339,0,0.0271,0.0332,0.0750]	-46.96	[-49.01,-46.18]	4.7433e9
(1,0,0,0)	[0.2708,1.3329,0,0,0]	[0.0712,0.1787,0,0,0]	-55.74	[-61.64,-54.06]	7.2942e5
(1,0,0,1)	[0.3230,1.0124,0,0,0.7485]	[0.0567,0.0776,0,0,0.1033]	-52.44	[-59.29,-50.97]	1.9776e7
(1,0,1,0)	[0.2837,1.2129,0,0.4350,0]	[0.0553,0.0573,0,0.0572,0]	-53.84	[-57.48,-52.65]	4.8768e6
(1,0,1,1)	[0.3652,1.0603,0,0.4021,0.7744]	[0,0,0,0,0]	-50.02	[-50.02,-50.02]	2.2240e8
(1,1,0,0)	[0.4958,0.9898,1.0612,0,0]	[0.1127,0.1134,0.1460,0,0]	-48.63	[-56.57,-46.50]	8.9291e8



(1,1,0,1)	[0.6043,0.8305,1.0877,0,0.7049]	[0,0,0,0,0]	-44.79	[-44.79,-44.79]	4.1543e10
(1,1,1,0)	[0.5784,0.9363,1.1591,0.4673,0]	[0,0,0,0,0]	-45.42	[-45.42,-45.42]	2.2126e10
(1,1,1,1)	[0.6328,0.7390,1.1137,0.4781,0.6944]	[0,0,0,0,0]	-43.83	[-43.83,-43.83]	1.0850e11

In summary, based on the results of Table 4-7, we can easily find that the full model (intercept and  $X_1, X_2, X_3, X_4$  included) performs the best, as opposed to other model/variable selection, with the largest likelihood  $\ln P(y|M_{\gamma=(1,1,1,1)})$  and the highest Bayesian factor  $BF(M_{\gamma=(1,1,1,1)}:M_0)$ . In addition, RWMH for importance sampling from a proposal pdf that is multivariate normal with mean equal to the posterior mode and covariance matrix taken to be the sample covariance matrix performs better than the classic RWMH algorithm. In general, whether the classic RWMH algorithm or the RWMH for importance sampling, the scenario of  $\sigma = 2$  performs better than the scenario of  $\sigma \sim Ca^+(0,1)$ , in terms of the data likelihood and Bayesian factor. For a single variable, we find that the variable  $X_2$  is more important than the variables  $X_1, X_4, X_3$  in predicting  $Y$ . In terms of dual variables, the combination of the variables  $X_1, X_2$  performs better than others. For the combination of three variables, the variables  $X_1, X_2, X_4$  perform the best. However, all these combinations of different variables are worse than the full model when predicting the variable  $Y$ .

**Problem 4: Rejection sampling and importance sampling**

**4.1** The smallest value of the bounding constant  $M$  is 2.29 so that  $f(x) \leq M \cdot g(x)$  for every  $x > 0$ . The efficiency of the rejection sampler is  $\frac{1}{M} = 0.437$ . Based on the simulations, we calculated the acceptance rate of the rejection sampler is 0.48.

Problem 4:

(4.1) The pdf of a r.v.  $X$  is  $f(x) \propto (1+x^2)^{-1.75} \mathbb{I}(x>0)$

Using numeric integration,  $\int_{-\infty}^{+\infty} f(x) dx \approx 0.874$

The proposal pdf is  $g(x) = 0.5g_1(x) + 0.5g_2(x)$

$$= 0.5 \mathbb{I}(0 < x < 1) + 0.5 \cdot \frac{x^{-3} \mathbb{I}(x > 1)}{\int_1^{\infty} x^{-3} dx}$$

$$= 0.5 \mathbb{I}(0 < x < 1) + x^{-3} \mathbb{I}(x > 1)$$

So, the normalized pdfs of  $f(x), g(x)$  are

$$f(x) \approx \frac{(1+x^2)^{-1.75} \mathbb{I}(x>0)}{0.874}$$

$$g(x) = 0.5 \mathbb{I}(0 < x < 1) + x^{-3} \mathbb{I}(x > 1)$$

Since  $f(x) \leq M \cdot g(x)$  for every  $x \geq 0$ ,

$$\text{the optimal } M \text{ is } M = \sup_x \frac{f(x)}{g(x)} = \sup_x \frac{\frac{(1+x^2)^{-1.75} \mathbb{I}(x>0)}{0.874}}{0.5 \mathbb{I}(0 < x < 1) + x^{-3} \mathbb{I}(x > 1)}$$

When  $x \leq 0$ ,  $f(x) \equiv 0$ ,  $g(x) \equiv 0$ , so there is no constraints for  $M$ .

$$\text{When } 0 < x < 1, M = \sup_x \frac{(1+x^2)^{-1.75} \mathbb{I}(x>0)}{0.5 * 0.874} = 2.29$$

$$\text{When } x \geq 1, M = \sup_x \frac{(1+x^2)^{-1.75} \mathbb{I}(x>0)}{0.874 * x^{-3}} \approx 0.56$$

