PHY604 Lecture 19

October 28, 2021

Review: More accurate approximations: Crank-Nicholson

- As we saw before, numerically stable does not mean accurate
- More accurate scheme: Crank-Nicholson
  - Average of implicit and explicit FTCS:

$$i\hbar\frac{\psi_j^{n+1}-\psi_j^n}{\tau}=\frac{1}{2}\sum_{k=0}^{N-1}H_{jk}(\psi_k^n+\psi_k^{n+1})$$

  - Where:

$$H_{jk}=-\frac{\hbar^2}{2m}\frac{\delta_{j+1,k}+\delta_{j-1,k}-2\delta_{jk}}{h^2}+V_j\delta_{jk}$$

- Isolating the *n*+1 term:

$$\Psi^{n+1}=\left(\mathbf{I}+\frac{i\tau}{2\hbar}\mathbf{H}\right)^{-1}\left(\mathbf{I}-\frac{i\tau}{2\hbar}\mathbf{H}\right)\Psi^n$$

Review: Crank-Nicolson for tridiagonal matrices

$$\Psi^{n+1} = \mathbf{Q}^{-1}\Psi^{n} - \Psi^{n}, \quad \mathbf{Q} = \frac{1}{2}\left[\mathbf{I} + \frac{i\tau}{2\hbar}\mathbf{H}\right]$$

- Now we can solve for the next timestep by solving the linear system:

$$\mathbf{Q}\chi = \Psi^{n}$$

- And then:

$$\Psi^{n+1} = \chi - \Psi^{n}$$

- Recall that for banded matrices, solving linear systems via, e.g., Gaussian elimination, is particularly efficient

Example: Numerical solution of the Schrödinger equation

- Initial conditions: Gaussian wave packet
  - Localized around x_0
  - Width of σ_0
  - Average momentum of: $p_0 = \hbar k_0$

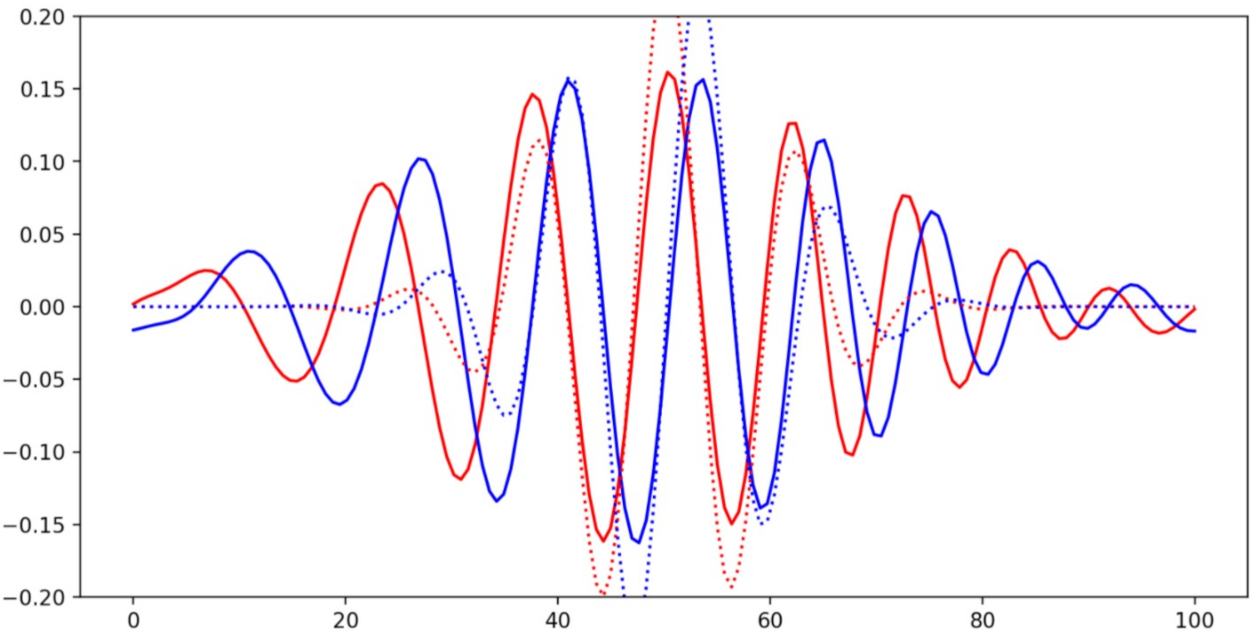
$$\psi(x, t=0) = \frac{1}{\sqrt{\sigma_0 \sqrt{\pi}}} \exp\left(ik_0 x\right) \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right]$$

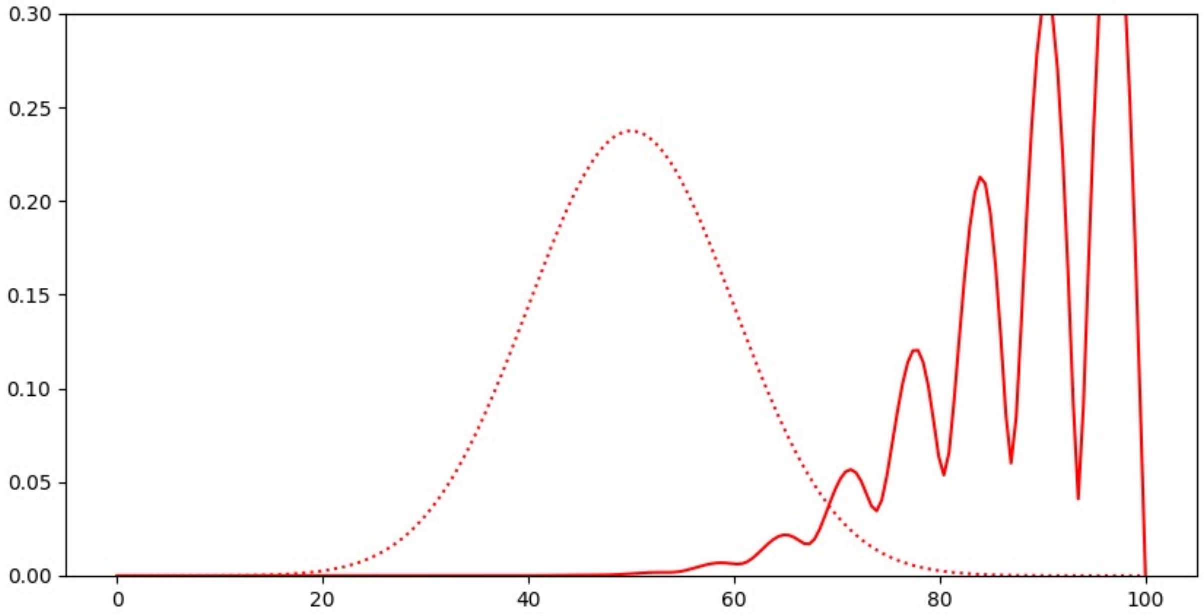
- Which is normalized so that:

