Monte Carlo Integration Calculator

An Honors Project for Prof. Bognar's STAT:2020 by Aidan McGrane

The intuition behind Monte Carlo integration begins with the definition of the average value of a function f, which is given by:

$$\overline{f} = \frac{1}{b-a} \int_a^b f(x)dx$$

Our goal is to evaluate the integral, so we rearrange to get:

$$\int_a^b f(x)dx = (b-a) \cdot \overline{f}$$

So, we know that we can approximate the value of the integral by approximating the average value of the function.

The Monte Carlo approach to approximating $\overline{f}$ takes a sample of N uniformly distributed independent random points over the interval $[a, b]$.

For each random point $X_i \in [a, b]$, we evaluate the function values at these points, giving us $f(X_1), f(X_2), \ldots, f(X_N)$.

Taking the average of these function values provides our estimate of the true average function value, which can be described by:

$$\overline{f} \approx \frac{1}{N} \sum_{i=1}^{N} f(X_i)$$

> By the Law of Large Numbers, this sample mean approaches the true average function value as $N \to \infty$.

We can now update our previous integral formula to utilize this estimate, and we have the

Monte Carlo integration formula:

$$\int_a^b f(x)dx \approx (b-a) \cdot \frac{1}{N} \sum_{i=1}^{N} f(X_i)$$

Implementing this formula in Python is a straightforward process with four steps.

1. Generate N random points $X_1, X_2, \ldots, X_N$ uniformly in the interval $[a, b]$.
2. Evaluate $f(X_i)$ for each point X_i.
3. Compute the average of these function values.
4. Multiply by $(b - a)$ to approximate the integral.

In [2]:
```
import numpy as np
#function to be integrated
def f(x):
    return (np.sin(x)) #we'll try f(x) = sin(x)

#integrates f(x) from a to b using N random samples
def monteCarloIntegration(a, b, N):
    xrand = np.random.uniform(a, b, N)  #1
    fxrand = f(xrand)                   #2
    averagefx = np.sum(fxrand) / N      #3
    answer = (b - a) * averagefx        #4
    return answer
```

> Note: `np.random.uniform(a, b, N)` technically uses the interval $[a, b)$, but $P(X_i = b) = 0$ for $X_i \sim U[a, b]$ anyway, so this is fine.

Let's test it out! We know $\int_0^{2\pi} \sin(x)dx = 0$, so we can see how close our new calculator gets.

In [17]:
```
#inputs
a = 0
b = 2 * np.pi
N = 100000

monteCarloIntegration(a, b, N)
```

Out[17]:
```
np.float64(-0.019867451723017260)
```

That seems pretty good. However, "seems pretty good" for a single trial isn't a great measure of performance.

So, we will analyze our estimation by looking at its distribution.

Our Monte Carlo integration estimate is a random variable, given by $I \sim \mathcal{N}\left(\mu_I, \sigma_I^2\right)$.

> We know it follows a Normal distribution using the Central Limit Theorem, because our sample size N is much larger than 30, but we'll show it later.

Expected Value

Since each X_i is i.i.d., each $f(X_i)$ is also i.i.d., which means that

$\mathbb{E}\left[\sum_{i=1}^{N} f(X_i)\right] = N \cdot \mathbb{E}[f(X)]$.

So, the expected value of our integral estimate I is given by $\mathbb{E}[I] = (b-a) \cdot \mathbb{E}[f(X)]$.

This relationship can be summarized by:

$$\mathbb{E}[I] = \mu_I = (b-a) \cdot \mathbb{E}[f(X)] = \int_a^b f(x)dx$$

Variance

Since the variance of a sum of independent variables is the sum of their variances, it follows that

$\mathrm{Var}\left[\sum_{i=1}^{N} f(X_i)\right] = N \cdot \mathrm{Var}[f(X)]$.

I is defined as $I = (b-a) \cdot \frac{1}{N} \sum_{i=1}^{N} f(X_i)$ from our Monte Carlo integration formula.

Applying the property that $\mathrm{Var}[cX] = c^2 \mathrm{Var}[X]$ to this equation gives $\mathrm{Var}[I] = \left(\frac{b-a}{N}\right)^2 \cdot N \cdot \mathrm{Var}[f(X)]$, which simplifies to:

$$\mathrm{Var}[I] = \sigma_I^2 = \frac{(b-a)^2}{N} \cdot \mathrm{Var}[f(X)]$$

Distribution

We can now see that the distribution of I is given by:

$$I \sim \mathcal{N}\left(\mu_I = (b-a) \cdot \mathbb{E}[f(X)], \sigma_I^2 = \frac{(b-a)^2}{N} \cdot \mathrm{Var}[f(X)]\right)$$

μ_I equals the value of the integral of our function f, as desired.

Variance is equivalent to squared error, so we can define our error as $\sigma_I = \sqrt{\frac{(b-a)^2 \cdot \mathrm{Var}[f(X)]}{N}}$.

b, a, and $\mathrm{Var}[f(X)]$ are all constant values based on inputs, so we can define a constant c such that $c = (b-a)^2 \cdot \mathrm{Var}[f(X)]$.

This gives us $\sigma_I = \frac{\sqrt{c}}{\sqrt{N}}$.

Thus, it becomes clear that as we increase our sample size N, our error decreases at a rate proportional to $\sqrt{N}$.

Our convergence rate of I can therefore be described as

$$\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

Now, we have a fuller understanding of the accuracy of our Monte Carlo integration calculator.

Testing Results

With this computation done, we can now test to see if experimental results back up the answers we found.