So, the smallest value of the bounding constant  $M$  is 2.29 so that

$$f(x) \leq M \cdot g(x) \text{ for every } x \geq 0.$$

The probability of acceptance (efficiency of the rejection sampler) is

$$\frac{1}{M} = 0.437.$$

Then we use the rejection sampling method with the proposal  $g(x)$  to simulate  $X \sim f(x)$  and plot the samples in Fig. 15.

```

sampler_1 = function(n_points, w=0.5) {
  sample = matrix(0, nrow=n_points, ncol=1, byrow=TRUE)
  for (i in 1:n_points) {
    if (runif(1)<w) {sample[i] = runif(1)}
    else {sample[i] = sqrt(1/(1-runif(1)))}
  }
  return(sample)
}

# rejection sampling
set.seed(1)

M = 2/I_f$value
n = 10^2
d = data.frame(x = sampler_1(n),
               u = runif(n)) %>%
  mutate(u_scaled = u*M*g(x),
         accept = u_scaled < f(x)/I_f$value)

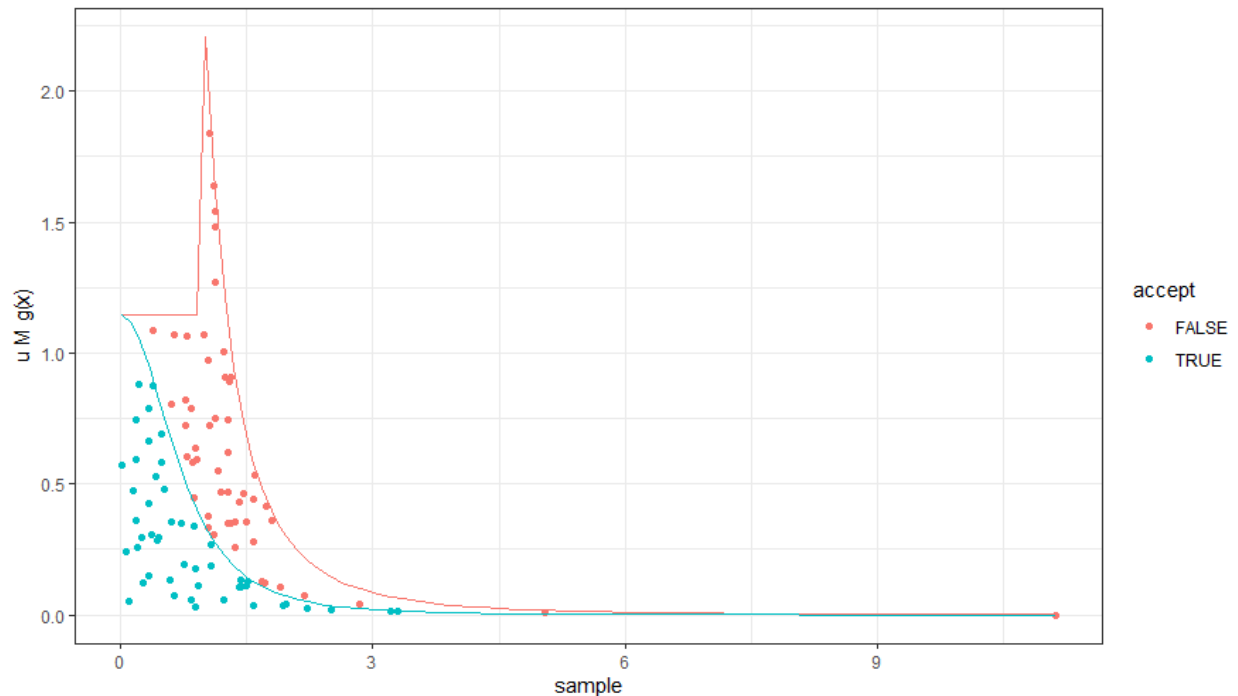
gg = ggplot(d, aes(x=x,y=u_scaled,col=accept)) +
  geom_point()

clrs = unique(ggplot_build(gg)$data[[1]]$colour)

gg + stat_function(fun=function(x) M*g(x), col=clrs[2]) +
  stat_function(fun=function(x) f(x)/I_f$value, col=clrs[1]) +
  labs(x="sample",y=expression(paste("u M g(",x,")"))) +
  theme_bw()

cat("Observed acceptance rate was",mean(d$accept))

```



**Fig. 15:** Plots of samples derived from the rejection samplers

## 4.2

(4.2)  $g(x) = w \cdot g_1(x) + (1-w) \cdot g_2(x)$ ,  $w \in (0,1)$ ,  $c > 0$ ,  $p > 1$

Since  $g_1(x) = c^{-1} \mathbb{I}(x \in [0, c])$ ,  $g_2(x) \propto x^{-p} \mathbb{I}(x > c)$ , then

$$\int_c^{+\infty} x^{-p} dx = \frac{1}{p-1} c^{1-p}$$

So  $g(x) = w \cdot c^{-1} \mathbb{I}(x \in [0, c]) + (1-w) \cdot \frac{x^{-p} \mathbb{I}(x > c)}{\frac{1}{p-1} c^{1-p}}$

$$= w \cdot c^{-1} \mathbb{I}(x \in [0, c]) + \frac{(1-w)(p-1)}{c^{1-p}} x^{-p} \mathbb{I}(x > c)$$

The following is about how to simulate  $X \sim g(x)$

Step 1: determine  $g_1(x)$  or  $g_2(x)$  is used for sampling

$\begin{cases} \text{if } (\text{runif}(1) < w) & g_1(x) \text{ is selected, go to step 2} \\ \text{else} & g_2(x) \text{ is selected, go to step 3} \end{cases}$

Step 2: for  $g_1(x) = \frac{1}{c} \mathbb{I}(x \in [0, c])$ ,  $X = \text{runif}(1) * c$

Step 3: for  $g_2(x) = \frac{p-1}{c^{1-p}} x^{-p} \mathbb{I}(x > c)$

$$F_n(x) = \text{cdf}(x) = \begin{cases} 0 & x \leq c \\ 1 - \frac{x^{1-p}}{c^{1-p}} & x > c \end{cases}$$

