

STAT 545 HW 4

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Assignment 4: Metropolis-Hastings algorithm

Exercise 5.7

Exhibit a Metropolis-Hastings algorithm to sample from a binomial distribution with parameters n and p . Use a proportional distribution that is uniform on $\{0, 1, \dots, n\}$.

Solution

We wish to construct a Metropolis-Hastings (MH) algorithm to sample from a Binomial distribution with parameters n and p , whose probability mass function is

$$\pi(k) = \mathbb{P}(X = k) = \binom{n}{k} p^k (1-p)^{n-k}, \quad k \in \{0, 1, \dots, n\}.$$

We are instructed to use a proposal distribution that is uniform on $\{0, 1, \dots, n\}$. Thus, for any current state x ,

$$q(y | x) = \frac{1}{n+1}, \quad y \in \{0, 1, \dots, n\}.$$

This is an independence proposal (it does not depend on x), and it is symmetric in the sense that

$$q(x | y) = q(y | x) = \frac{1}{n+1}.$$

The general Metropolis-Hastings acceptance probability is

$$\alpha(x, y) = \min \left(1, \frac{\pi(y) q(x | y)}{\pi(x) q(y | x)} \right).$$

Since the proposal is symmetric, $q(x | y) = q(y | x)$ and these terms cancel. Therefore,

$$\alpha(x, y) = \min \left(1, \frac{\pi(y)}{\pi(x)} \right).$$

Substituting the Binomial pmf,

$$\frac{\pi(y)}{\pi(x)} = \frac{\binom{n}{y} p^y (1-p)^{n-y}}{\binom{n}{x} p^x (1-p)^{n-x}} = \frac{\binom{n}{y}}{\binom{n}{x}} \left(\frac{p}{1-p} \right)^{y-x}.$$

Hence the acceptance probability is

$$\alpha(x, y) = \min \left(1, \frac{\binom{n}{y}}{\binom{n}{x}} \left(\frac{p}{1-p} \right)^{y-x} \right).$$

Let T be the total number of iterations, and choose an initial value $x_0 \in \{0, 1, \dots, n\}$.

For $t = 1, 2, \dots, T$:

1. Propose $y \sim \text{Unif}\{0, 1, \dots, n\}$.

2. Compute

$$\alpha = \min \left(1, \frac{\pi(y)}{\pi(x_{t-1})} \right).$$

3. Draw $u \sim \text{Unif}(0, 1)$.

4. If $u \leq \alpha$, set $x_t = y$ (accept).

5. Otherwise, set $x_t = x_{t-1}$ (reject).

The Markov chain $\{x_t\}$ constructed in this way has stationary distribution $\text{Binomial}(n, p)$. After discarding an initial burn-in period, the samples may be used as approximate draws from the target distribution.

Exercise 5.8

The Metropolis–Hastings algorithm is used to simulate a binomial random variable with parameters $n = 4$ and $p = \frac{1}{4}$. The proposal distribution is a simple symmetric random walk on $\{0, 1, 2, 3, 4\}$ with reflecting boundaries.

- Exhibit the T matrix.
- Exhibit the transition matrix for the Markov chain created by the Metropolis–Hastings algorithm.
- Show explicitly that this transition matrix gives a reversible Markov chain whose stationary distribution is the desired binomial distribution.

Solution

We want to simulate the target distribution

$$\pi(k) = \binom{4}{k} \left(\frac{1}{4}\right)^k \left(\frac{3}{4}\right)^{4-k}, \quad k \in \{0, 1, 2, 3, 4\},$$

using a Metropolis–Hastings (MH) chain whose proposal is a simple symmetric random walk on $\{0, 1, 2, 3, 4\}$ with reflecting boundaries.