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

- Also, has the special property that uncertainty produce $\Delta x \Delta t$ is minimized $(\hbar/2)$

Review: 1D Schrödinger equation



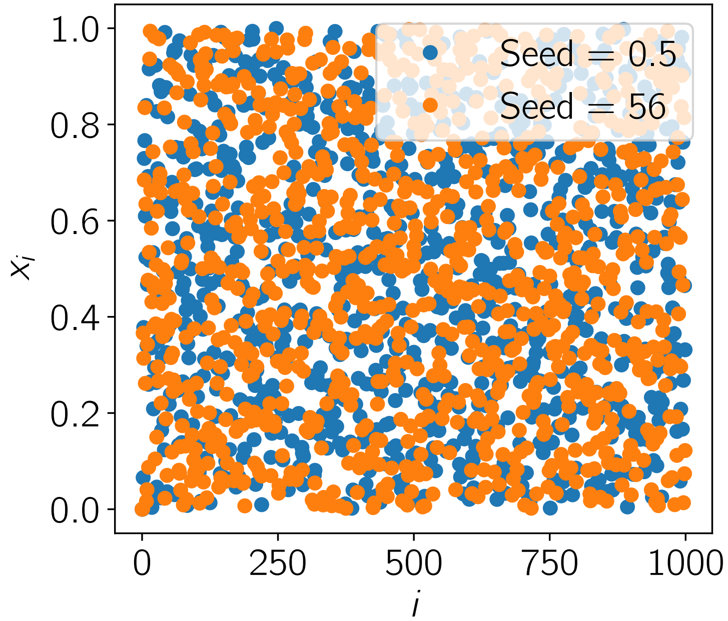


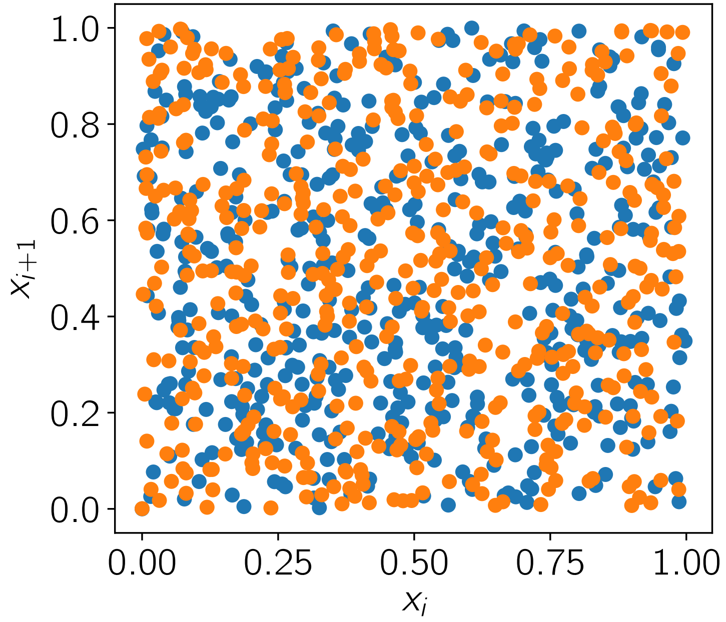
Review: Example of a simple random number generator

- Simplest generator made using the linear congruent scheme
- Random numbers are generated in sequence from the linear relation:

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

- *a*, *b*, and *c* are “magic numbers” which determine the quality of the generator
  - Typical choices: $a = 7^5$, $b = 0$, $c = 2^{31} - 1$
  - x_0 is the seed, allows for reproducibility





Review: Radioactive decay (see Newman Sec. 10.1)

- One of the quintessential random processes in physics
- Parent atoms decay with characteristic half-life τ
- We will consider ^{208}Tl, which decays to ^{208}Pb with τ = 183.18 sec.

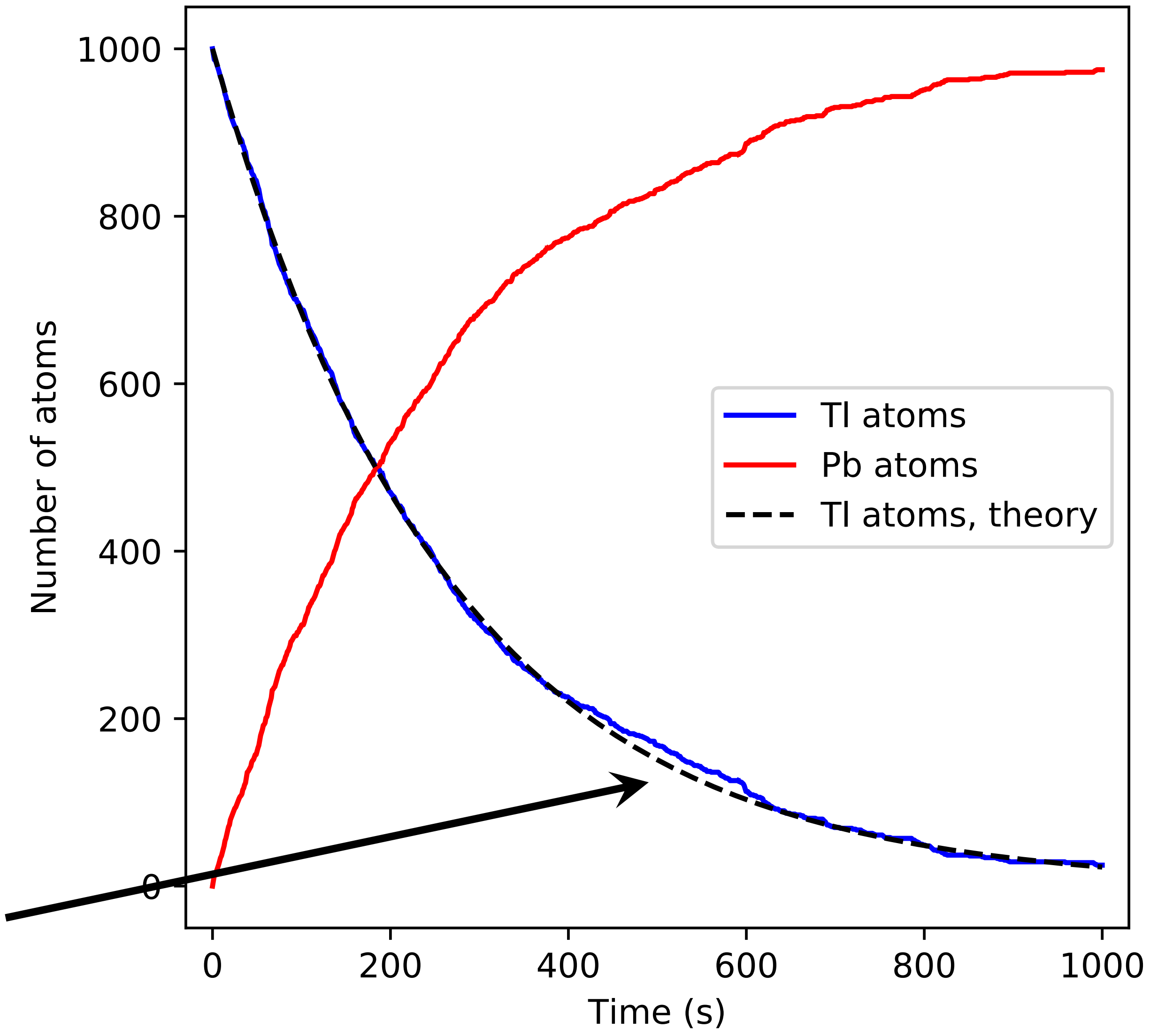
- Number of parent atoms falls off exponentially:

$$N(t) = N(0)2^{-t/\tau}$$

- Probability that a particular atom has decayed in a time interval *t*:

$$p(t) = 1 - 2^{-t/\tau}$$

Review: Radioactive decay



$$N(t) = N(0)2^{-t/\tau}$$

Today’s lecture:
Random numbers and Monte Carlo integration

- Random numbers

- Monte Carlo integration

Nonuniform distributions

- We can also select random numbers from a distribution that is not constant over the range
  - I.e., all numbers are not selected with equal probability
- Consider the radioactive decay example:
  - Probability of decay in time interval *dt* is:

$$p(t) = 1 - 2^{-dt/\tau} = 1 - \exp\left(-\frac{dt}{\tau}\ln 2\right) \simeq \frac{\ln 2}{\tau}dt$$

- What is the probability to decay in time window *t* + *dt*?
  - Needs to survive without decay until *t* (probability $2^{-t/\tau}$)
  - Then must decay in *dt*
  - Total probability is:

$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}dt$$

Nonuniform distribution for decay example

- Nonuniform probability distribution:

$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}dt$$

- Decay times t are distributed in proportion to $2^{-t/\tau}$
- We could calculate the decay of N atoms by drawing N random samples from this distribution
    - More efficient than previous method
    - Need to generate nonuniform distribution of random numbers
- Can generate nonuniform random numbers from a uniform distribution

Transformation method for changing distributions

- We have a source of random numbers *z* drawn from distribution *q*(*z*)
  - Probability of generating a number between *z* and *z*+d*z* is *q*(*z*)d*z*
- Now we choose a function *x* = *x*(*z*) whose distribution *p*(*x*) is the one we want
- We know that: $$p(x)dx = q(z)dz$$
- If our random numbers are drawn from a uniform distribution [0,1), *q*(*z*)=1 from 0 to 1, zero elsewhere
- Then:

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_0^z dz' = z$$

- We need to do the integral on the left and then solve for *x*(*z*)
  - Not always possible

Transformation method to exponential distribution

- Say we want to generate random real numbers that are > 0 with the distribution:

$$p(x) = \mu e^{-\mu x}$$

- μ is for normalization
- Then:

$$\mu \int_{-\infty}^{x(z)} e^{-\mu x'} dx' = 1 - e^{-\mu x} = z$$

- So:

$$x = -\frac{1}{\mu} \ln(1 - z)$$

Nonuniform distribution for decay example

- We can write the probability distribution for the decay example as

$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}dt = e^{-t\ln 2/\tau}\frac{\ln 2}{\tau}$$

- So:

$$x = -\frac{\tau}{\ln 2}\ln(1-z)$$

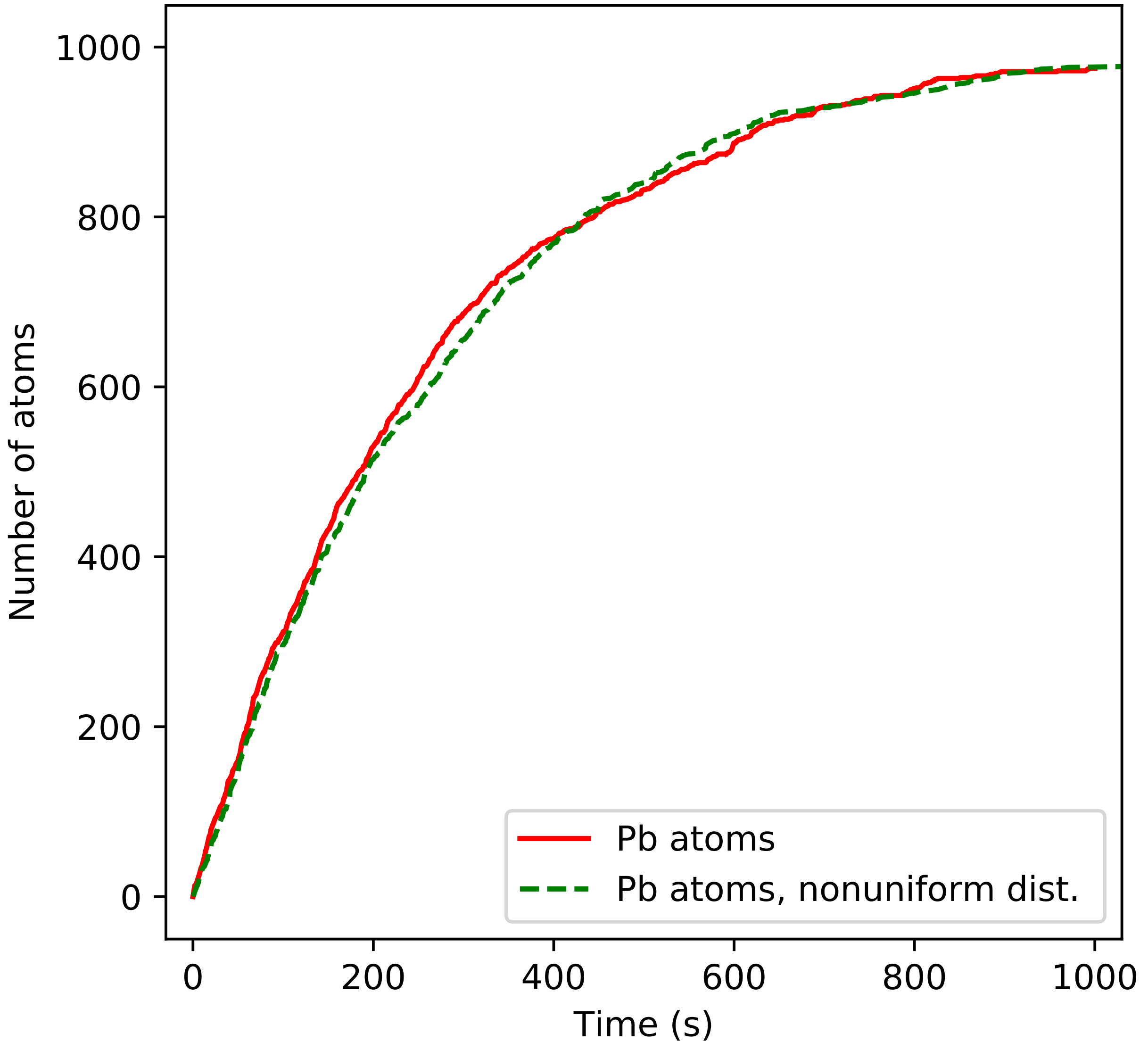
Nonuniform distribution for decay example

