PHY407 – University of Toronto
Lecture 10: Random Numbers and Numerical Integration

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Supporting textbook chapters for week 10: Chapters 10.1 and 10.2

Week 10, topics: * Random number generation * Monte Carlo integration

1 Random numbers

1.1 General requirements

Why we need random numbers:

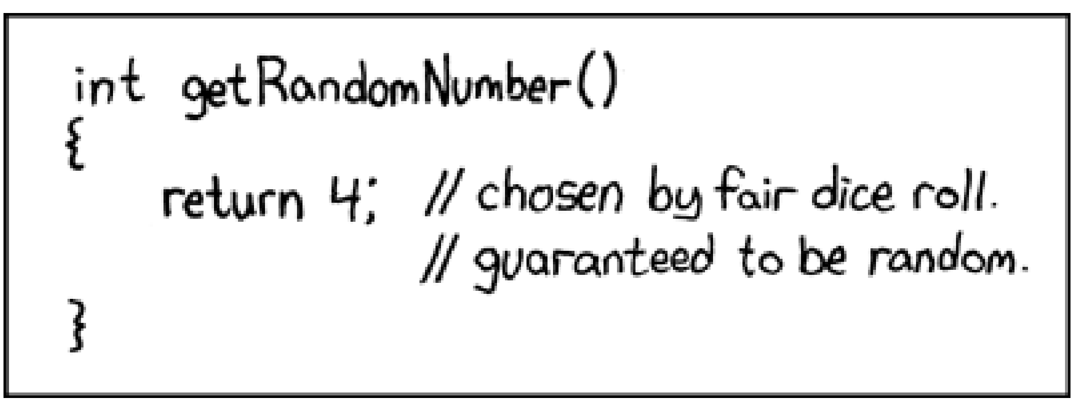
- For randomly sampling a domain (today)
- Monte Carlo integration (today)
- Monte Carlo simulations (next week)
- Stochastic algorithms (we'll see some next week)
- Cryptography

Q: How can a computer generate random numbers?

What is a useful random sequence of numbers? * Follows some desired distribution * Unpredictable on a number-by-number basis * Fast to generate (we may need billions of them) * Long period (we may need billions of them) * Uncorrelated

Problems with actually random numbers: * generally slow, expensive to generate, * hard/impossible to reproduce for debugging * Often hard to characterize underlying distribution

Q: How can a computer generate random numbers?



http://xkcd.com/211

Q: How can a computer generate random numbers? A: It can't!

The computer can't do anything randomly.

2 options: * find physical process that actually is random, have computer store info from that to provide a random number * Use an algorithm for generating a sequence of numbers that approximates the properties of random numbers. This is called a "Pseudorandom Number Generator" (PRNG) or a "Deterministic Random Bit Generator" (DRBG).