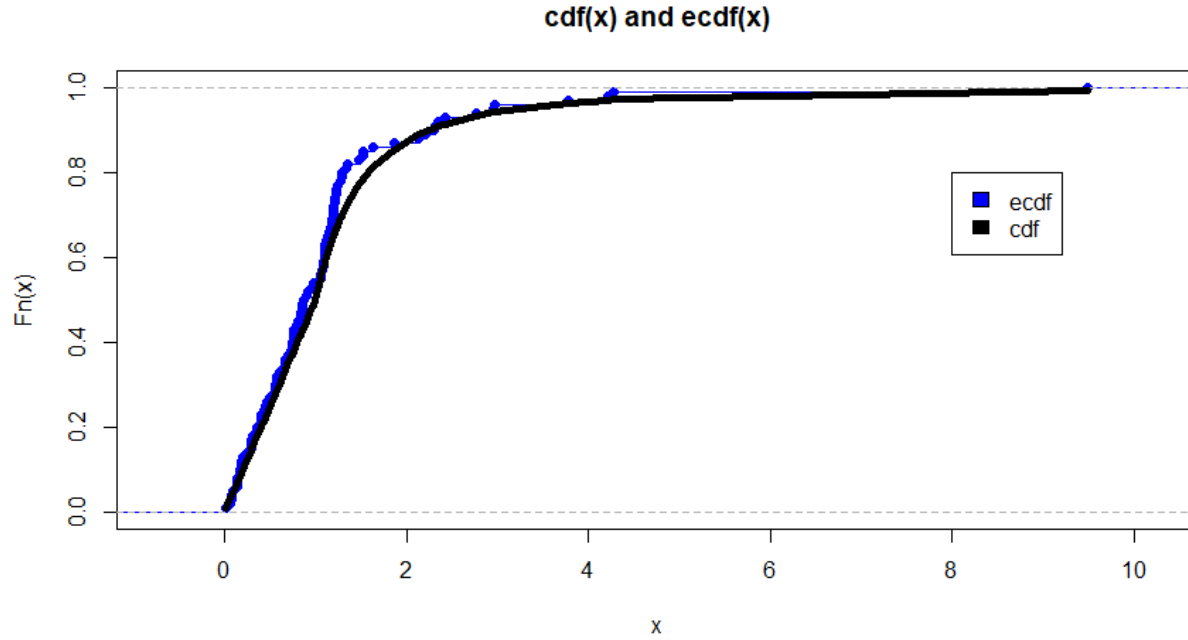
So, if  $U$  is  $\text{Unif}(0,1)$ ,  $U = \text{runif}(1)$ ,  $X = F^{-1}(u) = c(1-u)^{\frac{1}{1-p}}$ .

Step 4: run  $n$  iterations to obtain  $n$  samples.

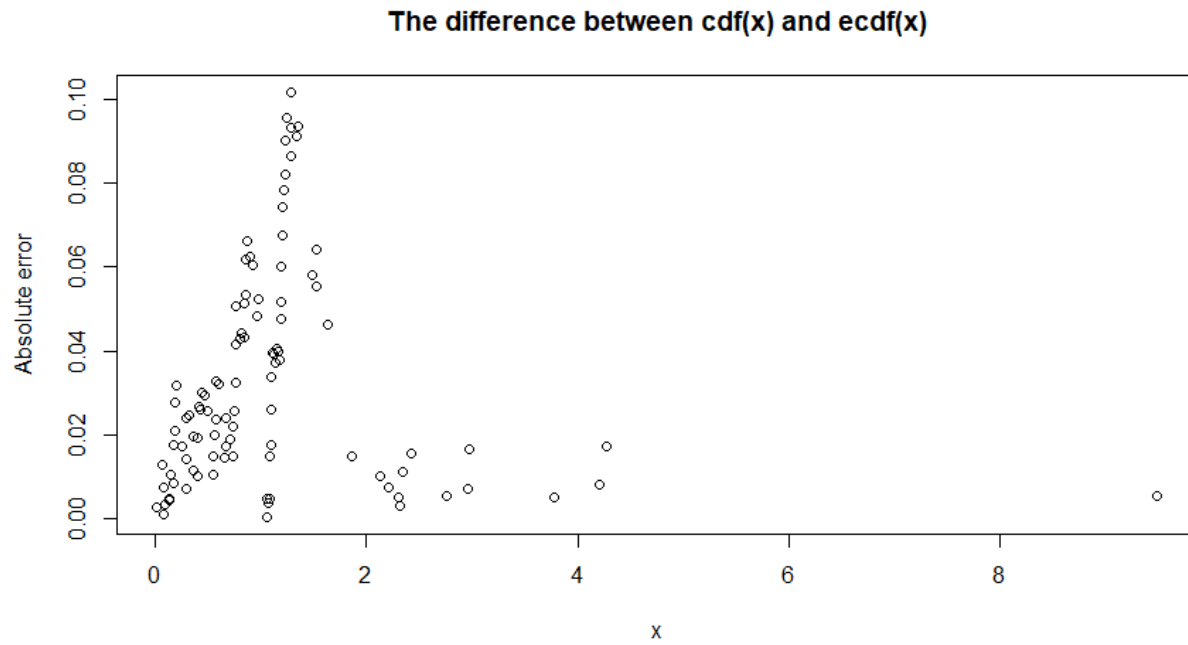
Specifically, the implementation of sampling from  $X \sim g$  is shown below:

```
sampler_2 = function(n_points, p, c, w) {
  sample = matrix(0, nrow=n_points, ncol=1, byrow=TRUE)
  for (i in 1:n_points) {
    if (runif(1) < w) {sample[i] = runif(1)*c}
    else {sample[i] = c*(1-runif(1))^(1/(1-p))}
  }
  return(sample)
}
```

To check the reliability of the sampler, we first assume  $w = 0.5$ ,  $p = 3$ ,  $c = 1$ ,  $n = 100$  and plot the cdf and ecdf based on the samples from of  $X \sim g$  in Fig. 16. Also, we plot the absolute error between the cdf and ecdf in Fig. 17. The two figures both suggest that the difference between the cdf and ecdf is tiny.



**Fig. 16:** Plots of the cdf and ecdf based on the simulations of  $X \sim g$



**Fig. 17:** Plots of absolute error between the cdf and ecdf

In addition, we use the rejection sampling method with the proposal  $g(x)$  to simulate  $X \sim f(x)$  and plot the samples in Fig. 18. Based on the simulations, we calculated the acceptance rate of the rejection sampler is 0.44. This figure and related results is almost the same as those in 4.1.