- We can write the probability distribution for the decay example as

$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}dt = e^{-t\ln 2/\tau}\frac{\ln 2}{\tau}$$

- So:

$$x = -\frac{\tau}{\ln 2}\ln(1-z)$$



Gaussian random numbers

- In many cases we would like to draw numbers from a Gaussian (i.e., normal) distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

- Let's try the transformation method:

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{x} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = z$$

- The solution to this integral and the resulting equation is complicated

Gaussian random numbers

- Trick: consider two random numbers *x* and *y*, both drawn from Gaussian distribution with the same standard deviation
- Probability that point with position (*x*,*y*) falls in some element d*x*d*y* on *xy* plane is:

$$p(x)dx \times (y)dy = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx \times \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{y^2}{2\sigma^2}\right) dy$$
$$= \frac{1}{2\pi\sigma^2} \exp\left(-\frac{x^2+y^2}{2\sigma^2}\right) dxdy$$

- Now convert to polar coordinates:

$$p(r,\theta)drd\theta = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) rdrd\theta = \frac{r}{\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) dr\frac{d\theta}{2\pi}$$

2D transformation method

$$p(r)dr \times p(\theta)d\theta = \frac{r}{\sigma^2}\exp\left(-\frac{r^2}{2\sigma^2}\right)dr\frac{d\theta}{2\pi}$$

- The point in polar coordinates will have the same distribution as the original point in cartesian (*x*,*y*)
  - Solving in polar coordinates and transforming back to Cartesian gives us two random points from a Gaussian distribution
- θ part is just a uniform distribution: $p(\theta) = 1/2\pi$
- Radial part can be treated with transformation method:

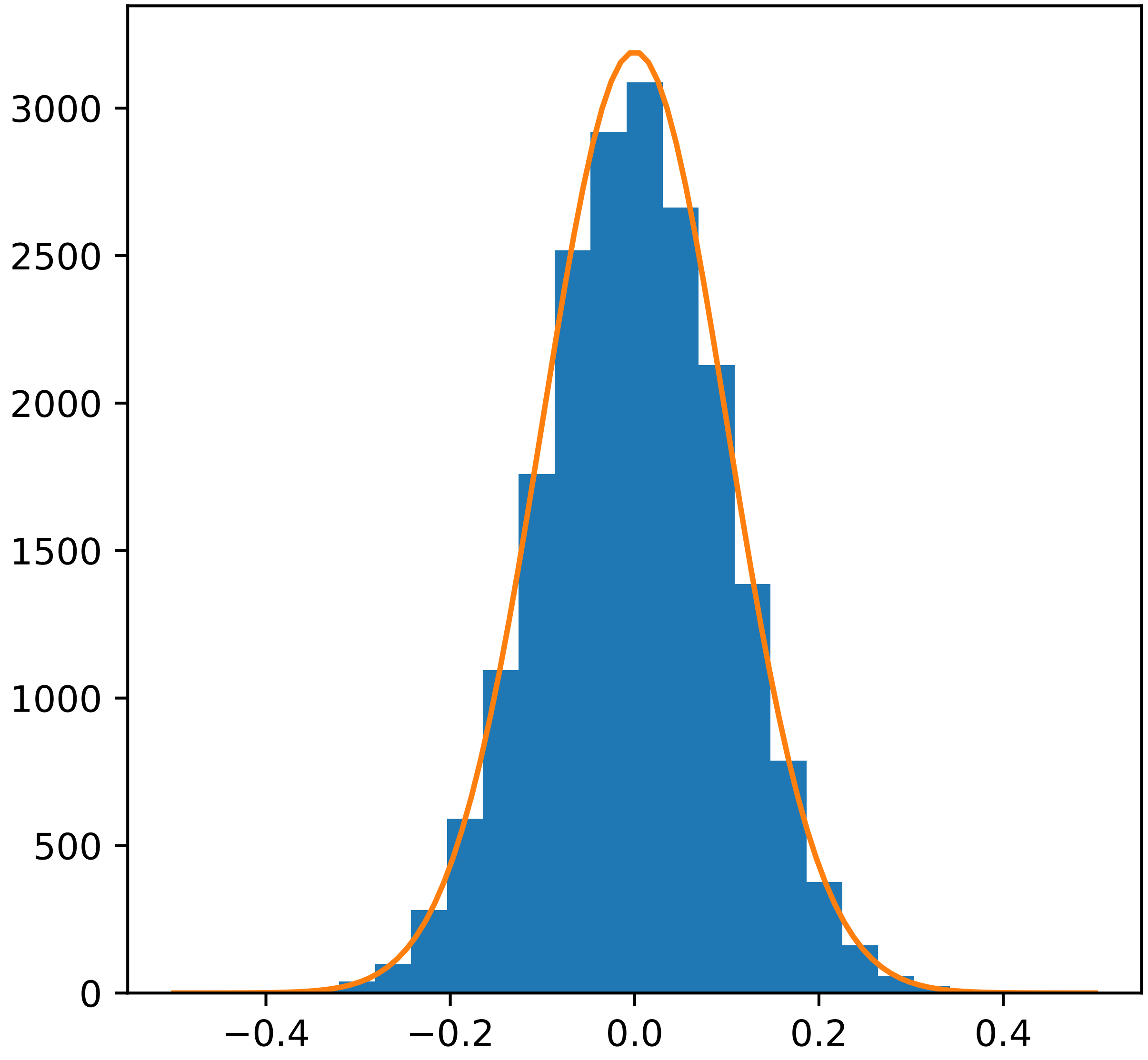
$$\frac{1}{\sigma^2}\int_0^r \exp\left(-\frac{r'^2}{2\sigma^2}\right)r'dr' = 1 - \exp\left(-\frac{r^2}{2\sigma^2}\right) = z$$

- So:

