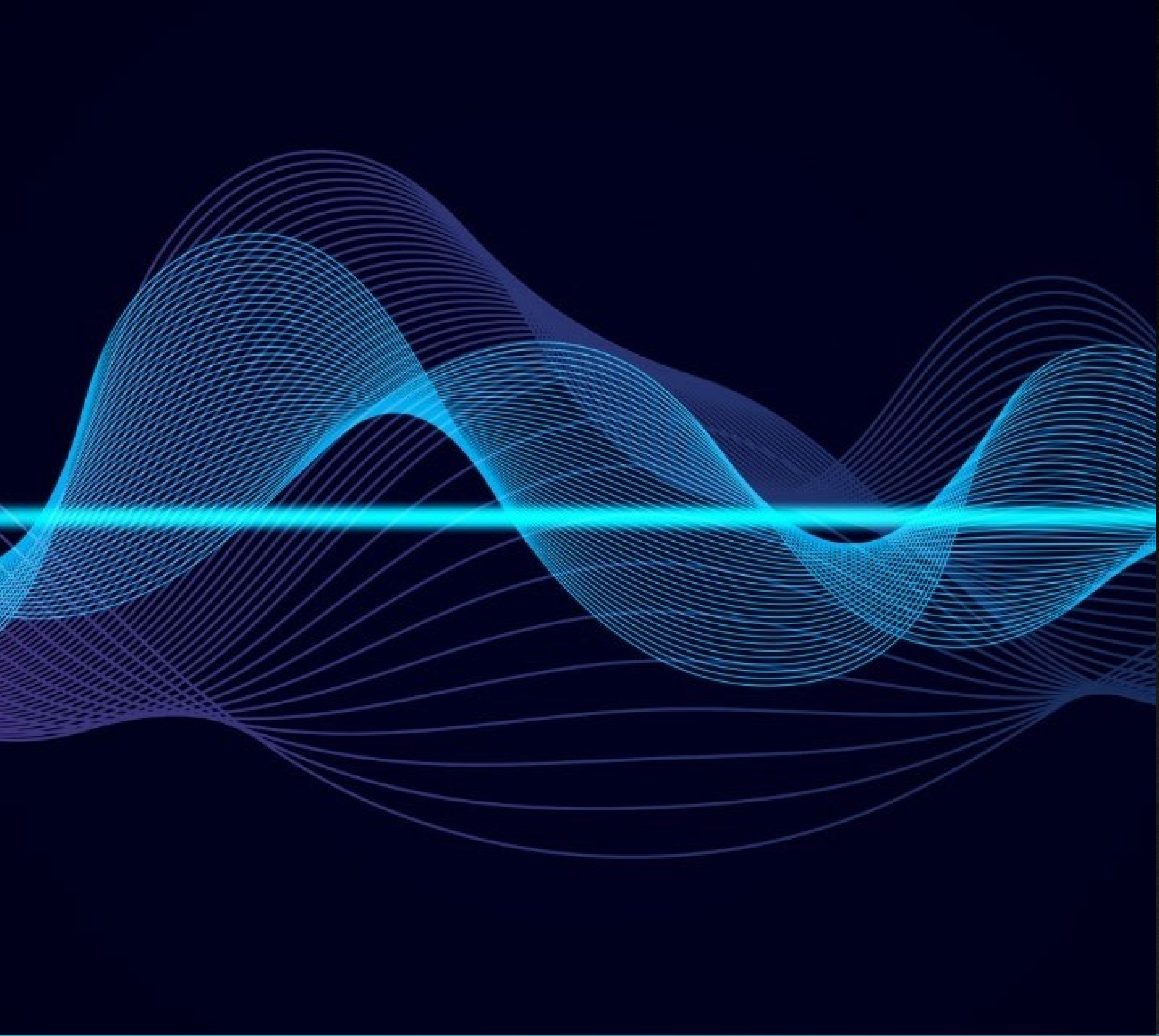


Computational Physics

PHYS 6260

Monte Carlo Integration

Announcements:

- HW4: Due Friday 2/7
- HW5: Due Friday 2/14
- Traveling next week. Will post recorded lectures on Teams.