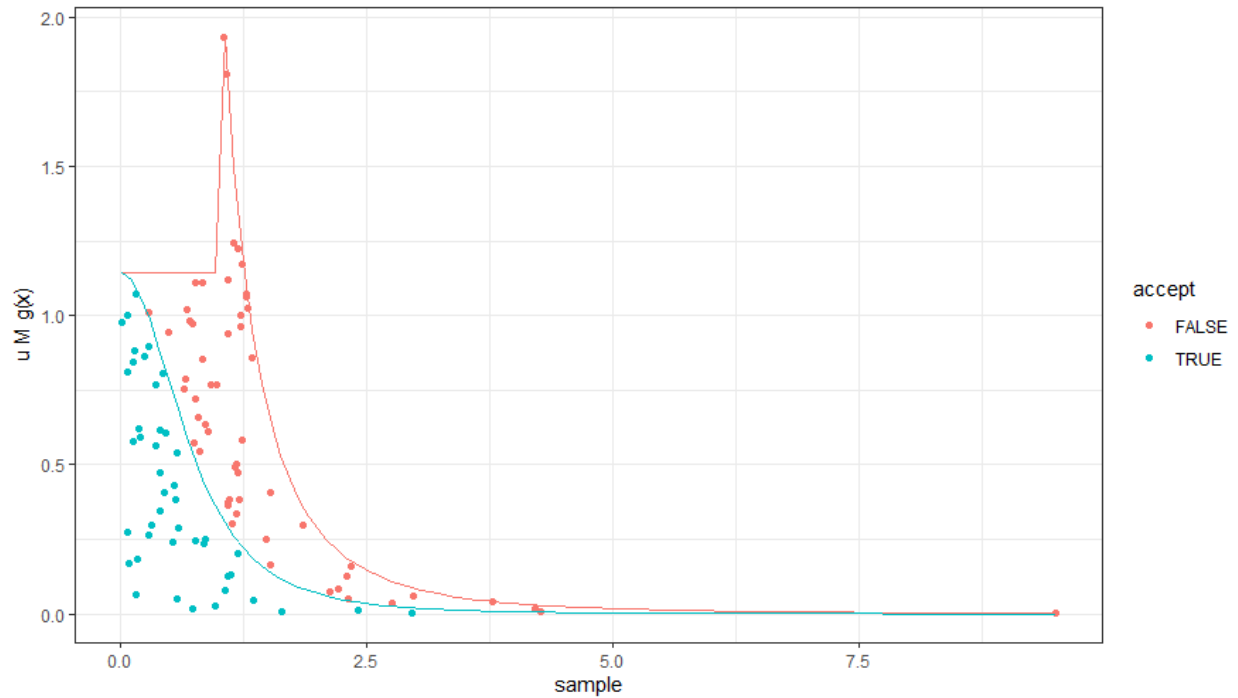


Fig. 18: Plots of samples derived from the rejection samplers

## 4.3

(4.3) For rejection sampling,  $f(x) \leq M \cdot g(x)$  for every  $x \geq 0$ .

$$\text{Since } f(x) \approx \frac{(1+x)^{-1.75} \mathbb{I}(x \leq c)}{0.874}$$

$$g(x) = w c^{-1} \mathbb{I}(0 \leq x < c) + \frac{(1-w)(p-1)}{c^{1-p}} x^{-p} \mathbb{I}(x \geq c)$$

when  $x \leq 0$ ,  $f(x) \equiv 0$ ,  $g(x) \equiv 0$ , so, there is no constraint for  $M$

$$\text{when } 0 < x < c, M = \sup_x \frac{\frac{(1+x)^{-1.75}}{0.874}}{w c^{-1}} = \frac{c}{0.874 w}$$

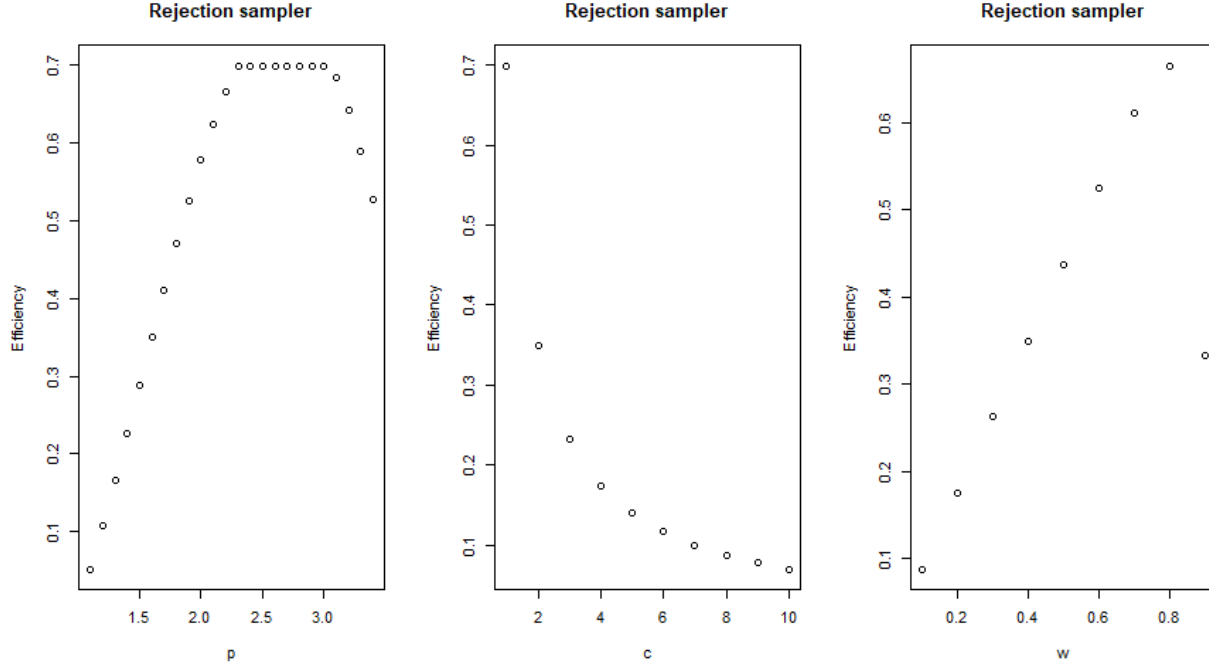
$$\text{when } x \geq c, M = \sup_x \frac{\frac{(1+x)^{-1.75}}{0.874}}{\frac{(1-w)(p-1)}{c^{1-p}} x^{-p}} \begin{cases} \text{① when } p > 3.5, M = +\infty, \\ \text{so this situation should be avoided.} \end{cases}$$