$$r = \sqrt{-2\sigma^2\ln(1-z)}$$

- And random numbers are: $x = r\cos\theta, \quad y = r\sin\theta$

Random numbers from Gaussian distribution



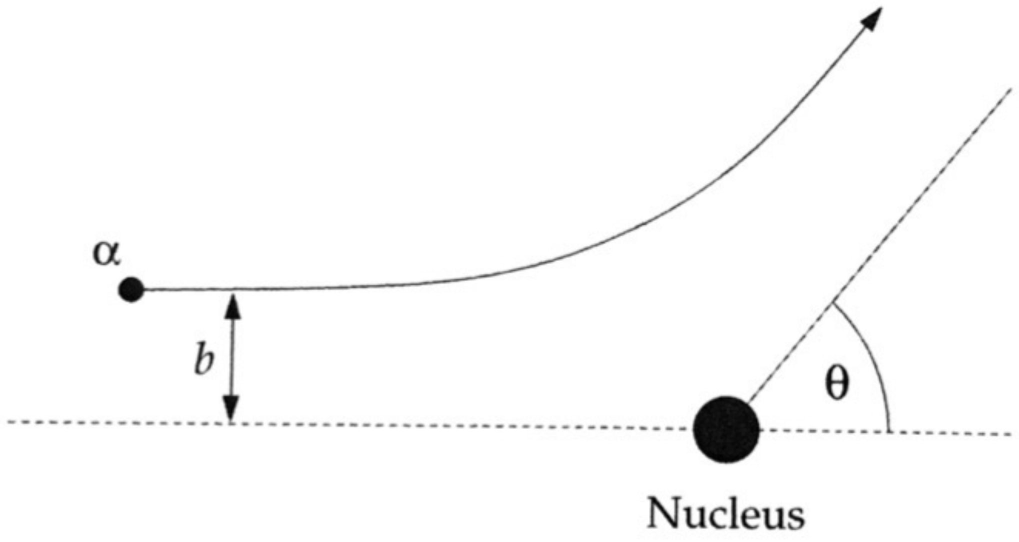
Example: Rutherford scattering

- α particles (helium nuclei) scatter when they pass close to an atom with angle:

$$\tan\left(\frac{\theta}{2}\right) = \frac{Ze^2}{2\pi\epsilon_0 Eb}$$

- *E* is the kinetic energy of the α particle, *b* is the impact parameter
- Consider Gaussian beam of particles with σ=a_0/100 and *E*=7.7MeV fired at a gold atom
- How many “bounce back” (scattering angle > 90 degrees)?

$$b \leq \frac{Ze^2}{2\pi\epsilon_0 E}$$



Analytic solution to Rutherford scattering

- The impact parameter (distance from gold atom) are radially distributed:

$$p(r) = \frac{r}{\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

- Thus, the probability of scattering by more that 90 degrees is:

$$\frac{1}{\sigma^2} \int_0^b \exp\left(-\frac{r'^2}{2\sigma^2}\right) r' dr' = 1 - \exp\left(-\frac{b^2}{2\sigma^2}\right) = 1 - \exp\left(-\frac{Z^2 e^4}{8\pi^2 \epsilon_0^2 \sigma^2 E^2}\right)$$

- Exact solution: 1557 particles backscattered out of 1,000,000
  - In good agreement with our stochastic calculation

Today’s lecture:
Random numbers and Monte Carlo integration

- Random numbers

- Monte Carlo integration

Monte Carlo integration

- Let’s come back to the Rutherford scattering example
- One way to look at: Our stochastic solution was in good agreement with the exact one
- Another way to look at it: Using a random process, we obtained an approximate solution to the integral:

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

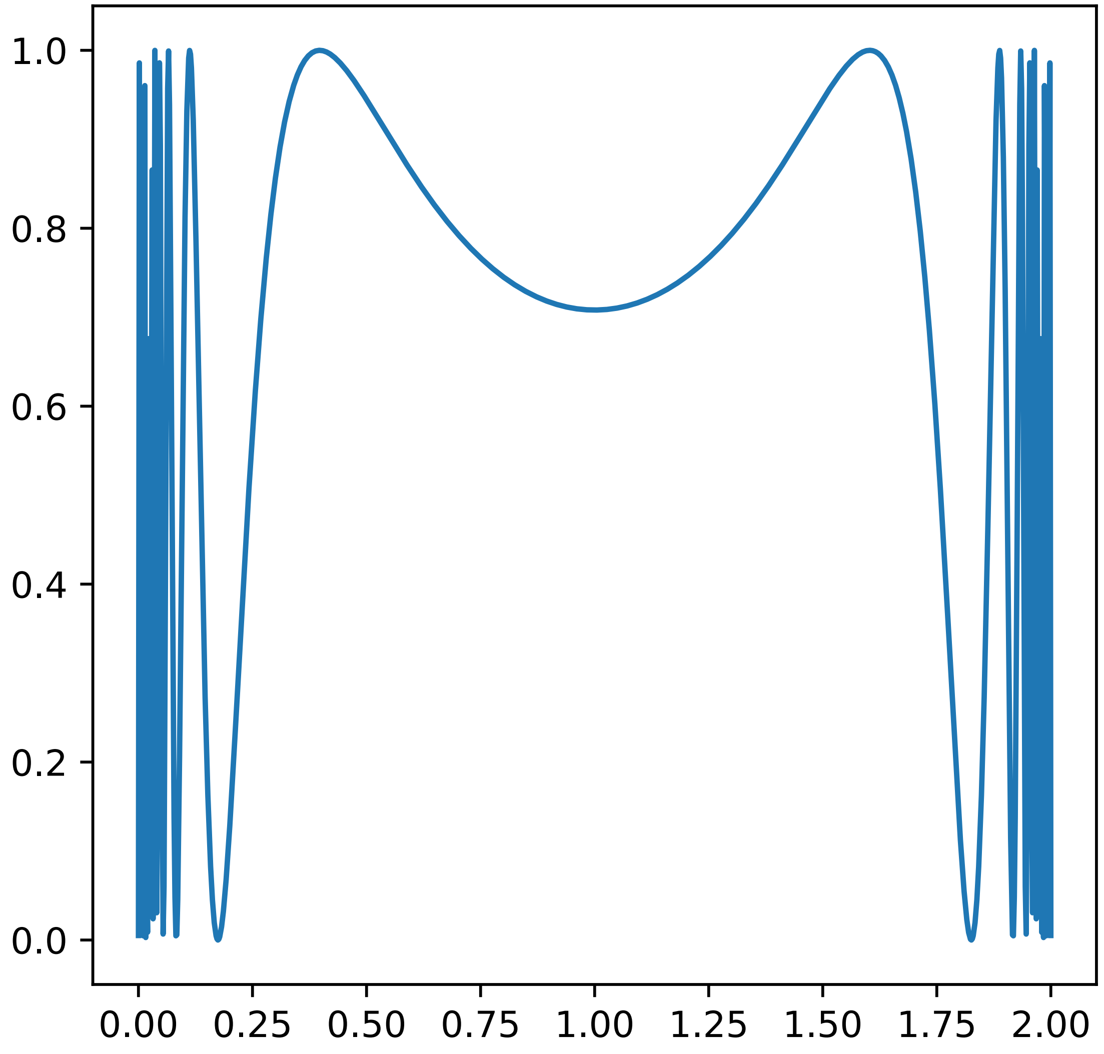
- **Monte Carlo integration**: Approximate the value of an integral (which has an exact solution) with random calculations

Example: Challenging integral with exact solution in principle

- Consider the function:

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

- Finite over the range, must be less than 2x1=2
- Oscillates infinitely fast at the edges so very challenging for numerical integration

