# MSDM5004 Part II Assignment 2

## Due: 15 May 2022, 23:59

1. Consider the integral

$$I = \int_0^1 \sin^2 \sqrt{100x}\, dx$$

(a) Calculate $I$ by adaptive trapezoidal rule method to an approximate accuracy of $\epsilon = 10^{-6}$ (i.e., correct to six digits after the decimal point). Start with one single integration slice and work up from there to two, four, eight, and so forth. Have your program print out the number of slices, its estimate of the integral, and its estimate of the error on the integral, for each value of the number of slices $N$, until the target accuracy is reached.

(b) Calculate $I$ by adaptive Simpson's rule method to an approximate accuracy of $\epsilon = 10^{-6}$. Starting with two integration slices, work up from there to four, eight, and so forth, printing out the results at each step until the required accuracy is reached. Compare the results and the efficiency with that of part (a).

(c) Calculate $I$ by Romberg integration technique to an approximate accuracy of $\epsilon = 10^{-6}$. Have your program print out a triangular table of values, as in the lecture notes, of all the Romberg estimates of the integral. Compare the results and the efficiency with that of part (a) and (b).

2. Debye's theory of solids gives the heat capacity of a solid at temperature $T$ to be

$$C_V = 9V\rho k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\, dx$$

where $V$ is the volume of the solid, $\rho$ is the number density of atoms, $k_B$ is Boltzmann's constant, and $\theta_D$ is the so-called Debye temperature, a property of solids that depends on their density and speed of sound.

(a) Define dimensionless heat capacity by

$$\widetilde{C_V} = \frac{C_V}{9V\rho k_B}$$

and dimensionless temperature by

$$\tilde{T} = \frac{T}{\theta_D}$$

Write a Python function that calculates $\widetilde{C_V}$ for a given value of $\tilde{T}$ by Gaussian quadrature.

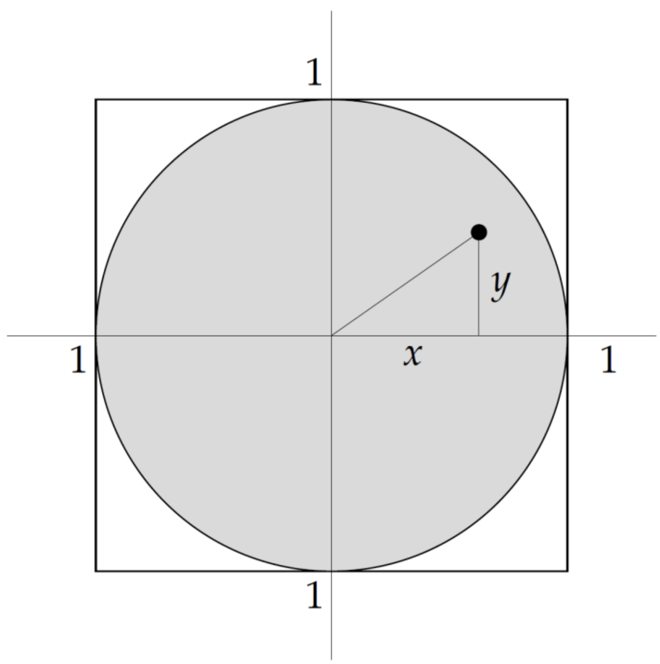
(b) You are asked to find the heat capacity of a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of $\rho = 6.022 \times 10^{28}\ \mathrm{m}^{-3}$ and a Debye temperature of $\theta_D = 428$ K.

Compute it by the program you wrote in (a) with $N = 50$ sample points. Make a graph of the heat capacity as a function of temperature from

$T = 5$ K to $T = 500$ K.

3. In this question you will estimate the volume of a sphere of unit radius in ten dimensions using a Monte Carlo method.

Consider the equivalent problem in two dimensions, the area of a circle of unit radius:




The area of the circle, the shaded area above, is given by the integral

$$\int_{-1}^{1}\int_{-1}^{1} f(x,y)\,dx\,dy$$

where $f(x,y) = 1$ everywhere inside the circle and zero everywhere outside. In other words,

$$f(x,y) = \begin{cases} 1 & \text{if } x^2 + y^2 \leq 1 \\ 0 & \text{Otherwise} \end{cases}$$

So if we didn't already know the area of the circle, we could calculate it by Monte Carlo integration. We would generate a set of $N$ random points ($x$, $y$), where both $x$ and $y$ are in the range from −1 to 1. Then the two-dimensional version for this calculation would be

$$I \approx \frac{4}{N} \sum_{i=1}^{N} f(x_i, y_i)$$

Generalize this method to the ten-dimensional case and write a program to perform a Monte Carlo calculation of the volume of a sphere of unit radius in ten dimensions.

If we had to do a ten-dimensional integral the traditional way, it would take a very long time. Even with only 100 points along each axis (which wouldn't give a very accurate result) we'd still have $100^{10} = 10^{20}$ points to sample, which is impossible on any computer. But using the Monte Carlo method we can get a pretty good result with a million points or so.

4. Consider the integral

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

(a) Set the artificial cutoff of the upper limit at $x = 10$ and evaluate the integral

$$I' = \int_0^{10} \frac{x^{1/2}}{e^x + 1} dx$$

by Monte Carlo integration.

State your answer as well as the error estimation. Use number of points

$N = 1000000$.

(b) State two shortcomings of the above direct simple Monte Carlo method.

Now let us evaluate the integral by sampling points with weight function

$$w(x) \propto \frac{1}{e^x + 1}$$

(c) Evaluate the integral $I$ by Monte Carlo integration using 1000000 points with weight function $w(x)$ sampled by the transformation method. State your answer and the error estimation. How do they compare with the results in (a)?

(d) For practice, also sample 1000000 points with weight $w(x)$ by Metropolis Algorithm to evaluate $I$. State your answer and the error estimation. How do they compare with the results of (a) and (c)?