Institute for Cross-Disciplinary Physics and Complex

Task 2

Simulation Methods

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1 Exercise 47

We want to design a rejection method in order to generate random values according to the pdf

$$f_{\hat{x}}(x) = \frac{x^{\alpha-1}e^{-x}}{\Gamma(\alpha)} \quad 0 \leq x \tag{1}$$

For $0 < \alpha < 1$ we aim to find a decomposition of the form $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$ where $0 \leq h(x) \leq 1$ and $g_{\hat{x}}(x)$ is another pdf. This task is more intricate than it might appear due to the divergence of the term $x^{\alpha-1}$ at $x = 0$. Consequently, it's clear that we must avoid this divergence in the probability function $h(x)$. However, if we were to choose $h(x) = e^{-x}$ and $g_{\hat{x}}(x) \propto x^{\alpha-1}$, then $g_{\hat{x}}(x)$ cannot be properly normalized over the entire interval $0 \leq x$. After this initial analysis, we realize that we need to account for different behaviors of the functions in various parts of the interval. This insight leads us to propose the following functions:

$$g_{\hat{x}}(x) = \frac{1}{C}\begin{cases} \frac{x^{\alpha-1}}{\Gamma(\alpha)} & \text{if } 0 \leq x \leq 1 \\ \frac{e^{-x}}{\Gamma(\alpha)} & \text{if } 1 < x \end{cases} \qquad h(x) = \begin{cases} e^{-x} & \text{if } 0 \leq x \leq 1 \\ x^{\alpha-1} & \text{if } 1 < x \end{cases} \tag{2}$$

where C is a normalization constant and it can be easily checked that $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$. The normalization constant can be easily calculated

$$\int_0^\infty g_{\hat{x}}(x)dx = \int_0^1 \frac{x^{\alpha-1}}{C\Gamma(\alpha)}dx + \int_1^\infty \frac{e^{-x}}{C\Gamma(\alpha)}dx = \frac{1}{C\Gamma(\alpha)}\left(\frac{1}{\alpha} + \frac{1}{e}\right) = 1. \tag{3}$$

Thus, $C = \frac{\alpha+e}{\Gamma(\alpha+1)e}$. Now, we need to generate random numbers according to $g_{\hat{x}}(x)$. In order to do that, we have calculated the cumulative distribution obtaining

$$G_{\hat{x}}(x) = \int_0^x g_{\hat{x}}(x')dx' = \frac{1}{C}\begin{cases} \frac{x^{\alpha}}{\Gamma(\alpha+1)} & \text{if } 0 \leq x \leq 1 \\ \frac{1}{\Gamma(\alpha)}\left(\frac{1}{\alpha} + \frac{1}{e} - e^{-x}\right) & \text{if } 1 < x \end{cases}. \tag{4}$$

Let $u = G_{\hat{x}}(x)$ where u is a $\hat{U}(0,1)$ random number. Then, we just need to invert the cumulative distribution $G_{\hat{x}}(x)$ to obtain x. This leads us to

$$x = \begin{cases} (uC\Gamma(\alpha+1))^{\frac{1}{\alpha}} & \text{if } 0 \leq u \leq G_{\hat{x}}(x=1) \\ -\ln\left(-uC\Gamma(\alpha) + \frac{1}{\alpha} + \frac{1}{e}\right) & \text{if } G_{\hat{x}}(x=1) < x \leq 1 \end{cases} \tag{5}$$

where the partition is obtained by calculating $G_{\hat{x}}(x=1)$ which depends on α. So, for generating random numbers according to the gamma distribution given by Eq. (1), we need to generate random numbers according to $g_{\hat{x}}(x)$ by using Eq. (5) and accept them with probability $h(x)$. We will use rejection with repetition. Result of the histogram obtained using this method is shown in Figs. 1, 2 and 3.