1.2 Common Tests

https://dilbert.com/strip/2001-10-25

1.2.1 Correlations

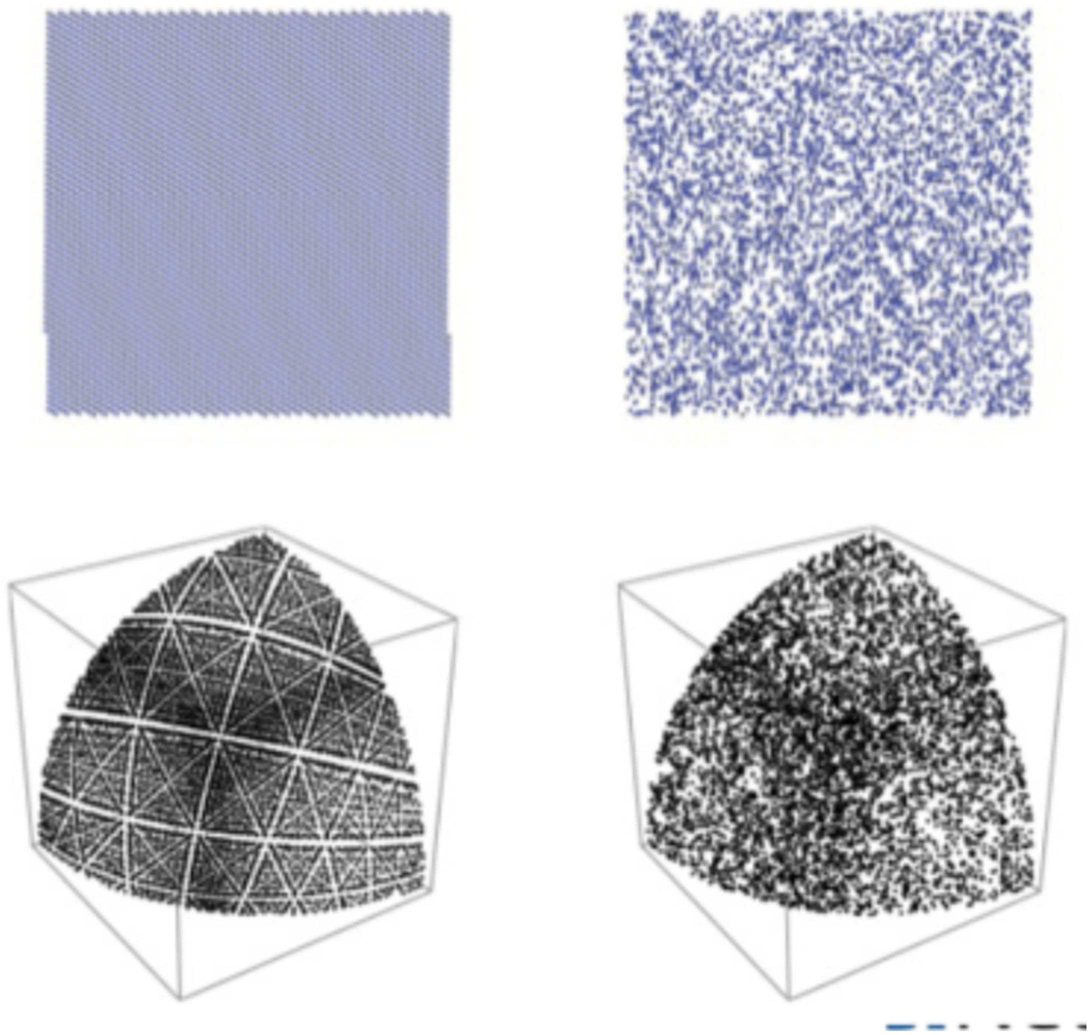
Simple pairwise correlations:

$$\epsilon(N, n) = \frac{1}{N}\sum_{i=1}^{N} x_i x_{i+n} - \mathrm{E}[x^2]$$

* N = number of data points * $n = $ correlation "distance" * $\mathrm{E}[x] = \sum_{i=1}^{N} x_i / N$, the expected value.

We want to avoid correlations between pairs of numbers.

Left: bad PRNG; right: Mersenne Twister



1.2.2 Moments

k^{th} moment of sequence of N elements, $\mu(N,k)$:

$$\mu(N,k) = \mathrm{E}[x^k]$$

We want to ensure moments of random number distributions also have desired properties.

1.2.3 Other tests

- Overlapping permutations:
  - For example, analyze orders of five consecutive random numbers. There are $5!(= 5 \times 4 \ldots)$ possible permutations. They should occur with equal probability.
- $\ldots$

1.3 Linear Congruential Generator

- The sequences of numbers produced by a PRNG seem random, but they are reproducible if you start with the same "seed" value.