Lecture Outline

We will cover these topics

- Basic Monte Carlo integration
- Mean value method
- Importance sampling

Monte Carlo Integration

- In the last class, we used Rutherford scatterings as an example for a calculation with randomness
- In essence, we were performing an integral to determine what fraction of particles were within some radius b

$$\frac{1}{\sigma^2}\int_0^b \exp\left(-\frac{r^2}{2\sigma^2}\right) r dr = 1 - \exp\left(-\frac{b^2}{2\sigma^2}\right)$$

$$= 1 - \exp\left(-\frac{Z^2 e^4}{8\pi^2\epsilon_0^2\sigma^2 E^2}\right) \simeq 0.156\%$$

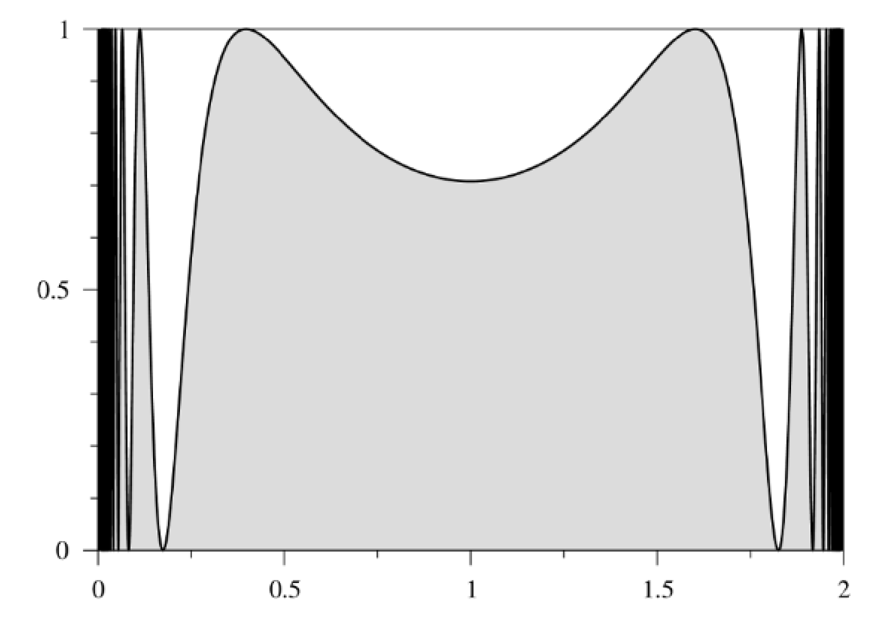
- We can model a system that has an analytical result by modeling it with random numbers
- This is a deep result

Monte Carlo Integration

- Let's do an example with an ill-behaved function

$$f(x) = \sin^2\left[\frac{1}{2(2-x)}\right]$$

- Integrate from x = 0 → 2
- Rapidly varies near the integration limits
- Notice that the function is bounded by y = [0,1]
- We can choose N random numbers within this rectangle with area A = 2
- Count how many (k) points lie below the function
- This ratio k/N should approach the integral I / A
- Thus $I \simeq kA/N$

