MCMC:HW2

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February 15, 2017

Problem 1

A chain with transition matrix P and stationary density π is reversible if

$$\pi_i \, p_{ij} = \pi_j \, p_{ji} \tag{1}$$

for all i, j. Show that this condition is satisfied for the P with elements

$$p_{ij} = \alpha_{ij} \, q_{ij} + (1 - r_i) \, \mathbf{1} \, (i = j) \tag{2}$$

where $\mathbf{1} \, (i = j)$ if $i = j$ and is 0 otherwise, and

$$\alpha_{ij} = \min \left\{1, \frac{\pi_j \, q_{ji}}{\pi_i \, q_{ij}}\right\} \tag{3}$$

and

$$r_i = \sum_{j=1}^{k} \alpha_{ij} \, q_{ij} \tag{4}$$

Here $(q_{ij})_{j=1}^{k}$ are a set of weights for each i.

Solution:

$$\begin{aligned}
\pi_i \, p_{ij} &= \pi_i [\alpha_{ij} \, q_{ij} + (1 - r_i) \, \mathbf{1} \, (i = j)] \\
&= \alpha_{ij} \, \pi_i \, q_{ij} + \pi_i \left(1 - \sum_{l=1}^{k} \alpha_{il} \, q_{il}\right) \mathbf{1} \, (i = j) \\
&= \min \left\{1, \frac{\pi_j \, q_{ji}}{\pi_i \, q_{ij}}\right\} \pi_i \, q_{ij} + \pi_i \left(1 - \sum_{l=1}^{k} \alpha_{il} \, q_{il}\right) \mathbf{1} \, (i = j) \\
&= \min \{\pi_i \, q_{ij}, \, \pi_j \, q_{ji}\} + \left(\pi_i - \sum_{l=1}^{k} \min \left\{1, \frac{\pi_l \, q_{li}}{\pi_i \, q_{il}}\right\} \pi_i \, q_{il}\right) \mathbf{1} \, (i = j) \\
&= \min \{\pi_i \, q_{ij}, \, \pi_j \, q_{ji}\} + \left(\pi_i - \sum_{l=1}^{k} \min \{\pi_i \, q_{il}, \, \pi_l \, q_{li}\}\right) \mathbf{1} \, (i = j)
\end{aligned} \tag{5}$$

On the other hand, by exchanging i and j in the above expression, one finds

$$\begin{aligned}
\pi_j \, p_{ji} &= \min \{\pi_j \, q_{ji}, \, \pi_i \, q_{ij}\} + \left(\pi_j - \sum_{l=1}^{k} \min \{\pi_j \, q_{jl}, \, \pi_l \, q_{lj}\}\right) \mathbf{1} \, (i = j) \\
&= \min \{\pi_j \, q_{ji}, \, \pi_i \, q_{ij}\} + \left(\pi_i - \sum_{l=1}^{k} \min \{\pi_i \, q_{il}, \, \pi_l \, q_{li}\}\right) \mathbf{1} \, (i = j) \\
&= \pi_i \, p_{ij}
\end{aligned} \tag{6}$$

Problem 2

Suppose that the joint density $f(x, q)$ is given by

$$f(x, q) = q^x (1 - q)^{1-x}, \; x \in \{0, 1\} \text{ and } 0 < q < 1. \tag{7}$$

Consider the transition density, with X_n, $X_{n+1} \in \{0, \; 1\}$,

$$p(X_{n+1} \mid X_n) = 2 \int_0^1 q^{X_n + X_{n+1}} (1 - q)^{2 - X_n - X_{n+1}} \, dq \tag{8}$$

Find the stationary density for this transition density. Generate the sequence (X_n), starting with $P(X_0 = 1) = 1/2$, and use this to confirm your finding on the stationary density.

Solution: According to the definition of the stationary condition,

$$f(X_{n+1}) = \sum_{X_n} P(X_{n+1} \mid X_n)\, f(X_n) \tag{9}$$

From Eq. (7), one can obtain the marginal density of x as

$$f(x) = \int_0^1 f(x,\, q)\, dq = \frac{\Gamma(1+x)\,\Gamma(2-x)}{\Gamma(3)} = \frac{x\,!\,(1-x)\,!}{2},\ x \in \{0,\ 1\} \tag{10}$$