- For example (actually a bad choice for a PRNG, but good for illustration): "Linear Congruential Random Number Generator":

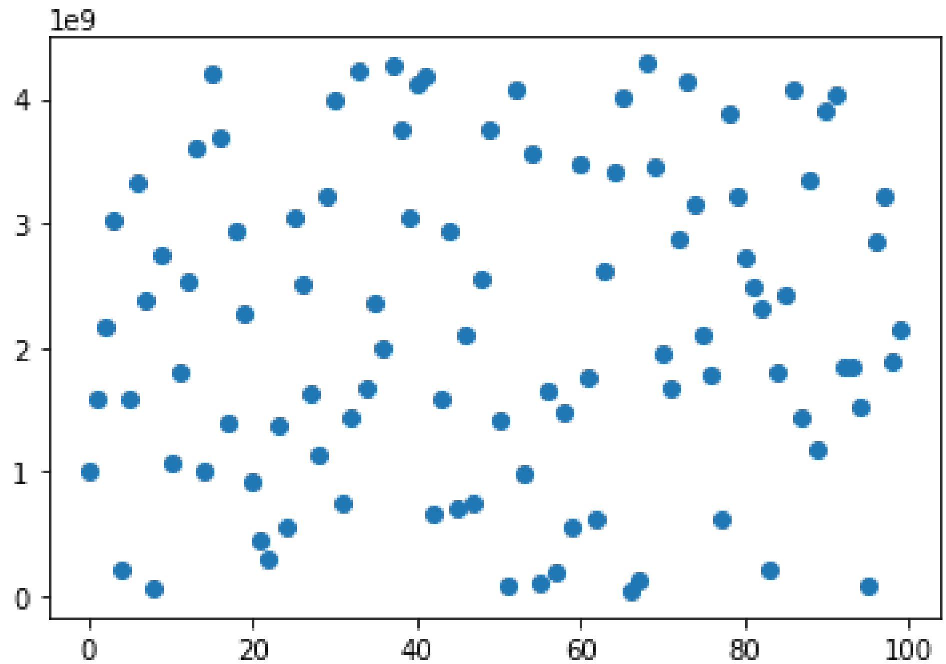
$$x_{i+1} = (ax_i + c) \mod m$$

  E.g. in Python: `x[i+1] = (a*x[i] + c) % m`.
- x_0 would be the seed,
- m: large integer, determines period,
- For good results:
  - c relatively prime to m,
  - $a - 1$ is a multiple of p for every prime divisor p of m (e.g., $a - 1$ is multiple of 4 if m is multiple of 4).
- How does computer pick seed x_0? Taking system time is common (dangerous in parallel if all processors use the same seed!).

[1]:
```python
# Newman's lcg.py
from pylab import plot, show

N = 100
a = 1664525
c = 1013904223
m = 4294967296
x = 1
results = []

for i in range(N):
    x = (a*x+c) % m
    results.append(x)
plot(results, "o")
show()
```



Benefits: * much faster than real random number generators * good for testing code since you can supply the same 'seed' for reproducible outcome using the `random.seed()` function:

`random.seed(4219)`

`x = random.random()`

`will always produce the same `x` (that is, 0.03738057695923325).`

- easy to generate many different sequences, just pick many different seeds.

Better methods?

- We want to avoid correlations between pairs of numbers
- Can do lots of test that PRNGs producing right "statistics" of random numbers!
- Python uses a Mersenne twister

Functions in `random.py` most likely to use (assuming `import random`): * `random()`: gives a random float uniformly distributed in a the range $[0, 1)$ (all values have equal probability of being selected), * `randrange(m, n)`: Gives a random integer from `m` to `n-1`, inclusive.

- If you need a uniformly distributed random float outside the range $[0, 1)$, say in range $[a, b)$, then just multiply your answer by $(b - a)$ and shift the argument. For example:

  `num = random()`

  `shiftnum = (b-a)*num + a`

More resources:

https://docs.scipy.org/doc/numpy-1.15.1/reference/routines.random.html

https://docs.python.org/3/library/random.html

[ ]:
```
# re-do random walk here in class
from random import randrange

# define function that moves left, right, up or down by one at each step␣
↪depending randrange
# start from position (x, y) = (0, 0)
# loop over 10 steps to see where you land.
```

1.4 Non-Uniform distributions

What if you need a random number from a non-uniform distribution?