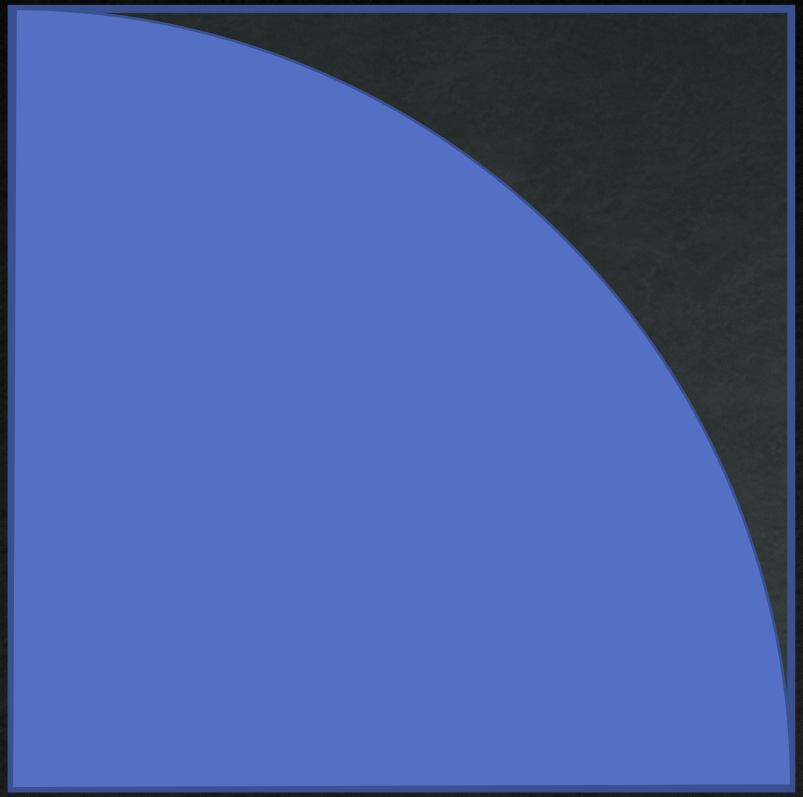



```python
from numpy.random import random
import numpy as np

def f(x):
    return (np.sin(1.0/(x*(2-x))))**2

N = 10000
x = 2*random(N)
y = random(N)
count = np.sum(y < f(x))
I = 2.0*count/N
print(I)
```

Monte Carlo Integration

In-class problem

- Classic problem: calculate π with Monte Carlo Integration
- Consider a quarter-circle with radius 1 in the 1st quadrant [x,y] = [0,0] → [1,1]
- Create a program from scratch to calculate π by choosing N random numbers
- Create a plot that shows the progression of your π estimate with respect to N (increase it by factors of 10, for example)



Monte Carlo Integration

- The problem with MC integration is that it's not accurate, even if we increased N dramatically. Let's inspect how the accuracy increases with N
- The probability that a point lies beneath the curve is p = I/A, where I is the integral and A is the domain area
- The probability that k and N-k points are beneath and above the curve is $p^k(1-p)^{N-k}$
- There are ${}_N C_k$ ways to choose k out of N points. So the total probability P(k) that we get exactly k points below the curve is

$$P(k) = \binom{N}{k} p^k (1-p)^{N-k}$$

- This is the binomial distribution

Monte Carlo Integration

$$P(k) = \binom{N}{k} p^k (1-p)^{N-k}$$

- The variance of a binomial distribution is

$$\sigma^2 = var(k) = Np(1-p) = N\frac{I}{A}\left(1 - \frac{I}{A}\right)$$

- Recall from our original example that the integral $I \simeq kA/N$
- Relate this to the error of the integral

Error = $\frac{\sigma_k A}{N} = \sqrt{\frac{I(A-I)}{N}}$

- The error decreases as $N^{-1/2}$
- This is much worse than any other integration method

Mean value method

- This most basic MC method may not give accurate results, but there are other methods that are more accurate
- The most common one is called the mean value method
- Calculates the average value of a function f(x) over the integration range

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

- This leads to $I = (b-a)\langle f \rangle = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$
- We can calculate the average value by taking random or uniform x-values