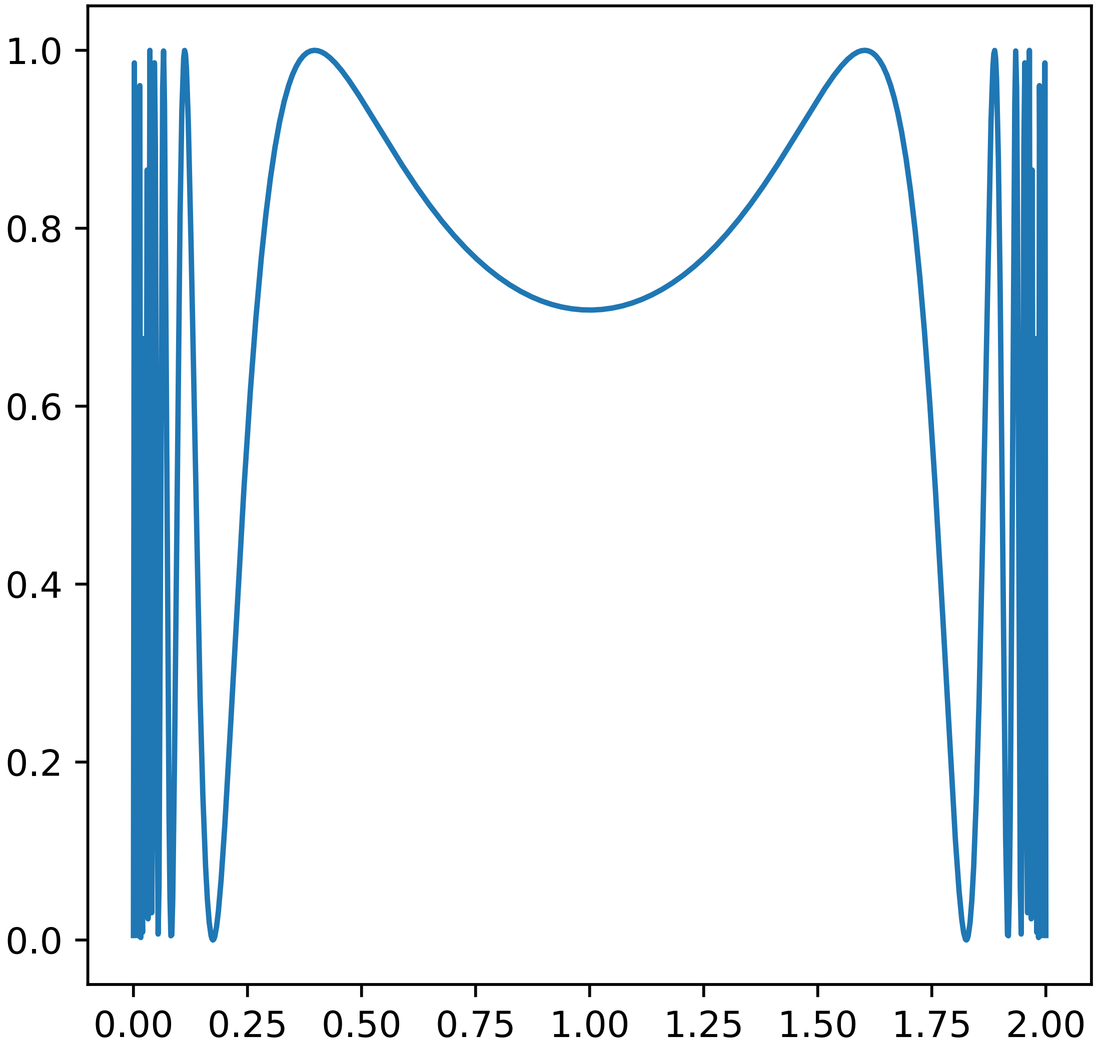


Monte Carlo Integration with random sampling

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

- Choose *N* random samples in the bounding rectangle with area *A*=2
- Check which lie under the curve
- Probability that point lies under the curve is *p* = *I*/*A*
- Fraction of points under the curve *k*/*N* should be approximately *p*
- So:

$$I \simeq \frac{kA}{N}$$



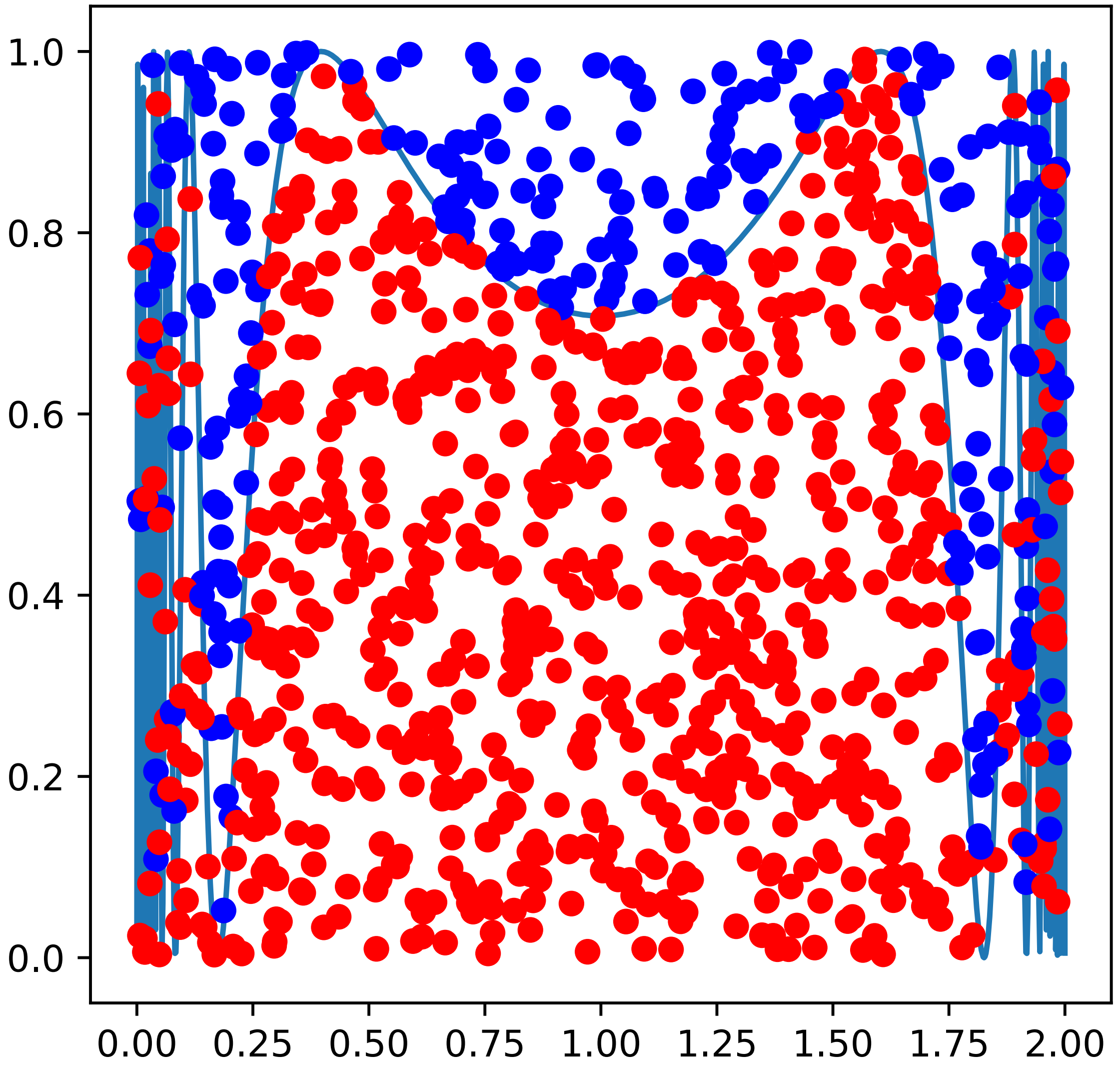
Errors in Monte Carlo method

- Normally gives worse results than, e.g., Simpson's or trapezoid rule for simple integrals
- Probability random point falls below the curve is *p*, above is 1-*p*
- Probability that *k* points fall below the curve is

$$p^k(1-p)^{N-k}$$

- There are *N* choose *k* ways to choose *k* points, so the probability to get *k* points under the curve is