- Get a uniformly distributed random number, then use a transformation to make it seem like it comes from a non-uniform distribution.
- Consider source of random floats z from a distribution with probability density $q(z)$, i.e., the probability of generating a number in the interval z to $z + \mathrm{d}z$ is:

$$q(z)\mathrm{d}z$$

- For a uniform distribution over [0, 1), $q(z) = 1$ because for all dz, equal probability of number being chosen.
- Now consider transformation of z into new variable, say x using:

$$x = x(z)$$

- Then x is also a random number, but will have some other probability distribution, call it $p(x)$.
- The probability of generating a value of x between x and $x + \mathrm{d}x$, with

$$\mathrm{d}x = \frac{\mathrm{d}x}{\mathrm{d}z}\mathrm{d}z,$$

  is by definition equal to the probability of generating a value of z between the corresponding z and $z + \mathrm{d}z$:

$$p(x)\mathrm{d}x = q(z)\mathrm{d}z, \quad \text{where } x = x(z)$$

- Goal: find a function $x(z)$ so that x has the distribution we want.
- Then we can use `random()` to get a uniformly distributed random number z and transform it to x using:

$$q(z) = 1 \quad \text{over} \quad [0, 1)$$
$$q(z)\mathrm{d}z = p(x)\mathrm{d}x$$
$$\Rightarrow \int_0^z 1\mathrm{d}z' = z = \int_0^{x(z)} p(x')\mathrm{d}x'.$$

- Plug in your $p(x)$ for the probability distribution you need and integrate to find $z(x)$ (if you can!)

- Even then: might not be possible to solve for $x(z)$.

Example: exponential distribution

$$q(z) = 1 \quad \text{over} \quad [0,1)$$

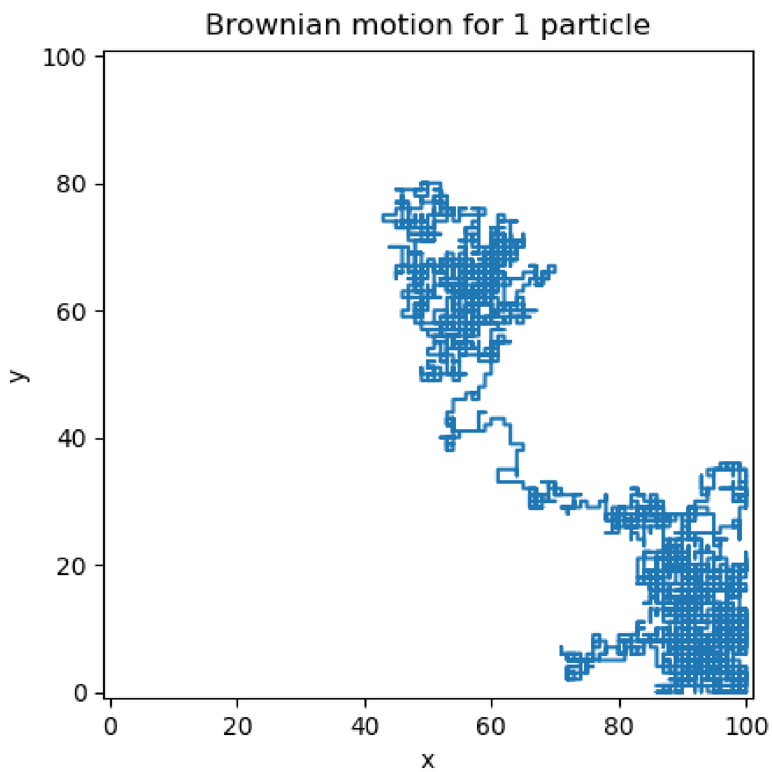
$$p(x) = a\exp(-ax) \quad \text{over} \quad [0,\infty)$$

$$\Rightarrow\ z = \int_0^{x(z)} a\exp(-ax')\mathrm{d}x' = 1 - \exp(-ax)$$

$$\Rightarrow\ x = -\frac{\ln(1-z)}{a}.$$

* Draw a number z in $[0,1)$, * $x(z)$ has the desired distribution.

