AA 372

Homework III

Please submit your codes together with your write-ups. Please email/meet me if something is unclear.

1. **Romberg Integration of improper integrals:** Numerically integrate the following equation:

$$I = \int_{-\infty}^{1} \frac{\sin x}{x} dx. \tag{1}$$

Since $(\sin x/x)$ is symmetric about $x = 0$,

$$I = I_1 + 2I_2, \tag{2}$$

where

$$I_1 = \int_{1}^{\infty} \frac{\sin x}{x} dx, \ \& \ I_2 = \int_{0}^{1} \frac{\sin x}{x} dx. \tag{3}$$

Now we should evaluate I_1 and I_2 separately. Its simple to evaluate I_2 via the mid-point rule (we do not want to use the trapezoidal rule here because function evaluation at $x = 0$ is numerically ill-posed) because we have to integrate over a finite interval, unlike in I_1. Use Romberg's method to evaluate I_2 correct to 8 decimal places.

Recall that the sinc function $(\sin x/x)$ has zeros at $x = n\pi$. The range $2n\pi < x < (2n+1)\pi$ contributes positively to the integral and $(2n-1)\pi < x < 2n\pi$ contributes negatively. The absolute value of the area contributed by the interval $[n\pi, (n+1)\pi]$ decreases with x due to $1/x$ factor in the integrand. However, the integrand decreases rather slowly with increasing x. Therefore we need to integrate to large values of x to get I_1 to several significant digits.

Plot the sinc function $\sin x/x$ and approximate I_1 as

$$I_{1,n} = \int_{1}^{(2n+1)\pi} \frac{\sin x}{x} dx. \tag{4}$$

Evaluate $I_{1,n}$ using the mid-point method combined with Romberg for $n = 10, 100, 1000, 10000$. How much do the results differ for different n? Can you use Richardson extrapolation to estimate how $I_{1,n}$ varies with n? *Hint:* Assume that $I = I_n + cn^{-\alpha} + dn^{-\beta} + ...$ (where

c, d, α, β are arbitrary constants); find α, β, etc. by taking appropriate combinations of $I_{1,n}$, $I_{1,2n}$, etc. Can you get a good estimate of I_1 by combining $I_{1,n}$ for several n's? Try to obtain I_1 correct to 8 decimal places using above hints. Now calculate the integral by combining I_1 and I_2 via Eq. 2.

I mentioned in the class that for improper integrals its better to change variables such that the integral is over a finite domain. You can change the variable to $s = 1/x$ and

$$I_1 = \int_0^1 \frac{\sin(1/x)}{x} dx,$$

however the integrand oscillates wildly near $x = 0$ and this integral is not that easy to evaluate (try this!) because $\sin(1/x)$ is unresolved close to $x = 0$. Therefore, the tricks mentioned in class should not be used blindly; its best to plot the integrand and have a feel for how the integral behaves throughout the domain.

Recall that $\int_0^\infty (\sin x/x) dx = \pi/2$; this is obtained via contour integration in the complex plane. So, to obtain result good to 8 decimal places, you can combine this result with I_2 which is evaluated much more easily than I_1. You can verify if your answer is correct to 8 deicmal places using this fact.

2. **MonteCarlo Integration:** Find the volume of the domain formed by the intersection of a sphere of radius 2 and a cylinder of radius 1 passing through the center of the sphere. The equation for points lying within the sphere is $x^2 + y^2 + z^2 < 4$ and the equation for points lying within the cylinder is $x^2 + y^2 < 1$. The volume is given by the integral

$$I = \int\int\int_V dxdxdz, \tag{5}$$

where the integral is over the domain of interest (satisfying $x^2+y^2+z^2 < 4$ & $x^2 + y^2 < 1$). We can consider a cube of side 4 circumscribing the sphere and generate random numbers representing x, y, z (even if the numbers are not random we will get the right answer, as long as they are uniformly distributed within the cube) uniformly distributed over the cube. The integral is given by

$$I \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}, \tag{6}$$

where $\langle f \rangle$ is the average value of f (recall $f = 1$ for points within the desired domain and zero outside it) over the known volume V (=64 in case of a cube of side 4) sampled with N uniformly distributed random numbers. The default random number generators in C, Fortran, and MATLAB are not good enough to get accurate answers. Use the NR subroutine ran2 for generating random numbers.

Another way of evaluating the integral is

$$I = \int\int\int_V r^2 dr \sin\theta d\theta d\phi = \int\int\int_V d(r^3/3)\theta d(\cos\theta) d\phi, \qquad (7)$$

where you can calculate $\langle f \rangle$ either by choosing random points uniformly distributed in r, θ and ϕ (in that case $f = r^2 \sin\theta$ if the random point lies within the volume of interest and $f = 0$ otherwise) or by choosing points uniformly distributed in $r^3/3$, $\cos\theta$ and ϕ (in this case $f = 1$ if the random point lies inside the domain of interest and $f = 0$ otherwise). Notice that in these cases the volume of the domain over which we are distributing the random numbers is sphere of radius 2. Which of the three methods (choosing a cube, sphere with points uniformly distributed in (r, θ, ϕ), or sphere with points uniformly distributed in $r^3/3$, $\cos\theta$ and ϕ) is better and why? *Hint:* recall that the error in the MonteCarlo method is given by the second term on the RHS of Eq. 6. You should calculate this expected error in each case and see if this gives a good error estimate (i.e., are you within one standard deviation of the correct answer?).

An even better choice of domain is the cylinder going from $z = -2$ to 2. We know the volume of this cylinder and most of the points will contribute to the integral and the error will be much smaller (why?). Implement this and compare with previous choices. Integral in this case is

$$I = \int\int\int_V d\phi dz d(R^2/2). \qquad (8)$$

Plot the volume as a function of number of random points. Does the result converge to a constant value with increasing N, as it should if the random numbers are good enough (i.e., really uniformly distributed). You can analytically calculate this integral and compare your numerical results.

3. π**:** Calculate π using the Monte Carlo method. Assume a 2-D square domain $[0, 1] \times [0, 1]$. The value of π is given by four times the area of the quarter-circle. Using a good random number generator (e.g., ran2) calculate the value of π for $N \times N$ uniformly distributed guess points ($N = 2^k$, where $k = 1, 2, ..., 13$). Plot the value of π as a function of number of guess points. Calculate the error estimate of the Monte Carlo method and compare with the actual error. Does it go like N^{-1}, as expected (the expected trend is N^{-1} and not $N^{-1/2}$ because there are N^2 sampling points)? **Bonus:** Do the same exercise in 3-D (by considering 1/8th of a unit sphere) and show how the error converges with number of grid points. Which method (2-D or 3-D) is more efficient?