Mean value method

- This method is more accurate for slowly varying functions
- We can calculate the integration error from its variance

$$var(f) = \langle f^2 \rangle - \langle f \rangle^2$$

- The variance of the average (sum/N) is N times the variance of a single term, N*var(f), and the standard deviation (error) is the square root of it

$$\sigma = \frac{b-a}{N}\sqrt{N\,var(f)} = (b-a)\sqrt{\frac{var(f)}{N}}$$

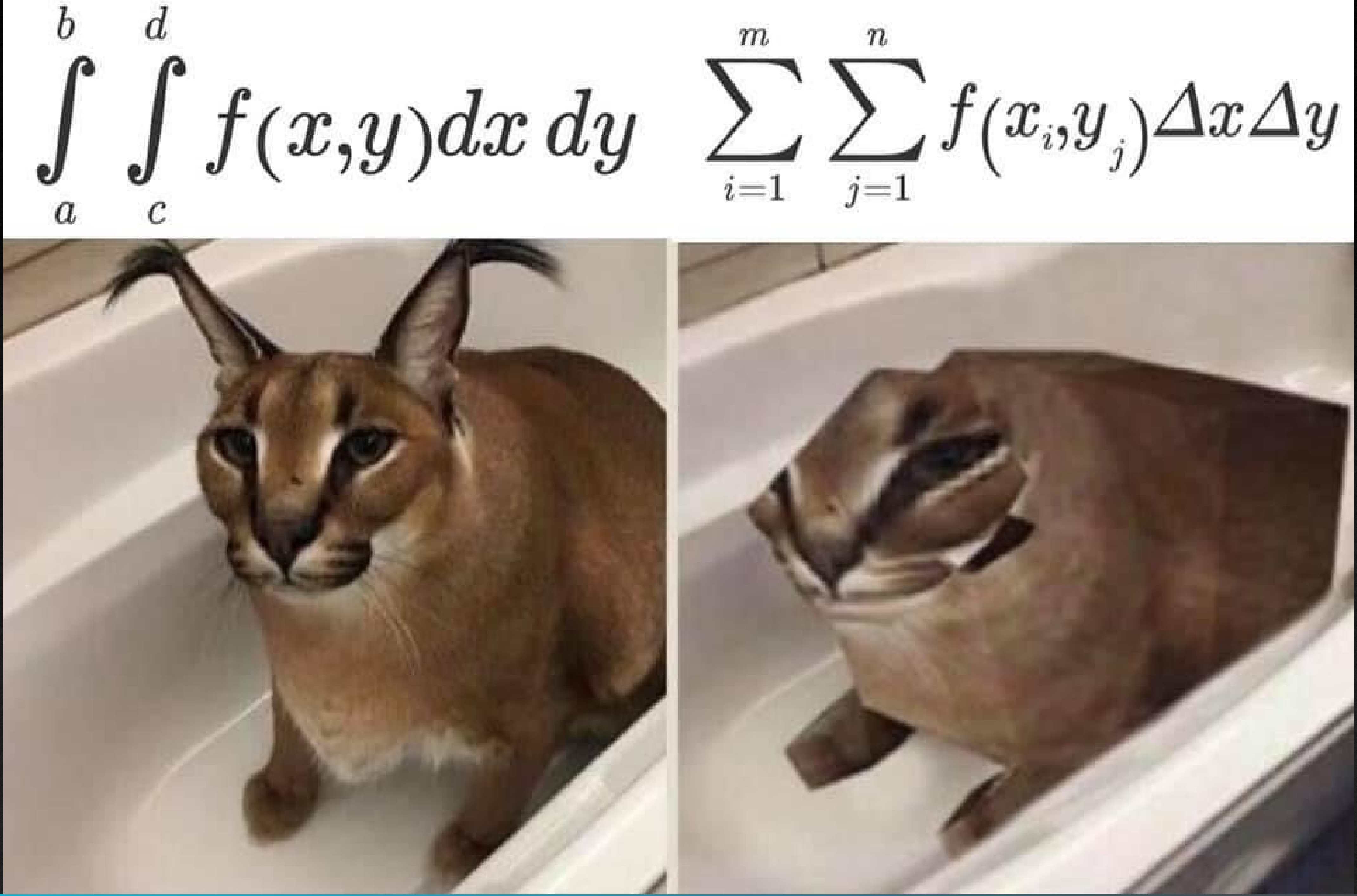
- The error still behaves as $N^{-1/2}$ but the factor is smaller than before