As a result,  $1 < p \leq 3.5$

$$\text{② when } 1 < p \leq 3.5, M = \max \left\{ \frac{c(1+c^2)^{-1.75}}{0.874(1-w)(p-1)}, \frac{c^{1-p} \left(\frac{p}{3.5-p}\right)^{\frac{p}{2}} (1+\frac{p}{3.5-p})^{-1.75}}{0.874(1-w)(p-1)} \right\}$$

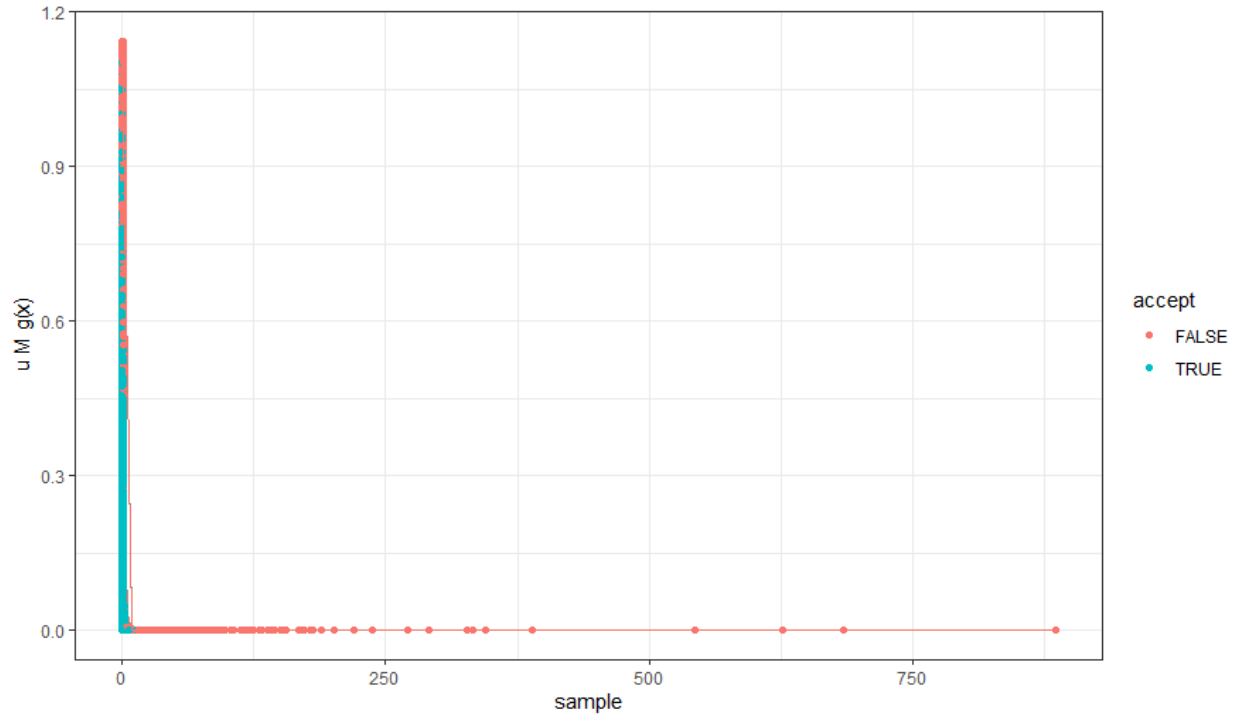
$$\text{So, } M = \max \left\{ \frac{c}{0.874 w}, \frac{c(1+c^2)^{-1.75}}{0.874(1-w)(p-1)}, \frac{c^{1-p} \left(\frac{p}{3.5-p}\right)^{\frac{p}{2}} (1+\frac{p}{3.5-p})^{-1.75}}{0.874(1-w)(p-1)} \right\}$$

Here, we vary the values of  $p, c, w$ , separately from 1.1 to 3.4, from 1 to 10, from 0.1 to 0.9, to determine their effects on the efficiency of the rejection sampler. We find that when  $c = 1, w = 0.8, p = 2.3$ , the rejection sampler is the most efficient (the smallest  $M$ ) among all cases.