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



Errors in Monte Carlo method

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

- This is a binomial distribution, which has variance:

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

- And standard deviation is: $\sqrt{\mathrm{var}k}$

- So, the error on the integral *I* is:

$$I_{\mathrm{error}} = \sqrt{\mathrm{var}k}\,\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}$$

Compare MC errors to quadrature rules

$$I_{\text{error}} = \sqrt{\text{var}k}\,\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}$$

- Errors for MC integration decrease like $N^{-1/2}$
- For the trapezoid rule, error was on the order of Δx^2, where Δx is the width of the integration slice:

$$\Delta x = \frac{b-a}{N}$$

- So, error decreases like N^{-2} much better than MC!
- For Simpson's rule, it decreases like N^{-4}

- **Monte Carlo methods should be used only when other methods break down!**

Can we do better? Mean value method

- Consider general integration problem: $I = \int_a^b f(x)dx$
- Average value of *f* in the range between *b* and *a* is:

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

- So, we can get the integral by finding the average of *f*:

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

- We can estimate the average by measuring *f*(*x*) at *N* points chosen at random between *a* and *b*
- Then:

$$I \simeq \frac{(b-a)}{N}\sum_{i=1}^{N} f(x_i)$$

Errors of the mean value method

- Can estimate the error using the general theorem: **The variance on the sum of *N* independent random numbers is the sum of the variances of the individual numbers**
  - Holds no matter what the distribution is
- So:

$$\operatorname{var} f \equiv \langle f^2 \rangle - \langle f \rangle^2$$

- Where:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i), \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

- And:

$$I_{\text{error}} = \frac{b-a}{N} \sqrt{N \operatorname{var} f} = (b-a) \frac{\sqrt{\operatorname{var} f}}{\sqrt{N}}$$

Still $N^{-1/2}$, but prefactor turns out to be smaller

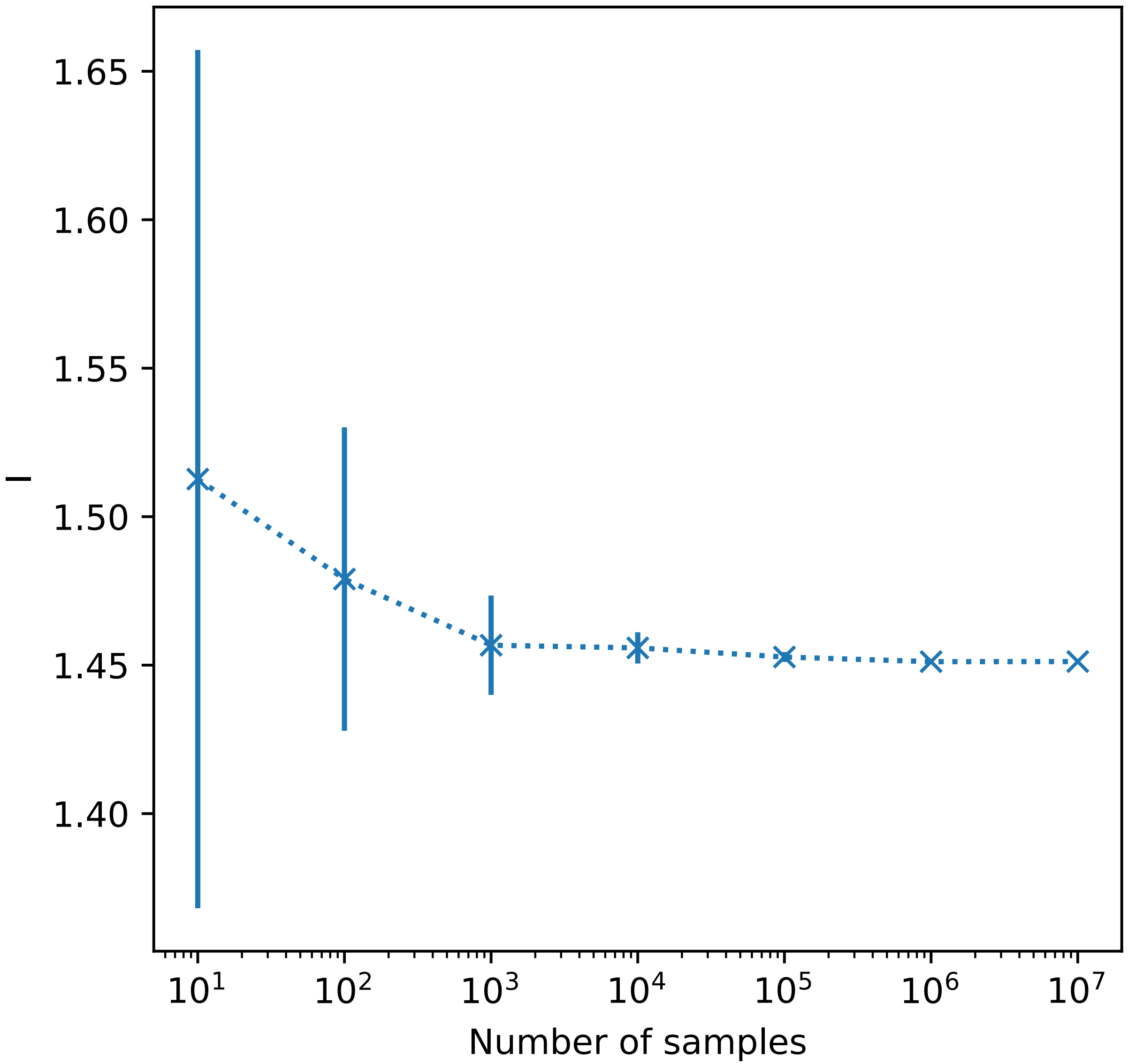
Mean value method

- Equation:

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

- Errors:

$$I_{\text{error}} = (b-a)\frac{\sqrt{\operatorname{var} f}}{\sqrt{N}}$$



When to use Monte Carlo integration? Multi-dimensional integrals

- If we have an integral over many dimensions (> 4), grid sizes get very large, scale as N^d
- Monte Carlo integration can give reasonable results with many fewer points
- Straightforward to generalize methods discussed to more dimensions
  - E.g., mean value method

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

Example: Volume of hypersphere

- Consider a hypersphere of unit radius in all dimensions:

$$f(\mathbf{r}) = \begin{cases} 1 & \text{if } \mathbf{r} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

- Let's use the mean value method to compute the integral of a 10-dimensional hypersphere
  - Trapezoid rule with 100 samples per dimension: 10^{20} grid points!