Then

$$\begin{aligned}
\sum_{X_n} P(X_{n+1} \mid X_n)\, f(X_n) &= \sum_{X_n} \frac{X_n\,!\,(1-X_n)\,!}{2}\, 2 \int_0^1 q'^{X_n + X_{n+1}} (1-q')^{2 - X_n - X_{n+1}}\, dq' \\
&= \sum_{X_n} X_n\,!\,(1-X_n)\,!\ \frac{\Gamma(1 + X_n + X_{n+1})\,\Gamma(3 - X_n - X_{n+1})}{\Gamma(4)} \\
&= \frac{\Gamma(1+X_{n+1})\,\Gamma(3-X_{n+1})}{\Gamma(4)} + \frac{\Gamma(2+X_{n+1})\,\Gamma(2-X_{n+1})}{\Gamma(4)} \\
&= \frac{\Gamma(1+X_{n+1})\,(2-X_{n+1})\,\Gamma(2-X_{n+1})}{\Gamma(4)} + \frac{(1+X_{n+1})\,\Gamma(1+X_{n+1})\,\Gamma(2-X_{n+1})}{\Gamma(4)} \\
&= \frac{2 - X_{n+1} + 1 + X_{n+1}}{\Gamma(4)}\,\Gamma(1+X_{n+1})\,\Gamma(2-X_{n+1}) \\
&= \frac{\Gamma(1+X_{n+1})\,\Gamma(2-X_{n+1})}{2} \\
&= \frac{X_{n+1}\,!\,(1-X_{n+1})\,!}{2},\ X_{n+1} \in \{0,\ 1\} = f(X_{n+1})
\end{aligned} \tag{11}$$

So we have verified that the stationary density for this transition is just

$$f(x) = \frac{1}{2},\ x \in \{0,\ 1\} \tag{12}$$

```
Integrate[x^n (1 - x)^m, {x, 0, 1}, Assumptions → {m ∈ Integers, n ∈ Integers}]
```

```
ConditionalExpression[Gamma[1 + m] Gamma[1 + n] / Gamma[2 + m + n], n ≥ 0 && m ≥ 0]
```

The Markov chain is discrete and we can write

$$P(X_{n+1} = j \mid X_n = i) = p_{ij} = 2\,\frac{\Gamma(1+i+j)\,\Gamma(3-i-j)}{\Gamma(4)} = \frac{(i+j)\,!\,(2-i-j)\,!}{3} \tag{13}$$

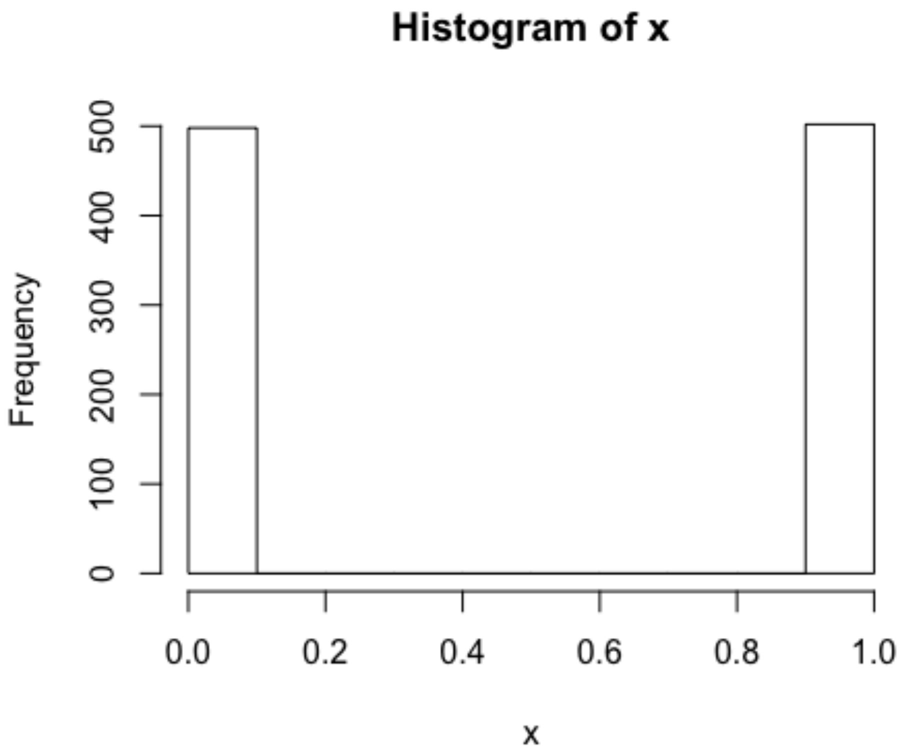
$$f(X_{n+1} = j) = f_j \tag{14}$$

In matrix notation,

$$P = \begin{pmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} \end{pmatrix},\ f = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \tag{15}$$

$$f_j = \sum_{i=0,1} f_i\, p_{ij} \tag{16}$$

The simulation results are given in the following histogram $\left(P_0(X = i) = \frac{1}{2}\right)$:



Problem 3

Consider the integral

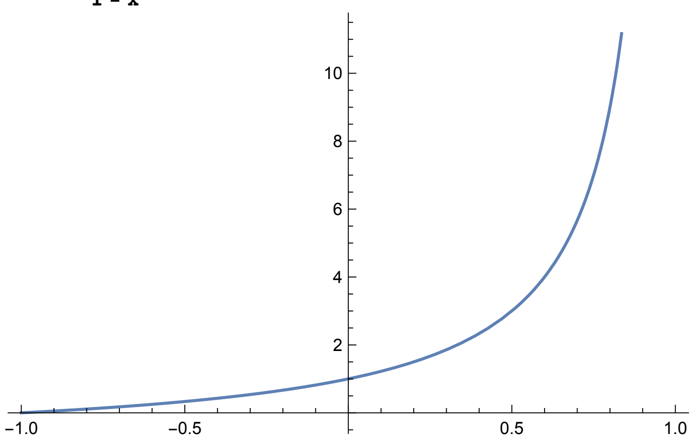
$$I = \int_{-\infty}^{\infty} \frac{1}{1+x^4} e^{-\frac{1}{2}x^2} \, dx \tag{17}$$

Evaluate this integral using a Markov chain sample (X_n) given by $X_{n+1} \sim N(\rho X_n, 1-\rho^2)$. What is the best ρ to use in this case and demonstrate via simulation.

```
NIntegrate[1/(1 + x^4) Exp[-1/2 x^2], {x, -∞, ∞}]
```

1.69639

```
Plot[(1 + x)/(1 - x), {x, -1, 1}]
```



Solution: The approximate value of the integral is

$$I = \int_{-\infty}^{\infty} \frac{1}{1+x^4} e^{-\frac{1}{2}x^2} \, dx \approx 1.69639 \tag{18}$$

The MCMC simulation can be performed based on the following form:

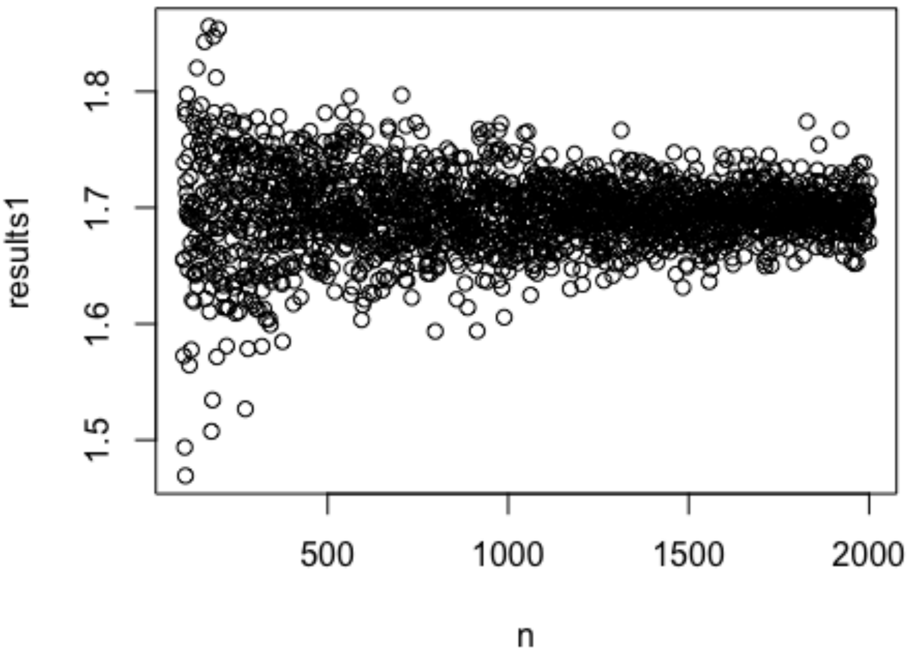
$$I = \int_{-\infty}^{\infty} g(x)\, f(x) \, dx \tag{19}$$

