

Exercise Set #3

due online Wednesday, April 25 at 10:10 AM

Please refer to the instructions from Exercise Set #1 about how to code and submit your work.

1. Importance sampling

- (a) Estimate the integral $\int_0^\pi \sin x \, dx$ and the uncertainty on the estimate by using uniform sampling over the interval.
- (b) Plot the uncertainty estimate (from uniform sampling) as a function of N , the number of points evaluated. How does the uncertainty change with N ?
- (c) Estimate the integral $\int_0^\pi \sin x \, dx$ and the uncertainty on the estimate by using importance sampling. (It may be helpful to note that $\sin x \approx \frac{4}{\pi^2} x(\pi - x)$ over the interval $[0, \pi]$.)
- (d) Plot the uncertainty estimate (from importance sampling) as a function of N , the number of points evaluated. How does the uncertainty change with N , and how does it compare to part (b)?

2. Acceptance/rejection method

Use the von Neumann (acceptance/rejection) method to estimate the following integrals numerically, including uncertainties. (Each of these integrals presents a new wrinkle in the calculation.) Motivate your choices of weighting functions for each of these integrals.

- (a) $\int_1^2 x^2 \, dx$
- (b) $4 \int_0^1 \sqrt{1 - x^2} \, dx$
- (c) $\int_0^2 (4 - x^2)^{1/2} \, dx$

3. Neutron scattering in a lead wall

We can use a random walk to estimate the probability for a low-energy neutron to penetrate a thick lead wall. This was actually one of the original uses of the Monte Carlo method when it was developed at Los Alamos.

Each neutron enters the lead wall in the x direction, at a right angle to the surface, and it travels a unit distance (arbitrary units). Then it collides with a lead atom and rebounds in a random direction. (Assume the scattering probability is uniform in θ .) It travels a unit distance again before colliding with another lead atom and scattering in a new direction. After 15 collisions, the neutron has lost all of its energy and does not move any more.

- (a) If an beam of neutrons is incident on a lead wall 5 units thick in the x direction and practically infinite in the y direction, what is the probability for a neutron to pass through to the other side of the wall? That is, how effective is the lead wall at shielding the neutrons?
- (b) Draw the random walk of a sample neutron that penetrates the wall.
- (c) Draw the histogram of the y coordinates where the neutrons exit the wall, assuming they enter at $y = 0$.
Hint: should the distribution be symmetric about 0? Why or why not?

4. Metropolis method

Use the Metropolis algorithm to sample the normal (Gaussian) distribution in one dimension.

- (a) For various step sizes, calculate the acceptance ratio (fraction of steps accepted) and the near-neighbor correlation functions $C(k)$ (for $k = 1, 2, 3$ only). Why do the neighboring points of the random walk seem to be correlated?
- (b) Use the random numbers you generated during the sampling to calculate

$$\int_{-\infty}^{\infty} x^2 e^{-\frac{1}{2}x^2} dx$$

5. Landau 17.4.2 (Thermodynamic properties of ferromagnetic 1-D Ising model in equilibrium)

- (a) Calculate the internal energy U and the magnetization \mathcal{M} for the chain with $N = 100$.
- (b) Plot the results as a function of kT and check them against Figure 17.3.
- (c) Show that the agreement with the analytic results in Section 17.3.1 is better for $N = 2000$ than for $N = 100$.