PHYS 3142 HW 6

Due date: 11:59 PM 27^{th} Mar. 2022

- Submit a report that includes your results and your python scripts
- Make sure your code can run
- Write comments in your code
- If you submit the assignment after the deadline or the report is missing, you can only get at most 80% of the full marks.
- If there is any kind of plagiarism, all students involved will get zero marks.

1 Monte Carlo integration for improper integral (80 points)

Integrate the following integral with the three types of Monte Carlo integration.

$$I = \int_0^1 \frac{\sqrt{\sin x}}{x} dx \tag{1}$$

First, plot histograms to show the distribution of the two types of random numbers, use 10^6 many sampling. Then, use 100 sampling of random numbers to estimate I. Repeat this for 50000 times (50000 different estimates of I) to evaluate the standard deviation σ. Plot the estimates of I as histograms (e.g., with `plt.hist`) for the two types of random numbers specified below.

Define the bins uniformly with keyword argument `bins = np.linspace( np.min(data),` `np.max(data), 501 )`, where `data` is either the sampling of random numbers or a list containing the estimates of I. And use `plt.vlines` to draw two grey vertical lines at $x = \mu - \sigma_{\bar{x}}$ and $x = \mu + \sigma_{\bar{x}}$, where μ is the average of the 50000 estimates of I, $\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{100}}$ is the standard deviation. You can use a value smaller than 50000 the computation time is too long. And draw a vertical red line to indicate the accurate solution obtained using `scipy.integrate.quad`. Use $(\mu - 2\sigma, \mu + 2\sigma)$ as the range for the x axis.

1.a. Use uniform random numbers. From the histogram, does the true value lie between $x = \mu - \sigma_{\bar{x}}$ and $x = \mu + \sigma_{\bar{x}}$?

1.b. Use nonuniform random numbers with $w(x) = \frac{1}{\sqrt{x}}$. From the histogram, does the true value lie between $x = \mu - \sigma_{\bar{x}}$ and $x = \mu + \sigma_{\bar{x}}$? In addition to the plot, write down $\sigma^a_{\bar{x}}/\sigma^b_{\bar{x}}$. $\sigma^a_{\bar{x}}$ is the standard error obtained in part a using uniform random numbers and $\sigma^b_{\bar{x}}$ is the standard error for nonuniform random numbers.

1.c. Use the Metropolis algorithm with $p(x) = \frac{1}{\sqrt{x}}$. If the integrand is $f(x)$, then the mean value is for $g(x) = \frac{f(x)}{p(x)}$. From the histogram, does the true value lie between $x = \mu - \sigma_{\bar{x}}$ and $x = \mu + \sigma_{\bar{x}}$? In addition to the plot, write down $\sigma^a_{\bar{x}}/\sigma^c_{\bar{x}}$. $\sigma^a_{\bar{x}}$ is the standard error obtained in part a using uniform random numbers and $\sigma^c_{\bar{x}}$ is the standard error for Metropolis algorithm.

In total, you need to include 5 figures for Q1, sampling of uniform random numbers, that for the non-uniform random numbers and 3 more histograms for the integration in 1.a to 1.c. One histogram is given below for reference.

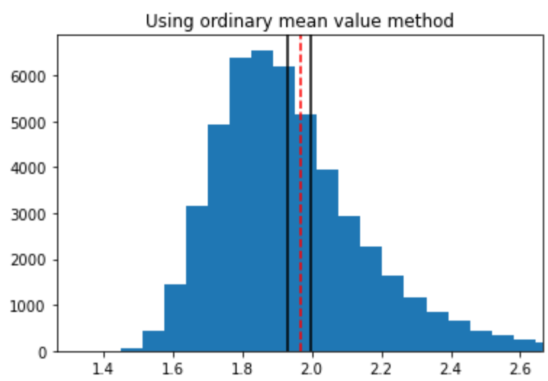

FIG. 1 The histogram of the Monte Carlo integration using uniform sampling. The integrand and the parameters for plotting are chosen to show the asymmetry of the distribution.

2 Detailed balance principle in Metropolis algorithm (20 points)

In Metropolis algorithm, the transition matrix is

$$T(x_i \to x_j) = \min\left\{1, \frac{p(x_j)}{p(x_i)}\right\} \tag{2}$$

2.a. Given a distribution

$$p = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \tag{3}$$

with $a_1 < a_2 < a_3$. Use the Metropolis algorithm to write down the transition matrix. Show that this obeys the detailed balance principle for $(i, j) = (1, 2), (2, 3), (1, 3)$.

2.b. Show that in general, the Metropolis algorithm obeys the detailed balance principle.

$$T(x_i \to x_j)p(x_j) = T(x_j \to x_i)p(x_i) \tag{4}$$

Optional

3 Detailed balance principle and balance principle (10 points)

The detailed balance principle is a sufficient but not a necessary condition for the balance principle. Meaning that if the detailed balance principle is valid, the balance principle must be true. But the balance principle can be valid even if the detailed balance principle is violated. For a system with the distribution

$$p = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} \tag{5}$$

Write down two matrices (denote as A and B), A satisfies the detailed balance principle $T_{ij}p(x_j) =$

$T_{ji}p(x_i)$ and B does not. And restrict the elements to be only $0, \frac{1}{6}, \frac{1}{3}, \frac{1}{2}$, or $\frac{2}{3}$ to simplify your guesses. Show that both matrices describe Markov chains as they are required to satisfy these conditions:

1. They are stochastic matrices, each column add up to 1, $\sum_{i=1}^{3} T_{ij} = 1$.

2. They obey the ergodic condition, for some power n (e.g. 2), show that all elements in T^n are nonzero.

3. They both satisfy the balance principle, $Tp = p$.

Note that you cannot just use the Metropolis algorithm to obtain the transition matrix.