- We can compare to the exact solution:

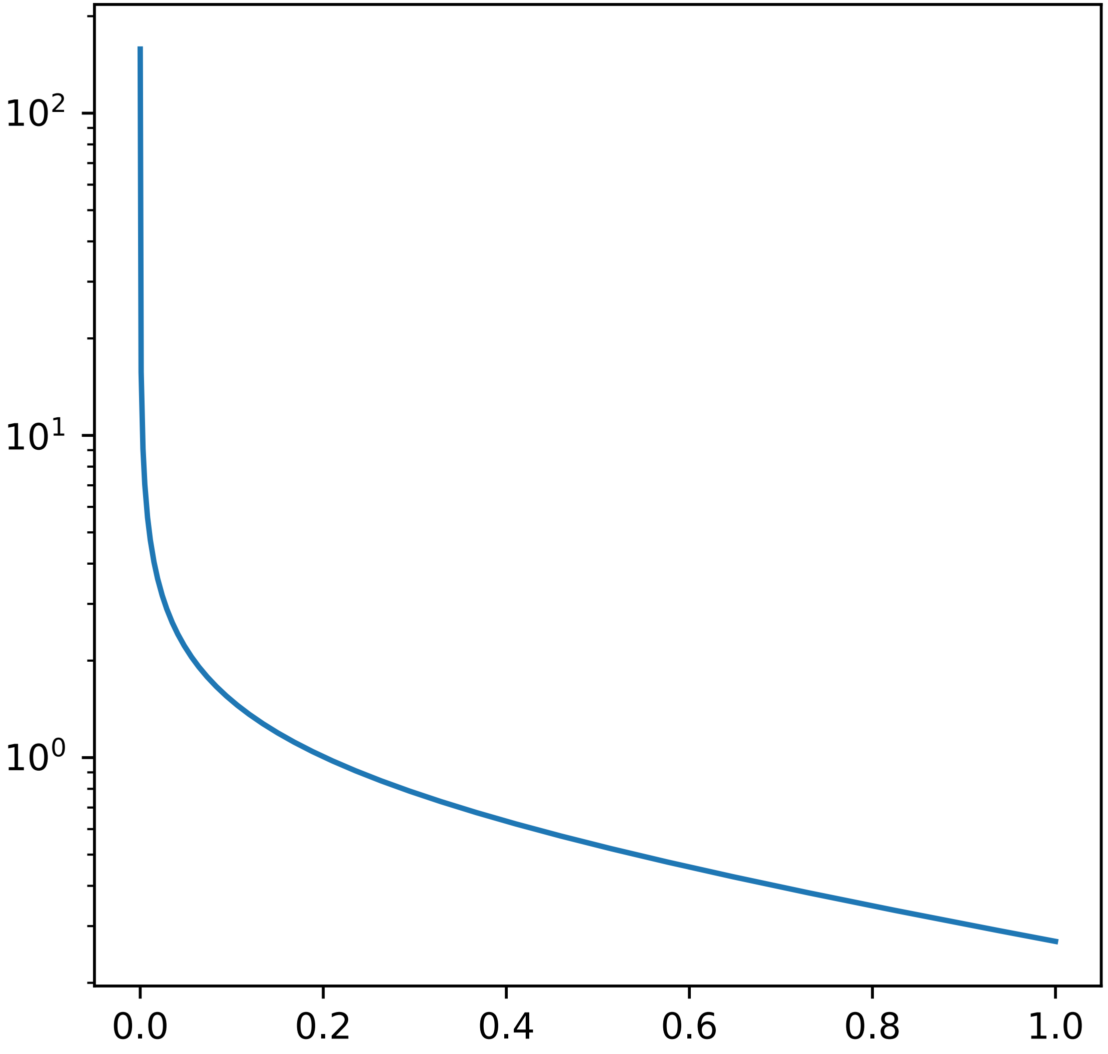
$$V_d(r) = \frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} r^d$$

Monte Carlo integration with divergences

- Monte Carlo integration fails for some pathological functions, e.g., those that contain divergences
- Consider:

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

- Function diverges at x=0, but integral is finite
- E.g., for mean value method, will occasionally get a very large contribution
  - Estimate varies widely between runs



Importance sampling

- Can get around these issues by drawing points nonuniformly
- For a general function *g*(*x*) can define a weighted average:

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

- *w*(*x*) is a weighting function
- If we want to solve a general 1D integral: $I = \int_a^b f(x) dx$
- We set *g*(*x*)=*f*(*x*)/*w*(*x*):

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

Importance sampling, 1D integral

- Thus, we have:

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

- Equivalent to the mean value method, but from a weighted average
- How do we calculate the weighted average?
- Define probability density function as normalized *w*(*x*)

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

- So

$$\langle g \rangle_w = \int_a^b p(x)g(x)dx$$

Importance sampling, 1D integral

- Now let's sample *N* random points in the interval with the distribution *p*(x). Then:

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

- So:

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

- Where x_i are chosen from the distribution:

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

Importance sampling, 1D integral

- Putting everything together:

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

- Generalization of mean value method, which is where *w*(*x*)=1
- *w*(*x*) can be any function that we choose
    - Can be chosen to remove pathologies in the integrand

- However, now we need to draw from a nonuniform distribution

Error on importance sampling method

- Error is given by:

$$I_{\mathrm{error}} = \frac{\sqrt{\mathrm{var}_w(f/w)}}{\sqrt{N}} \int_a^b w(x)dx$$

- Where:

$$\mathrm{var}_w g = \langle g^2 \rangle_w - \langle g \rangle_w^2$$

- Still goes like $N^{-1/2}$

Importance sampling for pathological function

- Let's return to the integral: $I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$
- Choose: $w(x) = x^{-1/2}$
- Then: $f(x)/w(x) = (e^x + 1)^{-1}$
  - Finite and well-behaved over the range
- Probability distribution is:

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

- So, using the transformation method:

$$\int_0^x \frac{1}{2\sqrt{x'}} dx' = \sqrt{x} = z \quad \Longrightarrow \quad x = z^2$$

Importance sampling for pathological function

- So finally, we need to sample:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{e^{x_i}+1}\int_0^1 \frac{1}{\sqrt{x}}dx = \frac{1}{N}\sum_{i=1}^{N}\frac{2}{e^{x_i}+1}$$

- With the distribution $x = z^2$

After class tasks

- Homework 3 is graded, see GRADES.md in your repo
- Homework 4 due today
- Homework 5 posted soon

- Readings:
  - Newman Sec. 10.2