- Simulate random physical processes like diffusion, radioactive decay, Brownian motion.



2 Monte Carlo integration

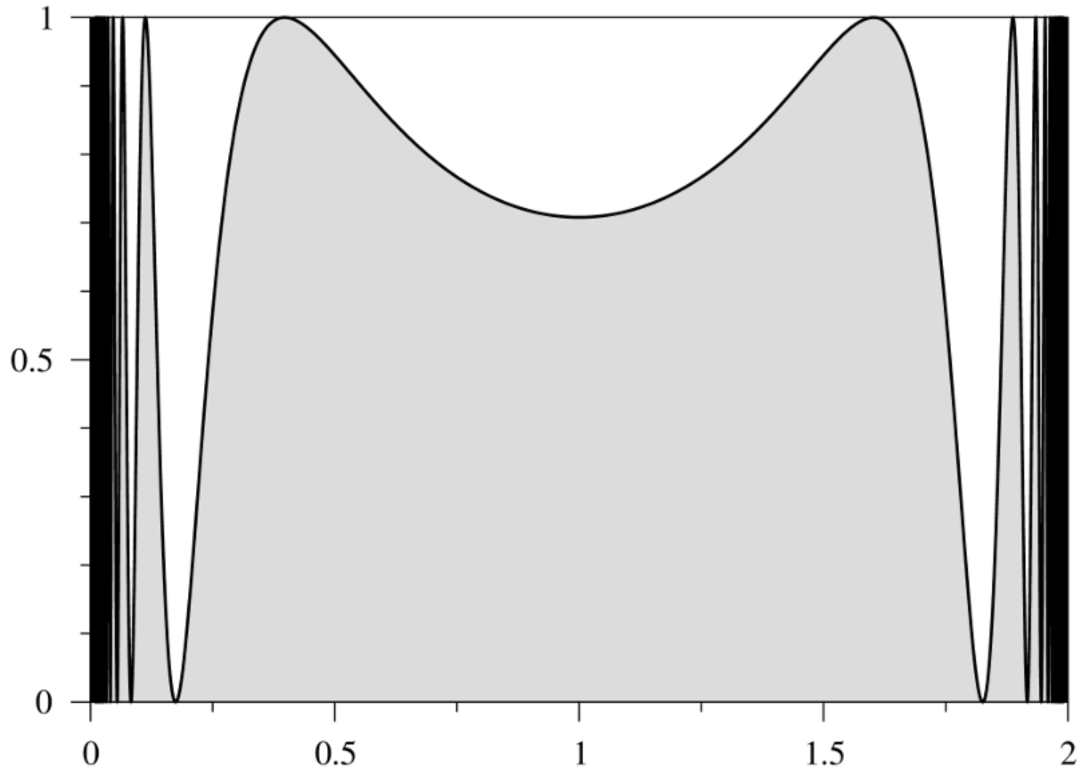
Monaco and Monte-Carlo. The casino is right below the small, almost-closed harbour if you extrapolate the ridge line on top of the picture.

2.1 What it is

Solving Integrals: "Monte Carlo Integration" * Sounds great in theory. Would never work in practice without computers. * 3 Monte Carlo techniques you will use in the lab: * "hit or miss" or "standard" Monte Carlo * "mean value" Monte Carlo * "importance sampling" Monte Carlo

You've already learned a bunch of different methods for integrating, why introduce another one? (Especially since its convergence/error properties are worse than the other methods):

Reason 1: Good for pathological functions or just fast-varying functions.



Reason 2: MUCH faster for multi-dimensional integrals.

The "curse of dimensionality": * For a dimension d integral, you need $O(n^d)$ grid points. * E.g. with trapezoid, Simpson or Gaussian integration: for $n = 1000$ points, a 10-d integral need 10^{30} grid points!

