

# Markov Chain Monte Carlo

As the question, the Markov Chain Monte Carlo in Metropolis-Hastings algorithm with probability density function given

$$f(x) = \frac{1}{2} \exp(-|x|)$$

where  $x$  takes values in the real line and  $|x|$  denotes the absolute value of  $x$  to generate  $x_1, x_1, \dots, x_N$

Because  $|x|$  reaches its minimum value of 0 at  $x = 0$ ,  $\exp(-|x|)$  reaches its maximum value of 1 at this point.

Thus,  $f(x)$  reaches its maximum value of  $\frac{1}{2}$  at  $x = 0$ . Theoretically, this distribution is symmetric about  $x = 0$ , with the shape on both sides of the distribution being mirror images of each other. The tails of the Laplace distribution decay faster than those of a normal distribution, and the Laplace distribution is sharper near the center.

First, conceptualize this distribution: The Laplace probability density function is defined as

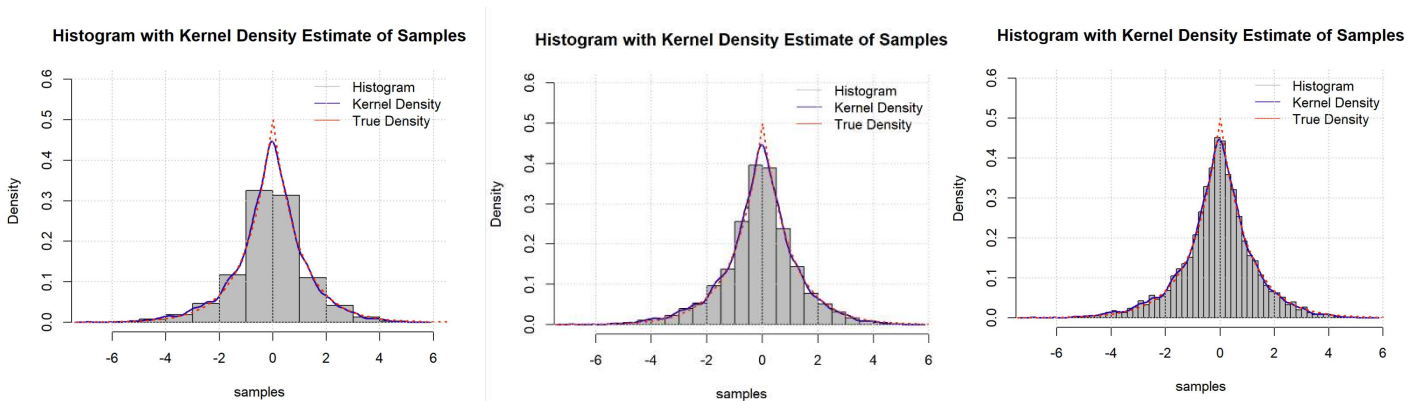
$$f(x) = \frac{1}{2b} \exp\left(-\frac{|x - \mu|}{b}\right)$$

where  $\mu$  is the location parameter here is equal to 0, and  $b$  is the scale parameter as 1, which is very similar to the given function. Therefore, the peak at  $x = 0$ .

## (a) Converged random walk Metropolis algorithm

In this plot, a histogram and a kernel density were constructed using the *random walk Metropolis algorithm*, with  $N$  set to 10000 and  $s$  set to 1. We used the generated samples  $(x_1, \dots, x_N)$ , and these plots provide estimates of  $f(x)$ .

The first histogram does not show an obvious concentration trend, although the high peak in the middle suggests a



concentration of data near zero. However, there is also a relatively large amount of data on both sides, making the overall distribution appear quite flat. However, more detail may also introduce noise issues, so it is more reasonable to use a break of 50. After increasing the number of groups, the middle graph, the histogram shows a clearer bimodal distribution, which may indicate that the sample data consists of two main clusters, each clustered around a central value. The right-side histogram and the kernel density estimate match very well, showing a clear unimodal trend with the peak at zero, indicating that most of the data is tightly clustered around zero.

```
> cat(" Monte Carlo estimates Mean:", sample_mean, "\n")  
Monte Carlo estimates Mean: -0.08561803
```