Continuing with our example of $\int_0^{2\pi} \sin(x)dx$, we can run our calculator repeatedly, and see if results center around 0 and match our calculated variance.

We can calculate the variance of $\sin(x)$ over the interval $[0, 2\pi]$ as follows:

$$\begin{aligned}
\mathbb{E}[f(X)^2] &= \frac{1}{b-a}\int_a^b f^2(x)dx &&= \frac{1}{b-a}\int_a^b \sin^2(x)dx &&= \frac{1}{2} \quad (1)\\
(\mathbb{E}[f(X)])^2 &= \left(\frac{1}{b-a}\int_a^b f(x)dx\right)^2 &&= \left(\frac{1}{b-a}\int_a^b \sin(x)dx\right)^2 &&= 0 \quad (2)\\
\text{Var}[f(X)] &= \mathbb{E}[f(X)^2] - (\mathbb{E}[f(X)])^2 &&= \frac{1}{2} - 0 &&= \frac{1}{2} \quad (3)
\end{aligned}$$

Now, we can find the variance of our integral estimate I as:

$$\sigma_I^2 = \frac{(b-a)^2}{N} \cdot \text{Var}[\sin(X)] = \frac{4\pi^2}{100000} \cdot \frac{1}{2} = \frac{\pi^2}{50000} \approx 0.000197392$$

So, we can write our distribution for I for $\sin(x)$ as:

$$I \sim \mathcal{N}\left(\mu_I = 0, \sigma_I^2 = 0.000197392\right)$$

Let's check if our calculator closely matches this over 1000 trials.

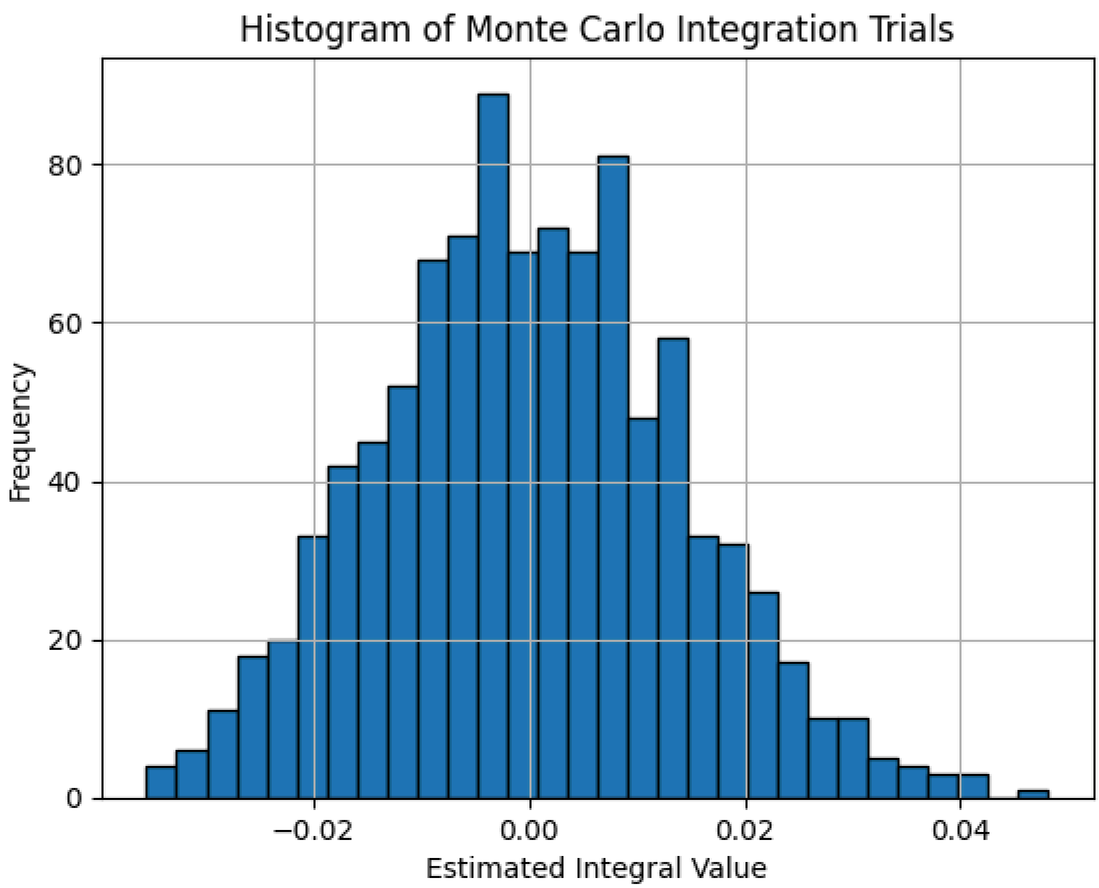
In [40]:
```
#same inputs as before
trials = np.zeros(1000)
for i in range(1000):
    trials[i] = monteCarloIntegration(a, b, N)
```

```python
print("mean: ")
print(np.mean(trials))
print("var: ")
print(np.var(trials))
```

```
mean: 
3.6169760003265215e-05
var: 
0.00019692474804538764
```

We can see that it does!

In [41]:
```python
import matplotlib.pyplot as plt
#plot histogram
plt.hist(trials, bins=30, edgecolor='black')
plt.title("Histogram of Monte Carlo Integration Trials")
plt.xlabel("Estimated Integral Value")
plt.ylabel("Frequency")
plt.grid(True)
plt.show()
```



Plotting our trials confirms our results visually, as we can clearly see a Normal Distribution curve centered around 0.

Additionally, this Normal curve supports our use of the Central Limit Theorem!