Part A:

A simple symmetric random walk proposes moving one step left or right with probability $1/2$ when in an interior state. At the boundaries, an attempted move outside the state space is reflected, assuming reflected boundaries implies the chain stays put with probability $1/2$ and moves inward with probability $1/2$. Thus, with states ordered as $0, 1, 2, 3, 4$, the proposal matrix $T = T(i, j)$ is

$$T = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

Part B:

First compute the target probabilities:

$$\begin{aligned} \pi(0) &= \left(\frac{3}{4}\right)^4 = \frac{81}{256}, & \pi(1) &= 4 \left(\frac{1}{4}\right) \left(\frac{3}{4}\right)^3 = \frac{27}{64}, \\ \pi(2) &= 6 \left(\frac{1}{4}\right)^2 \left(\frac{3}{4}\right)^2 = \frac{27}{128}, & \pi(3) &= 4 \left(\frac{1}{4}\right)^3 \left(\frac{3}{4}\right) = \frac{3}{64}, \\ \pi(4) &= \left(\frac{1}{4}\right)^4 = \frac{1}{256}. \end{aligned}$$

Since the proposal is symmetric ($T(i, j) = T(j, i)$), the MH acceptance probability is

$$\alpha(i, j) = \min\left(1, \frac{\pi(j)}{\pi(i)}\right).$$

For neighboring moves this gives:

$$\begin{aligned} \alpha(0, 1) &= 1, & \alpha(1, 0) &= \frac{3}{4}; & \alpha(1, 2) &= \frac{1}{2}, & \alpha(2, 1) &= 1; \\ \alpha(2, 3) &= \frac{2}{9}, & \alpha(3, 2) &= 1; & \alpha(3, 4) &= \frac{1}{12}, & \alpha(4, 3) &= 1. \end{aligned}$$

The MH transition probabilities for $i \neq j$ are

$$P(i, j) = T(i, j) \alpha(i, j),$$

and the diagonal entries are

$$P(i, i) = 1 - \sum_{j \neq i} P(i, j).$$

Therefore,

$$P(0, 1) = \frac{1}{2} \cdot 1 = \frac{1}{2}, \quad P(0, 0) = \frac{1}{2}.$$

$$\begin{aligned}
P(1,0) &= \frac{1}{2} \cdot \frac{3}{4} = \frac{3}{8}, & P(1,2) &= \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}, & P(1,1) &= 1 - \frac{3}{8} - \frac{1}{4} = \frac{3}{8}. \\
P(2,1) &= \frac{1}{2} \cdot 1 = \frac{1}{2}, & P(2,3) &= \frac{1}{2} \cdot \frac{2}{9} = \frac{1}{9}, & P(2,2) &= 1 - \frac{1}{2} - \frac{1}{9} = \frac{7}{18}. \\
P(3,2) &= \frac{1}{2} \cdot 1 = \frac{1}{2}, & P(3,4) &= \frac{1}{2} \cdot \frac{1}{12} = \frac{1}{24}, & P(3,3) &= 1 - \frac{1}{2} - \frac{1}{24} = \frac{11}{24}. \\
P(4,3) &= \frac{1}{2} \cdot 1 = \frac{1}{2}, & P(4,4) &= \frac{1}{2}.
\end{aligned}$$

Hence, with state order 0, 1, 2, 3, 4,

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{3}{8} & \frac{7}{18} & \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{9} & \frac{1}{24} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{11}{24} & \frac{1}{24} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

Part C:

To show reversibility, we verify the detailed balance equations:

$$\pi(i)P(i,j) = \pi(j)P(j,i) \quad \text{for all } i, j.$$

Since transitions only occur between neighbors, it suffices to check the pairs (0, 1), (1, 2), (2, 3), (3, 4).