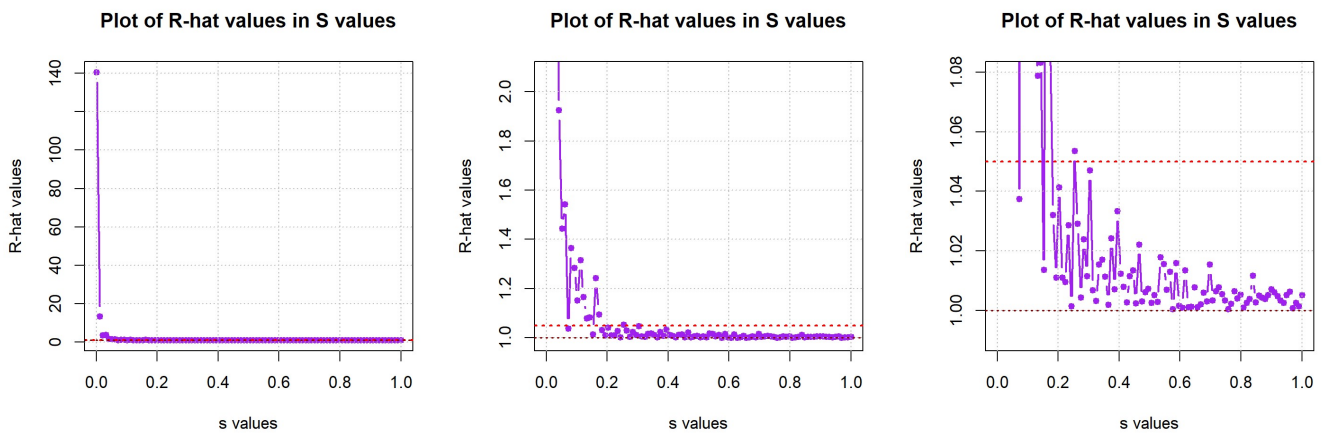
```
> cat(" Montecarlo estimates Standard Deviation:",  
sample_sd, "\n")  
Montecarlo estimates Standard Deviation: 1.348437
```

## (b) Diagnostics in Convergence by $\hat{R}$ value.

In general, values of  $(\hat{R})$  close to 1 indicate *convergence*, and it is usually desired for  $(\hat{R})$  to be lower than 1.05. Calculate the  $(\hat{R})$  for the Random Walk Metropolis algorithm with  $N = 2000$ ,  $s = 0.001$  and  $J = 4$ .

$$\begin{array}{l} M_j = \frac{1}{N} \sum_{i=1}^N x_i^{(j)} \\ V_j = \frac{1}{N} \sum_{i=1}^N (x_i^{(j)} - M_j)^2 \end{array} \quad \left| \quad \begin{array}{l} W = \frac{1}{J} \sum_{j=1}^J V_j \\ M = \frac{1}{J} \sum_{j=1}^J M_j \end{array} \right| \quad \begin{array}{l} B = \frac{1}{J} \sum_{j=1}^J (M_j - M)^2 \\ \hat{R} = \sqrt{\frac{B + W}{W}} \end{array}$$

These three graphs illustrate the convergence behavior of the random walk Metropolis algorithm at different  $s$  values. As  $s$  increases, the  $\hat{R}$  value gradually decreases and stabilizes, particularly when  $s$  is above 0.5, where the  $\hat{R}$  value is closer to 1, indicating that the *algorithm* is nearing *convergence*.



The first graph shows the overall trend of  $\hat{R}$  values as  $s$  ranges from 0 to 1. It can be seen that when  $s$  is small, the  $\hat{R}$  value is very high; as  $s$  *increases*, the  $\hat{R}$  value drops rapidly and remains low and stable for most of the  $s$  range. The second graph provides a more detailed depiction of the changes in  $\hat{R}$  values in the low  $s$  region. It shows that when  $s$  is extremely small, the  $\hat{R}$  value fluctuates significantly, but as  $s$  increases, these fluctuations gradually diminish and tend to *stabilize* around a level close to the *convergence* criterion (*around 1.05*). The third graph focuses on a narrower range of  $\hat{R}$  values (*from 1.0 to 1.08*), magnifying the subtle changes, thereby more intuitively reflecting the variations within a specific  $s$  value interval.