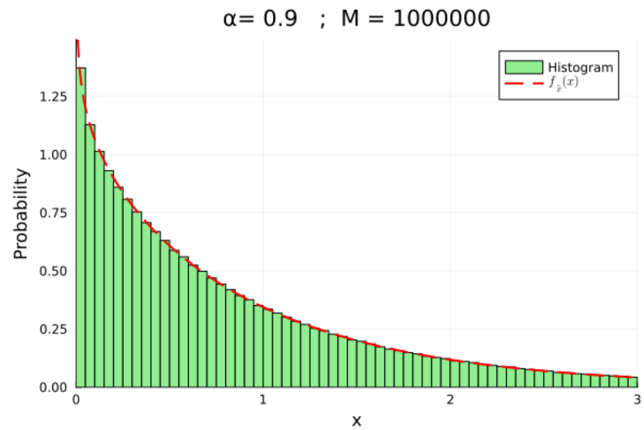

Figure 1: Histogram for $M = 10^6$ random numbers generated according to $f_{\hat{x}}(x)$ using $\alpha = 0.9$.

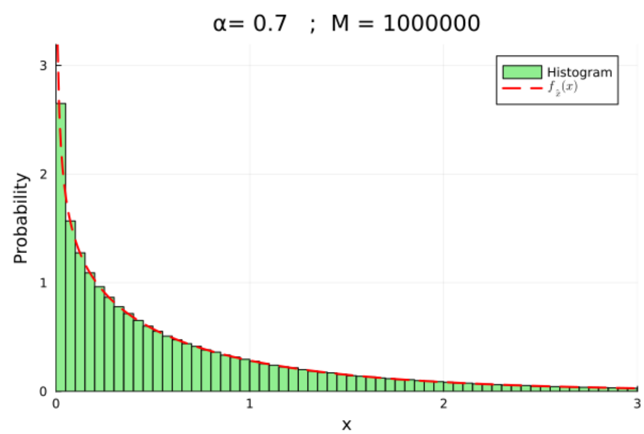

Figure 2: Histogram for $M = 10^6$ random numbers generated according to $f_{\hat{x}}(x)$ using $\alpha = 0.7$.

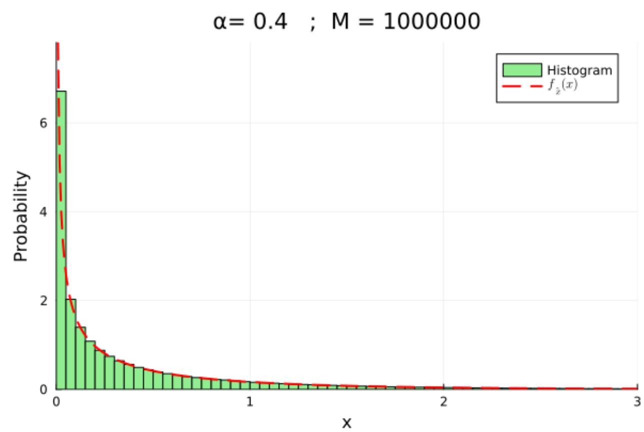

Figure 3: Histogram for $M = 10^6$ random numbers generated according to $f_{\hat{x}}(x)$ using $\alpha = 0.4$.

2 Exercise 49

We want to design a rejection method in order to generate random values according to the pdf

$$f_{\hat{x}}(x) = Ce^{-\frac{1}{2}x^2 - x^4} \tag{6}$$

so we propose the following decomposition of the form $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$

$$g_{\hat{x}}(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}} \qquad h(x) = e^{-x^4} \tag{7}$$

where $0 \leq h(x) \leq 1$ and $g_{\hat{x}}(x)$ is another pdf. Thus, the idea is to generate random numbers according to $g_{\hat{x}}(x)$ and accept them with probability $h(x)$. For obtaining the normalization constant we do the following calculation

$$\int_{-\infty}^{\infty} f_{\hat{x}}(x) = 1 \quad \longrightarrow \quad \sqrt{2\pi}C\int_{-\infty}^{\infty} g_{\hat{x}}(x)h(x) = 1 \quad \longrightarrow \quad C = \frac{1}{\epsilon\sqrt{2\pi}} \tag{8}$$

where ϵ is the acceptance probability given by the integral of $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$. Using the HCubature package for doing the numerical integration [1], we obtain

$$\begin{aligned} \epsilon &= 0.620282559595(39) \\ C_\epsilon &= 0.643162175416(40) \\ C_f &= 0.643162175415(16) \end{aligned} \tag{9}$$

where C_ϵ is the constant obtained by using the acceptance probability and C_f is computed directly by just integrating $f_{\hat{x}}(x)$. We see that the results are almost identical. Result of the histogram obtained using this method is shown in Fig. 4.