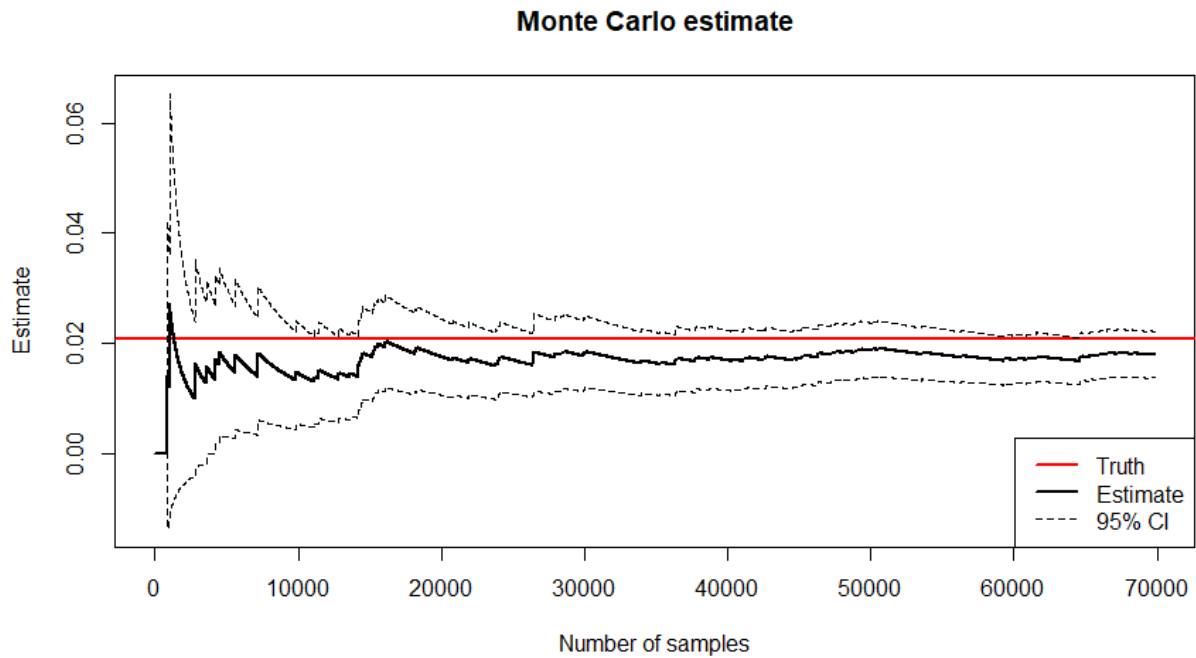


**Fig. 19:** Plot of effects of  $p, c, w$  on the efficiency of the rejection sampler

**4.4** We use the rejection sampling method with the proposal  $g(x)$  from 4.3 where  $c = 1, w = 0.8, p = 2.3, J = 10^5$  to simulate  $X \sim f(x)$  and plot the samples in Fig. 20. Based on the simulations, we calculated the acceptance rate of the rejection sampler is 0.70. Since most samples fall into the range of  $[0, 10]$  and only a few samples are distributed in the range of  $[10, \infty]$ , the rejection sampling method with proposal  $g(x)$  from 4.3 is not very appropriate or attractive for estimating the expectation  $E(h(X)) = \int_{-\infty}^{+\infty} h(x)f(x) dx$  where  $h(x) = xI(x \geq 10)$ . In addition, Fig. 21 plots how the Monte Carlo estimate and 95% credible interval of  $E(h(X))$  vary with an increase in the sample size and based on the strong law of larger numbers, the Monte Carlo estimate of  $E(h(X))$  eventually converge to 0.018, which is very close to the analytical integration 0.021.



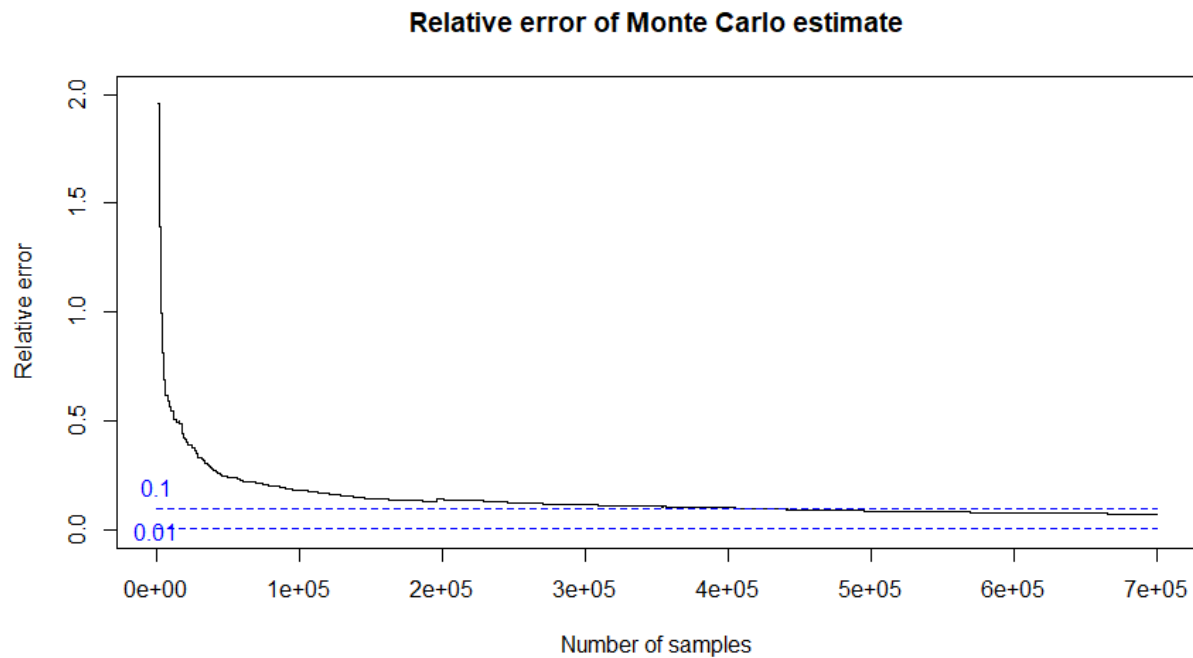
**Fig. 20:** Plots of samples derived from the rejection samplers with the proposal from 4.3



**Fig. 21:** Monte Carlo estimate and 95% credible interval of  $E(h(X))$



When we set the sample size  $J = 10^5$ , we find that the minimum of relative error is still higher than 10%. In other words, the Monte Carlo sample sizes required by the rejection sampling method is larger than  $10^5$  if we want the desired relative error is 10% and 1%. Therefore, we increase the sample size  $J$  from  $10^5$  to  $10^6$  and plot how the relative error varies by the sample size in Fig. 22. We conclude that if we want the desired relative error is 10%, the MC sample size required by the rejection sampling method is larger than 596529 (about  $6 \times 10^5$ ). If we want the desired relative error is 1%, the MC sample size required by the rejection sampling method must be larger than  $10^6$  (about  $5 \sim 6 \times 10^6$ ) because the minimum of relative error is 0.0744 when  $J = 10^6$ .