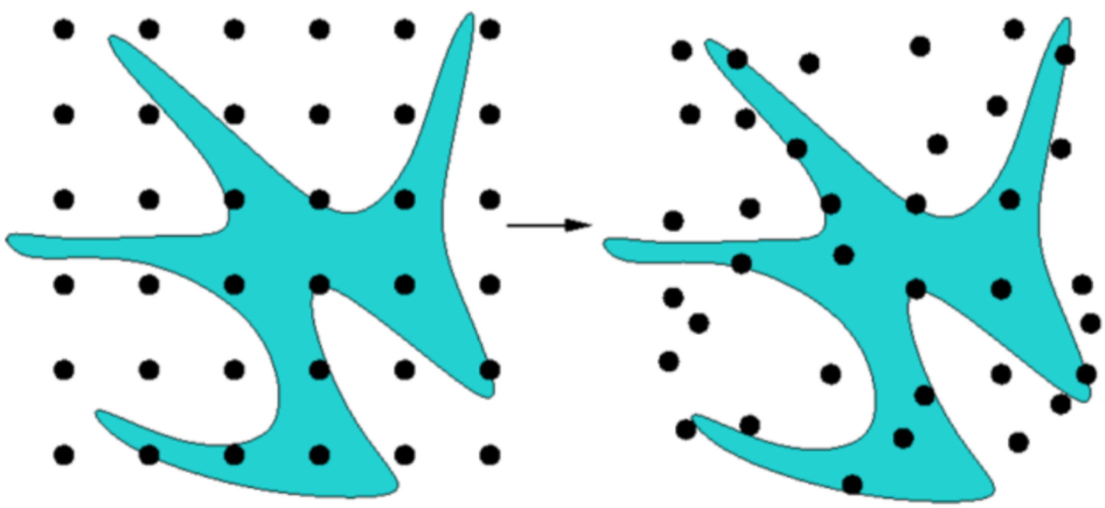
- Or: if you can afford N points, your grid has side length $O(N^{1/d})$.
- For trapezoid integration, error $\epsilon = O(h^2) \propto 1/N^{2/d}$.
- E.g., for a 10-d integral, $\epsilon \propto 1/N^{1/5}$.
- Monte Carlo: $\epsilon \propto 1/N^{1/2}$, regardless of d.

Reason 3: much easier to implement in complicated domains (i.e., complicated boundaries of integration).

Good luck finding the volume of the Blob with Gaussian quadrature!

2.2 Implementation

Use random numbers to pick points at which to evaluate integrand.

