A Wave Function

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1 Finding the probability of where a particle lies: A Wave Function Problem

DRAFT

Define the wave $\psi(x)$ function as:

$$\psi(x) = \begin{cases} 0 & if x < 0 \\ ce^{-x/L} & if x \geq 0 \end{cases}$$

Given the condition that $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$.
We can break the integral into two parts:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{0^-} |\psi(x)|^2 dx + \int_{0}^{\infty} |\psi(x)|^2 dx$$

The first integral is zero, as it comes from the definition of $\psi(x)$ where $\psi(x) = 0$ for $x < 0$. This simplifies the condition to an improper integral. Let's assume an arbitrary condition that $L = 1$.

We can integrate the function as follows:

$$\lim_{t\to\infty} \int_0^t |ce^{-x}|^2 dx = 1$$

$$c^2 \lim_{t\to\infty} \int_0^t e^{-2x} dx = 1$$

$$c^2 \lim_{t\to\infty} \left[-\frac{1}{2} e^{-2x} \right]_0^t = 1$$

$$c^2 \lim_{t\to\infty} \left(-\frac{1}{2} e^{-2t} - \left(-\frac{1}{2} e^0 \right) \right) = 1$$

$$c^2 \left(-\frac{1}{2}(0) - \left(-\frac{1}{2}(1) \right) \right) = 1$$

$$c^2 \left(\frac{1}{2} \right) = 1$$

$$\frac{c^2}{2} = 1$$
$$c^2 = 2$$

Therefore, $c = \sqrt{2}$. (Note: Since $|\psi(x)|^2$ is involved, c can be $\sqrt{2}$ or $-\sqrt{2}$. For simplicity, we usually take the positive root for normalization constants unless specified.)

For $L = 1$, if we choose $c = \sqrt{2}$, then $\psi(x) = \sqrt{2}e^{-x}$ for $x \geq 0$.

Numerically, we will use Monte Carlo simulations in Python with this probability density function (PDF) to estimate the probability of a particle being found in the region $x \geq 1nm$.

Analytically, to find the probability of the particle being found when $x \geq 1nm$, we set the lower bound of the integral to 1 and repeat the calculation from above. That is, we compute:

$$P(x \geq 1nm) = \lim_{t\to\infty} \int_1^t \left|\sqrt{2}e^{-x}\right|^2 dx$$

We proceed with the integration:

$$\lim_{t\to\infty} \int_1^t 2e^{-2x} dx$$

$$= 2 \lim_{t\to\infty} \left[-\frac{1}{2}e^{-2x}\right]_1^t$$

$$= 2 \lim_{t\to\infty} \left(-\frac{1}{2}e^{-2t} - \left(-\frac{1}{2}e^{-2(1)}\right)\right)$$

$$= 2\left(-\frac{1}{2}(0) + \frac{1}{2}e^{-2}\right)$$

$$= e^{-2} \approx 0.135335283237$$

Thus, there is approximately a 13.53% probability of finding the particle when $x \geq 1nm$.

Using SciPy quad integrate in python, we want to find the upper limit, t, such that the integral of the PDF is .1328451140, the probability after running the Monte Carlo simulation with 5,000 randomized points using the Halton algorithm in Python when x ranges from 1 to 3 in the Monte Carlo simulation.

Suppose we do not know the upper limit of the integral (expected result ≈ 3).

Thus we want to find a real-value, t, such that:

$$\int_1^t 2e^{-2x} dx = .1328451140$$

$$= 2\left(-\frac{1}{2}e^{-2t} + \frac{1}{2}e^{-2}\right) = .1328451140$$

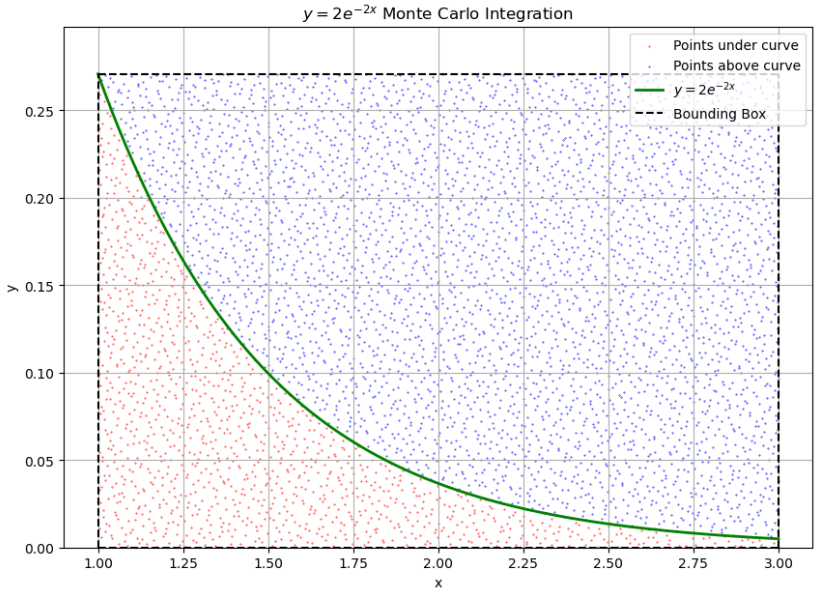

Figure 1: Monte Carlo simulation of PDF for n=5,000

$$= -e^{-2t} + e^{-2} = .1328451140$$

Solving this equation for t:

$$-e^{-2t} = .1328451140 - e^{-2}$$
$$e^{-2t} = -.1328451140 + e^{-2}$$
$$-2t = ln(-.1328451140 + e^{-2})$$
$$t = \frac{-ln(-.1328451140 + e^{-2})}{2} \approx 2.997702302$$

Thus, the integral

$$\int_1^t 2e^{-2x}dx \approx .1328451140$$

when

$$t \approx 2.997702302$$

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The relative error for this Monte Carlo simulation is

$$\approx .00859\%$$

The relative error for SciPy quad integrate over interval that gives the same PDF is $\approx 1.84\%$

We see that Monte Carlo simulation yields less relative error than SciPy quad integrate.

This gives us a comparison between two numerical methods of integration and the analytical calculation of the integral of the PDF. We can increase numerical precision of the Monte Carlo simulation by increasing the number of points, though marginally increasing the computational time for number of points less than 1,000,000 in the simulation.

References

[1] Slides and Python code edited from Dr. Biersach.

[2] Wikipedia. https://en.wikipedia.org/wiki/Exponential$_d istribution Exponential distribution$.

[3] Gemini AI for some code