**Fig. 22:** Plots of change of relative error by the number of samples

## 4.5

(4.5) Since  $f(x) \approx \frac{(1+x^2)^{-1.75} \cdot \mathbb{I}(x \geq 0)}{0.874}$

$$h(x) = x \mathbb{I}(x \geq 0)$$

the proposal:  $g_j(x) \propto x^{-j} \cdot \mathbb{I}(x \geq 0)$ ,  $j = 2, 3, 4$

the normalized pdf of the proposal is:

$$g_j(x) = \frac{x^{-j} \mathbb{I}(x \geq 0)}{\int_0^{\infty} x^{-j} dx} = \frac{(j-1)x^{-j} \mathbb{I}(x \geq 0)}{10^{1-j}}, \quad j = 2, 3, 4$$

notice  $E(h(X)) = \int_{\mathbb{R}} h(x)f(x)dx = \int_{\mathbb{R}} h(x) \frac{f(x)}{g_j(x)} g_j(x)dx$ ,

So we approximate the expectation via

$$E(h(X)) \approx \frac{1}{S} \sum_{s=1}^S w(X^{(s)}) h(X^{(s)})$$

where  $X^{(s)} \stackrel{iid}{\sim} g_j(x)$ ,  $j = 2, 3, 4$  and

$$w(X^{(s)}) = \frac{f(X^{(s)})}{g_j(X^{(s)})} \text{ is known as the importance weight.}$$

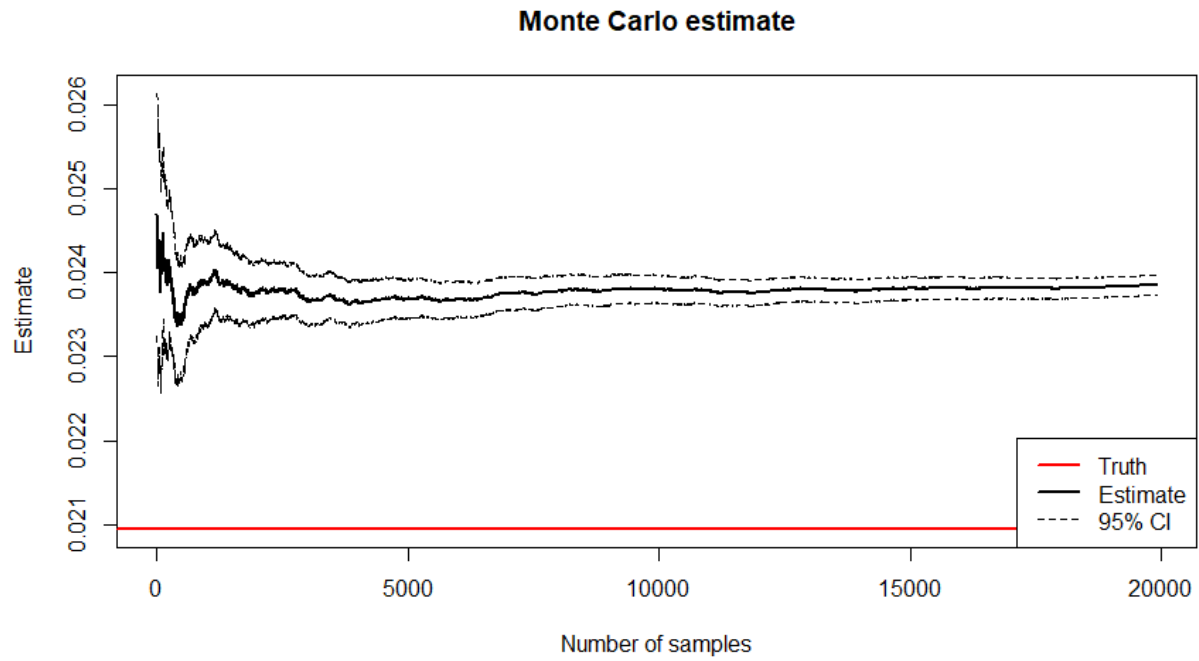
step 1: sample  $X^{(s)}$  from  $g_j(x)$ ,  $j = 2, 3, 4$ , i.e.,  $10 * (1 - \text{runif}(n))^{1/(1-j)}$

step 2: compute  $w(X^{(s)})$ ,  $h(X^{(s)})$

step 3: calculate  $E(h(X))$ ,  $\text{Var}(h(X))$ ,  $95\% \text{CI} = [E(h(X)) - q_{\text{norm}}(0.975) * \sqrt{\text{Var}(h(X))}, E(h(X)) + q_{\text{norm}}(0.975) * \sqrt{\text{Var}(h(X))}]$