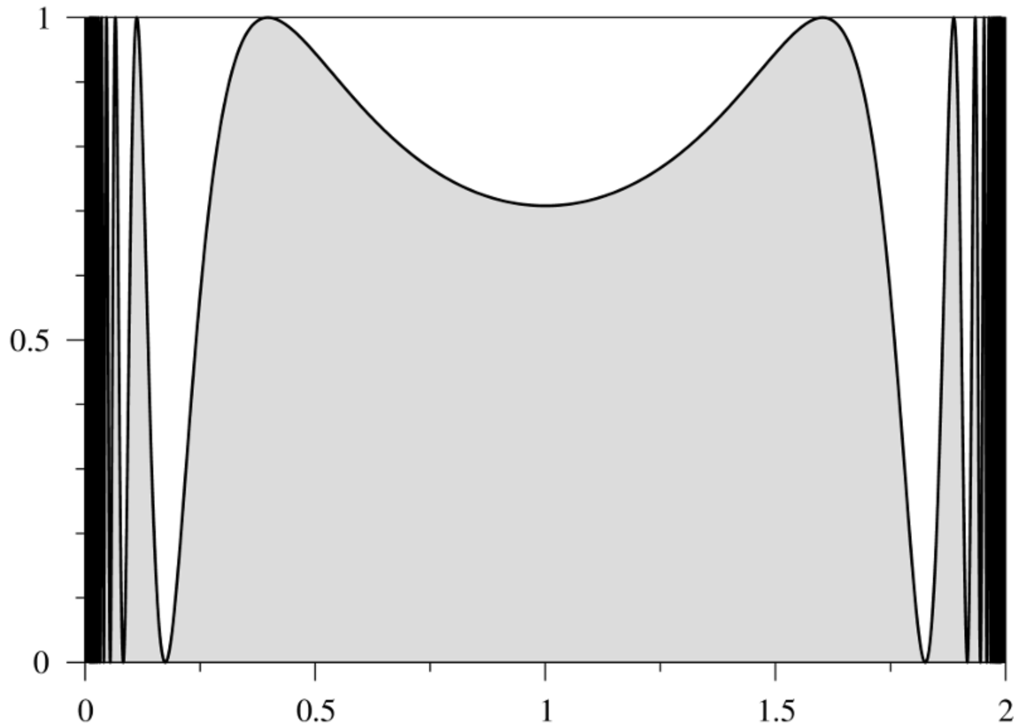


- Simple and flexible.
- Can generalize to focus on important parts.

2.2.1 Hit-or-miss MC

- If your function "fits" in a finite region where we want to integrate from $x = 0$ to $x = 2$:

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



- function fits in box of height 1, width 2.
- Define area of box: A (this is important! It is the piece of info we will leverage).
- Integral of function is shaded area in the box (call it I).

- Probability that your random point falls in the shaded region is $p = I/A$.
- Algorithm:
  1. Randomly pick N locations (x, y) in the box (lots of them).
  2. Count the number of locations that are in the shaded region (call the count k).
  3. The fraction of points in the shaded region is k/N. This approximates the probability p. Solve for I:
$$P = \frac{I}{A} \approx \frac{k}{N} \Rightarrow I \approx \frac{kA}{N}.$$

Can estimate the error on the integral (text gives derivation on page 467 from probability theory):

- The *Expected Error* (standard deviation):

$$\sigma = \sqrt{\frac{I(A-I)}{N}}.$$

- Notice it varies as $N^{-1/2}$. This is **very slow**!
- Compare:

  - Trapezoid Rule: error varies as N^{-2},
  - Simpson's Rule: error varies as N^{-4}.
- (but careful to compare apples with apples, see earlier!)
- This is why you only use Monte Carlo integration if you absolutely have to.

Example: exercise 10.5(a) from the text.

Write a program to evaluate

$$I = \int_0^2 \sin\left[\frac{1}{x(2-x)}\mathrm{d}x\right]$$

using the "hit-or-miss" method. * Use $N = 10^4$ points. * Also evaluate the error on your method.

[2]:
```python
# Re-do here in class
import numpy as np  # I'll use the numpy random functionalities

def f(x): return np.sin(1/((x-a)*(b-x)))**2  # the function to integrate

# define parameters

# loop over samples; in loop, have an if statement to check wether the point is␣
↪above of below the curve

# compute fraction of points below.

# compute error
```

2.3 Mean value MC

- Use the definition of an average (or mean value):

$$I = \int_a^b f(x)\mathrm{d}x,$$

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

$$\Rightarrow \; I = (b-a)\langle f \rangle$$

- Use random numbers for x to estimate $\langle f \rangle$. Evaluate f at N random x's, then calculate:

$$\langle f \rangle \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i) \;\Rightarrow\; I \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i).$$

- Different from "hit-or-miss": we chose N random point over (x, y).

Error estimate. * Can estimate the error on the integral (text gives derivation on pages 468-469 from probability theory): "Expected Error":

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

$$\mathrm{var} f = \langle f^2 \rangle - \langle f \rangle^2 .$$

* Notice it also varies as $N^{-1/2}$. However, it turns out the leading constant is smaller than with the hit or miss method. *Note: I have not been able to figure out if this result is always true, or usually true. Newman's wording seems to indicate that it is always true, but I can't quite figure out why.*

Example: exercise 10.5(b) from the text.