Pair (0, 1).

$$\pi(0)P(0,1) = \frac{81}{256} \cdot \frac{1}{2} = \frac{81}{512}, \quad \pi(1)P(1,0) = \frac{27}{64} \cdot \frac{3}{8} = \frac{81}{512}.$$

Pair (1, 2).

$$\pi(1)P(1,2) = \frac{27}{64} \cdot \frac{1}{4} = \frac{27}{256}, \quad \pi(2)P(2,1) = \frac{27}{128} \cdot \frac{1}{2} = \frac{27}{256}.$$

Pair (2, 3).

$$\pi(2)P(2,3) = \frac{27}{128} \cdot \frac{1}{9} = \frac{27}{1152}, \quad \pi(3)P(3,2) = \frac{3}{64} \cdot \frac{1}{2} = \frac{3}{128} = \frac{27}{1152}.$$

Pair (3, 4).

$$\pi(3)P(3,4) = \frac{3}{64} \cdot \frac{1}{24} = \frac{3}{1536} = \frac{1}{512}, \quad \pi(4)P(4,3) = \frac{1}{256} \cdot \frac{1}{2} = \frac{1}{512}.$$

Thus detailed balance holds for all possible moves, so the chain is reversible with respect to π . Finally, detailed balance implies stationarity: for each j ,

$$\sum_i \pi(i)P(i,j) = \sum_i \pi(j)P(j,i) = \pi(j) \sum_i P(j,i) = \pi(j),$$

so $\pi P = \pi$.

Exercise 5.18

A random variable X has density function, defined up to proportionality,

$$f(x) \propto e^{-(x-1)^2/2} + e^{-(x-4)^2/2}, \quad 0 < x < 5.$$

Implement a Metropolis–Hastings algorithm for simulating from the distribution. Use your algorithm to approximate the mean and variance of X .

Solution:

Input:

Listing 1: Metropolis-Hastings algorithm

```

1 ### Exercise 5.18
2
3 trials <- 1e6
4 sim <- numeric(trials)
5 sim[1] <- 2.45

```

```

6
7 # unnormalized target density on (0,5)
8 f_unnorm <- function(x) exp(-0.5 * (x - 1)^2) + exp(-0.5 * (x - 4)^2)
9
10 for (i in 2:trials) {
11   old <- sim[i - 1]
12   prop <- runif(1, 0, 5) # independence proposal q(prop) = Uniform(0,5)
13
14   acc <- f_unnorm(prop) / f_unnorm(old)
15   acc <- min(1, acc) # acceptance probability
16
17   sim[i] <- if (runif(1) < acc) prop else old
18 }
19
20 burn <- 10000
21 x <- sim[(burn + 1):trials]
22
23 mean(x)
24 var(x)

```

Output: Mean of 2.496 and Variance of 2.099.

Exercise 5.19

Implement the algorithm in Exercise 5.7 for $n = 50$ and $p = \frac{1}{4}$. Use your simulation to estimate

$$P(10 \leq X \leq 15),$$

where X has the given binomial distribution. Compare your estimate to the exact probability.

Solution

Input:

Listing 2: Metropolis-Hastings algorithm

```

1 ### Exercise 5.19
2
3 trials <- 1e6
4 n <- 50
5 p <- 1/4
6
7 sim <- numeric(trials)
8
9 for (k in 1:trials) {
10   state <- 0
11
12   # run chain for 60 steps to be near stationarity
13   for (i in 1:60) {
14     y <- sample(0:n, 1) # proposal: Uniform over {0,1,...,n}
15
16     # log acceptance ratio:
17     # [C(n,y) p^y (1-p)^(n-y)] / [C(n,state) p^state (1-p)^(n-state)]
18     log_acc <- (lchoose(n, y) - lchoose(n, state)) +
19       (y - state) * log(p / (1 - p))
20
21     acc <- min(1, exp(log_acc))
22
23     if (runif(1) < acc) state <- y
24   }
25
26   sim[k] <- as.integer(state >= 10 && state <= 15)
27 }
28
29 mean(sim) # estimate of P(10 <= X <= 15)
30
31 pbinom(15,n,p)-pbinom(9,n,p)

```

Output: Estimate = 0.671, Exact = .673