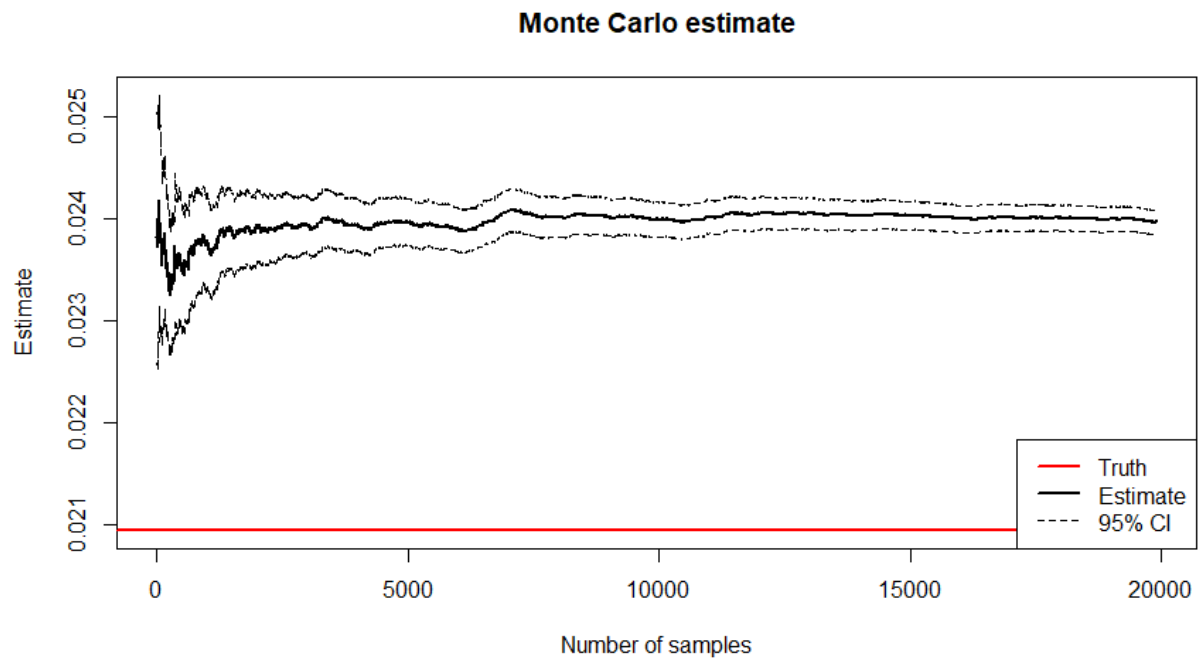
Then we let  $j = 2, 3, 4$ , estimate  $E(h(X))$  and its accuracy, (i.e., 95% equal-tailed approximate confidence interval, CI) by importance sampling using each  $g_j$ , and further plot the estimates and the corresponding CIs in Fig. 23-25.

(1)  $j = 2$ :



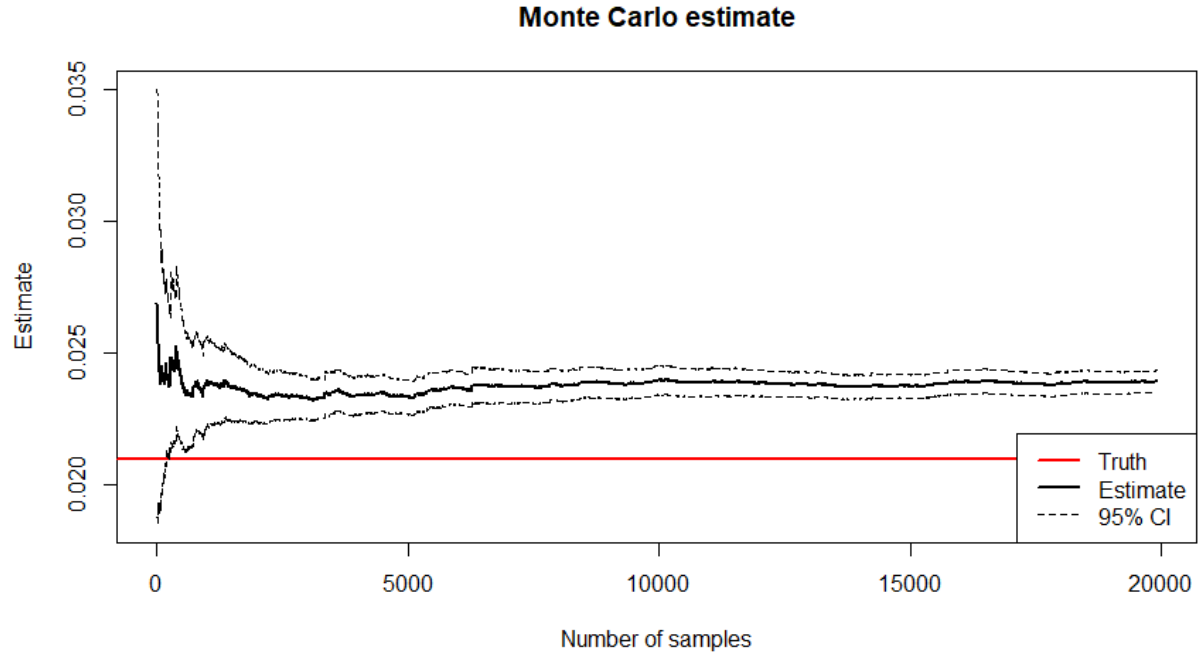
**Fig. 23:** MC estimates and 95% credible intervals of  $E(h(X))$  by importance sampling using  $g_2$

(2)  $j = 3$ :



**Fig. 24:** MC estimates and 95% credible intervals of  $E(h(X))$  by importance sampling using  $g_3$

(3)  $j = 4$ :



**Fig. 24:** MC estimates and 95% credible intervals of  $E(h(X))$  by importance sampling using  $g_4$

Whether  $g_2, g_3$  or  $g_4$ , the Monte Carlo estimates of  $E(h(X))$  based on importance sampling using the proposal  $g$  all eventually converge to 0.024 with an increase in the number of samples, which is very close to the analytical integration 0.021. In addition, these results follow the strong law of larger numbers (SLLN), reaching convergence rather than divergence. The length of 95% equal-tailed approximate credible intervals (CIs) is very small and densely concentrated in the MC estimates, which is significantly smaller than those derived from 4.4 (shown in Fig. 21), indicating that the importance sampling method is very efficient in approximating the expectation of  $h(X)$  and estimating  $E(h(X))$ .