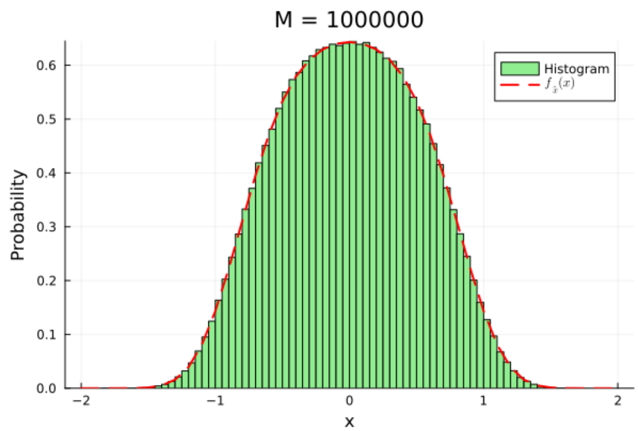

Figure 4: Histogram for $M = 10^6$ random numbers generated according to $f_{\hat{x}}(x)$.

3 Exercise 50

We want to design a rejection method in order to generate random values according to the pdf

$$f_{\hat{x}}(x) = Ce^{-\frac{1}{2}x^2 - x^4} \tag{10}$$

so we propose the following decomposition of the form $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$

$$g_{\hat{x}}(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}} \qquad h(x) = C'e^{x^2 - x^4} \tag{11}$$

where $0 \leq h(x) \leq 1$ and $g_{\hat{x}}(x)$ is another pdf. In order to fulfill the condition $0 \leq h(x) \leq 1$, we must obtain C' by calculating the maximun of the corresponding exponential

$$\frac{d}{dx}(e^{x^2 - x^4}) = 0 \quad \longrightarrow \quad x_{max} = \pm\sqrt{\frac{1}{2}} \quad \longrightarrow \quad h(x_{max}) = e^{1/4}. \tag{12}$$

Thus, $C' = e^{-1/4}$. For obtaining the normalization constant we do the following calculation

$$\int_{-\infty}^{\infty} f_{\hat{x}}(x) = 1 \quad \longrightarrow \quad \frac{\sqrt{2\pi}C}{C'} \int_{-\infty}^{\infty} g_{\hat{x}}(x)h(x) = 1 \quad \longrightarrow \quad C = \frac{C'}{\epsilon\sqrt{2\pi}} \tag{13}$$

where ϵ is the acceptance probability given by the integral of $f_{\hat{x}}(x) \propto g_{\hat{x}}(x)h(x)$. Using the HCubature package for doing the numerical integration [1], we obtain

$$\begin{aligned} \epsilon &= 0.6795241611(15) \\ C_\epsilon &= 0.4572266568(13) \\ C_f &= 0.4572266568(10) \end{aligned} \tag{14}$$

where C_ϵ is the constant obtained by using the acceptance probability and C_f is computed directly by just integrating $f_{\hat{x}}(x)$. We see that the results are almost identical. Result of the histogram obtained using this method is shown in Fig. 5.

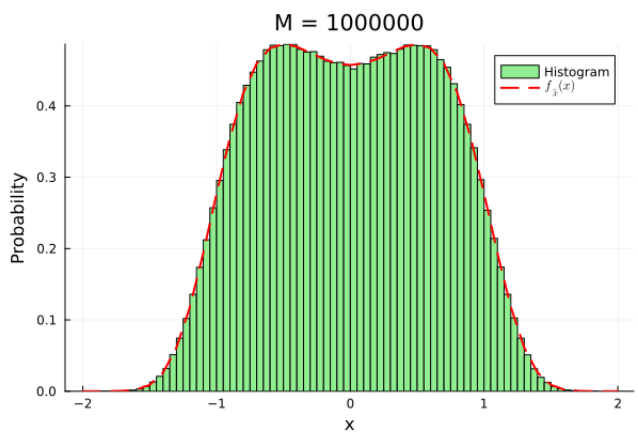

Figure 5: Histogram for $M = 10^6$ random numbers generated according to $f_{\hat{x}}(x)$.

References

[1] Julia: HCubature Package