Integrals in many dimensions

- Both the basic and mean value MC integration methods extend easily to multiple dimensions
- When we use conventional methods, we require an N-dimensional grid
- This is not computationally tractable with N > 3
- Example: 6-D phase space (position & velocity), we'd need $100^6 = 10^{12}$ points if the accuracy required 100 points in each dimension
- But with the mean value method, we can perform

$$I \simeq \frac{V}{N} \sum_{i=1}^{N} f(\vec{r}_i)$$

- Here $\vec{r}_i$ are random points chosen in the volume V


$\int_a^b \int_c^d f(x,y)\,dx\,dy$
$\sum_{i=1}^{m} \sum_{j=1}^{n} f(x_i,y_j)\Delta x \Delta y$

Importance sampling

- Sometimes functions diverge even if their integrals don't diverge, such as

$$I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$$

- This integral is applicable to Fermi gases (electrons in a white dwarf or neutrons in a neutron star)
- For MC integration, we want to favor x-values that don't overlap with the diverging portion (near x=0)

- Importance sampling draws a non-uniform random sample that avoids it

Importance sampling

- First consider a weighted mean of some function g(x)

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x)\, dx}{\int_a^b w(x)\, dx}.$$

- Taking $I = \int_a^b f(x)dx$ and g(x) = f(x)/w(x), we have

$$\left\langle \frac{f(x)}{w(x)} \right\rangle_w = \frac{\int_a^b w(x) f(x)/w(x)\, dx}{\int_a^b w(x)\, dx} = \frac{I}{\int_a^b w(x)\, dx}.$$

- Solve for the integral,

$$I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x)\, dx.$$

Importance sampling

$$I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x)\, dx.$$

- But how do we find the weighting function w(x)?

- We can equate the probability density function (set by the physics or math) as the normalized weighting function

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

- In practice, we want to pick w(x) that factors out the diverging portion
- The average number of samples between x and x+dx is Np(x)dx, so for g(x)

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b N p(x) g(x)\, dx.$$

Importance sampling

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b N p(x) g(x)\, dx.$$

- We can now write the general weighted average of the function g(x) as

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x)\, dx}{\int_a^b w(x)\, dx} = \int_a^b p(x) g(x)\, dx \simeq \frac{1}{N} \sum_{i=1}^{N} g(x_i),$$

- Where x_i are randomly chosen from p(x). Combining this with $I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x)\, dx.$ we arrive at

$$I \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \int_a^b w(x)\, dx.$$

- If we set w(x) = 1, we recover the mean value method
- The error still behaves as $N^{-1/2}$ but it can be smaller if the weighting function is chosen well

Importance sampling

- Let's apply this methodology to a Fermi gas

$$I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$$

- We want to avoid the diverging nature of the integrand, so we can choose $w(x) = x^{-1/2}$, giving

$$p(x) = \frac{x^{-\frac{1}{2}}}{\int_0^1 x^{-\frac{1}{2}} dx} = \frac{1}{2\sqrt{x}}$$

- We would choose random numbers from this distribution and use them in

$$I \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \int_a^b w(x)\, dx.$$

Importance sampling

- Importance sampling is useful when dealing with infinite domains, especially in multiple dimensions
- This is prevalent in statistical mechanics
- We can use an exponential weighting function w(x) = e^{-x} to place more importance on the sparsely populated regions (large x)
- The integral becomes

$$I \simeq \frac{1}{N}\sum_{i=1}^{N} \exp(x_i) f(x_i) \int_0^\infty e^x \, dx = \frac{1}{N}\sum_{i=1}^{N} \exp(x_i) f(x_i)$$