Write a program to evaluate

$$I = \int_0^2 \sin\left[\frac{1}{x(2-x)} \mathrm{d}x\right]$$

using the mean value method. * Use $N = 10000$ points. * Also evaluate the error on your method.

[ ]:
```python
import numpy as np

def f(x): return np.sin(1/((x-a)*(b-x)))**2

N = 10000
a = 0.
b = 2.
k = 0  # will contain the average
k2 = 0  # will be used for variance

for i in range(N):
    x = (b-a)*np.random.random()
    k += f(x)
    k2 += f(x)**2

I = k * (b-a) / N
print(I)

# error
var = k2/N - (k/N)**2  # variance <f**2> - <f>**2
sigma_MV = (b-a)*np.sqrt(var/N)  # MV stands for Mean Value
print('error = ', sigma_MV)
print('recall error in hit-or-miss = ', sigma_HM)
```

[ ]:
```python
# Re-do in class here (copy previous example and adjust):
def f(x): return np.sin(1/((x-a)*(b-x)))**2

# define parameters (re-use some from previous example)

# loop over samples; in loop, have an if statement to check wether the point is above of below the curve

# compute fraction of points below.

# compute error
```

2.4 Importance sampling MC

- Good to use when your integrand contains a divergence: want to place more points in region where the integrand is large to better estimate the integral, also when you want to integrate out to infinity
- Illustrative example (obviously a bad one for Monte-Carlo, but good for making my point):

$$f(x) = 1 \quad \text{for} \quad c < x < d, \qquad f(x) = 0 \quad \text{otherwise.}$$

[ ]:
```
import matplotlib.pyplot as plt
x = np.linspace(0, 1, 1000)
f = 0.*x
for i, xs in enumerate(x):
    if 0.33 < xs < 0.35:
        f[i] = 1.
plt.plot(x, f)
```

- Easy to miss the region between c and d with uniformly sampled points
- evaluating the integral many times using Mean Value or Hit/Miss MC (with different randomly sampled points) can give very different answers, much larger than the expected error
- Solution: sample "important" regions more frequently. I.e., come up with a non-uniformly distributed set of random numbers. This is called "Importance Sampling".
- Text shows that using a weight function $w(x)$, you can always write:

$$I = \int_a^b f(x)\mathrm{d}x = \underbrace{\left\langle \frac{f(x)}{w(x)} \right\rangle_w}_{weightedaverage} \int_a^b w(x)\mathrm{d}x.$$

- Goal: find a weight function that gets rid of pathologies in integrand $f(x)$. E.g., if $f(x)$ has a divergence, factor the divergence out and hence get a sum (in the $\langle\rangle$) that is well behaved (i.e. doesn't vary much each time you do the integral).

Example:

$$I = \int_0^1 \frac{x^{-1/2}}{1+\exp(x)}\mathrm{d}x,$$

diverges as $x \to 0$ because of numerator.

Fine, let $w(x) = numerator$. Then

$$\left\langle \frac{f(x)}{w(x)} \right\rangle = \frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} = \frac{1}{N}\sum_{i=1}^{N} \frac{1}{1+\exp(x_i)},$$

which is much better behaved than

$$\langle f(x) \rangle = \frac{1}{N}\sum_{i=1}^{N} \frac{x^{-1/2}}{1+\exp(x_i)}$$

- When you've chosen your weight function, you then need to make sure to randomly sample points from the non-uniform distribution:

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

  Use the transformation method described earlier in this lecture to take a uniformly distribution random z and find the corresponding x for this distribution.

- "Expected error":

$$\sigma = \sqrt{\frac{\mathrm{var}(f/w)}{N}} \int_a^b w(x)\mathrm{d}x.$$

  Yes, it also varies as $N^{-1/2}$. If you do the integral many times, your values should mostly fall within the expected error.