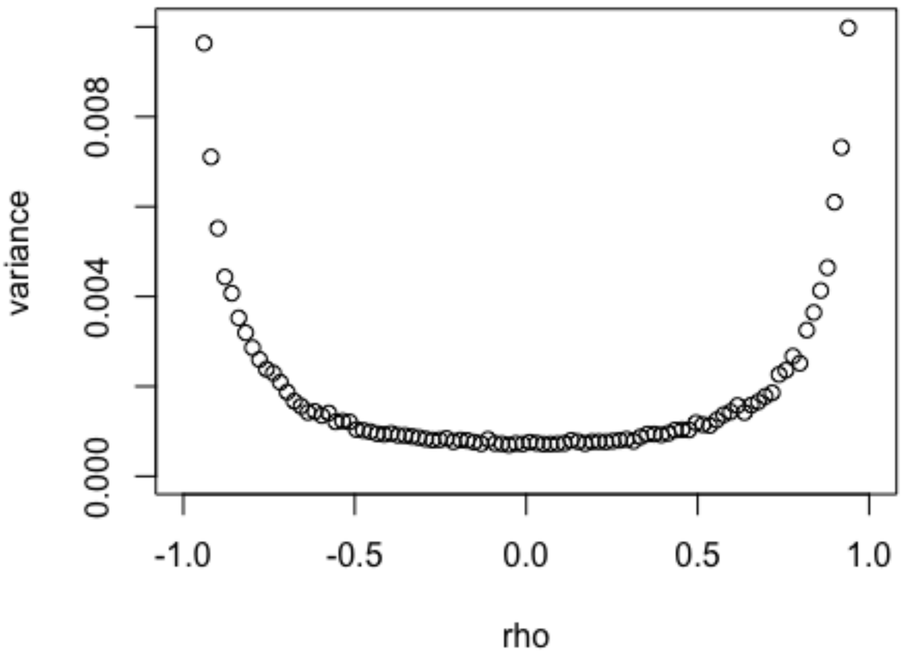
where

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \tag{20}$$

$$g(x) = \frac{\sqrt{2\pi}}{1+x^4} \tag{21}$$

The convergence and the variance plots are as follows





The simulation results gives

$$I \approx I_N = \frac{1}{N}\sum_{i=1}^{N} g(x_i) \approx 1.692704 \tag{22}$$

The best ρ to choose can be derived from minimization of variance:

$$\sigma^2 = \mathrm{Var}(g(X_1)) + 2\sum_{i=1}^{\infty}\mathrm{Cov}(g(X_1), g(X_i)) \tag{23}$$

If we plot the sample variance of size $m = 100$ integral results

$$S^2 = \frac{1}{m-1}\sum_{i=1}^{m}\left(I_N^i - \overline{I}_N\right)^2 \tag{24}$$

One finds $\rho = 0$ is the minimum. This is the case when $X_1, \ldots, X_n$ are i.i.d. $N(0, 1)$ and MCMC sampling is the same as the importance sampling.

Appendix: R-code

```
# problem 2
n<-1000
x<-array(dim=n)
# initialize
x[1]<-sample(0:1, 1, replace = TRUE)
for(i in 2:n){
  x[i]<-sample(c(0,1), 1, replace = TRUE, prob=c(factorial(x[i-1])*factorial(2-
x[i-1])/3,factorial(1+x[i-1])*factorial(1-x[i-1])/3))
}
hist(x)

# problem 3
n<-5000
```

```
x<-array(dim=n)
x[1] <- rnorm(1, 0, 1)
rho <- 0
for(i in 2:n){
  x[i]<-rnorm(1, rho*x[i-1], sqrt(1-rho**2))
}
g <- sqrt(2*pi)/(1+x**4)
I <- sum(g)/n
I

I_N_rho <- function(n,rho,x1){
  x<-array(dim=n)
  x[1] <- x1
  for(i in 2:n){
    x[i]<-rnorm(1, rho*x[i-1], sqrt(1-rho**2))
  }
  g <- sqrt(2*pi)/(1+x**4)
  return(sum(g)/n)
}

I_N <- function(n){
  return(I_N_rho(n,rho,rnorm(1, 0, 1)))
}

var_rho <- function(rho){
  g <-array(dim=1000)
  for(i in 1:1000){
    g[i] <- I_N_rho(1000,rho,rnorm(1, 0, 1))
  }
   return(sum((g-mean(g))**2)/(1000-1))
}

n = 100:2000
results1 <- lapply(n,I_N)
plot(n, results1)

m=100
rho=seq(from=-1, to=1,length.out=m)
variance <- lapply(rho,var_rho)
plot(rho, variance, ylim=c(0.000, 0.01))
```