Lab 2 : Using Random numbers

PH456

Semester 2, 2020–2021

1 Aim

The aims of this exercise is to perform and understand integration using Monte-Carlo sampling methods.

2 Tasks

1. Write a routine which takes inputs of 1) a reference to a function to be integrated (i.e. the integrand), 2) the limits of the integral and 3) the number of points to sample. It should return an estimate of the value of the integral the error in the estimate, using simple Monte Carlo integration from the notes about definite integrals.

   Think about how your function can to be written so that both one-dimensional and multi-dimensional integrals can be evaluated.

2. Using your function, evaluate the following definite integrals, and report the uncertainty in their evaluation. Investigate their convergence with the number of random points (**hint:** you may need to use many random numbers to get accurate values).

   $$\text{a)} \int_0^1 2\mathrm{d}x \quad \text{b)} \int_0^1 -x\mathrm{d}x \quad \text{c)} \int_{-2}^{2} x^2\mathrm{d}x \quad \text{d)} \int_0^1 \int_0^1 xy + x \ \mathrm{d}x\mathrm{d}y$$

   Evaluate these integrals analytically to check your numerical results.

3. Use your subroutine to evaluate the size of the region enclosed within an n-sphere of radius 2.0, for $n = 3$ (i.e. the volume of a ball of radius 1.5) and $n = 5$.

   hint: integrate the step function function $\Theta(r)$, where $\Theta(r > 2.0) = 0$ and $\Theta(r \leq 2.0) = 1$, where r is the distance from the origin.[1]. Using integral limits of -2 to 2 for each Cartesian direction

4. Evaluate, to at least 10% accuracy, the nine-dimensional integral

$$I = \int_0^1 \dots \int_0^1 \frac{\mathrm{d}a_x \mathrm{d}a_y \mathrm{d}a_z \mathrm{d}b_x \mathrm{d}b_y \mathrm{d}b_z \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z}{|(\mathbf{a}+\mathbf{b})\cdot\mathbf{c}|}$$

   where $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ each have 3 independent components.

5. Implement new code to apply importance sampling to evaluate one dimensional integrals. Use the Metropolis method to generate the non-uniform random sampling of the weighting function (and remember that the weighting function must be *normalised correctly*).

   Use this new function to evaluate the definite integrals

   (a) $\int_{-10}^{+10} 2e^{-x^2}\mathrm{d}x$ using $e^{-|x|}$ as the sampling function.

   (b) $\int_0^{\pi} 1.5\sin(x)\,\mathrm{d}x$, noting that $\sin(x) \approx \frac{4}{\pi^2}x(\pi - x)$ in this region.

   hint: when developing this code, it may be useful to plot a histogram of the values generated by the random walk (and remember that only $\sim$50 % of the steps should be accepted.

6. Evaluate both integrals in task 5 with uniform sampling – Compare your importance sampled result with the answer obtained using uniform sampling. You should compare and contrast the number of points required to achieve an answer of equal accuracy using the two methods.

[1]This is not a good way to integrate over hyperspheres, as the region in the 'corners' of a box grows rapidly with n.

3 Computational hints

1. Recall that the *variance* of the integrand can be used to estimate the error in determining the average value of a function within the limits of the integral (but remember the square root!).

4 Evaluation

You should hand in **at least** the following:

- A short report ($\sim$ 2 pages of text, plus extra materials) detailing what you did.
- Code listings with adequate documentation.
- Numerical answers to all integrals along with uncertainties.
- A display of the convergence of *selected* integrals as the number of sampling points increases.