COMPUTATIONAL METHODS IN RESEARCH

ASSIGNMENT 3

Exercise 1 (5.1 from book)

The file called `velocities.txt` contains two columns of numbers, the first representing time t in seconds and the second the x-velocity in meters per second of a particle, measured once every second from time $t = 0$ to $t = 100$. The first few lines look like this:

```
0        0
1        0.069478
2        0.137694
3        0.204332
4        0.269083
5        0.331656
```

Write a program to do the following:

1. Read in the data and, using the trapezoidal rule, calculate from them the approximate distance traveled by the particle in the x direction as a function of time.
2. Extend your program to make a graph that shows, on the same plot, both the original velocity curve and the distance traveled as a function of time.

Exercise 2 (5.3 from book)

Consider the integral

$$E(x) = \int_0^x e^{-t^2}\, dt.$$

1. Write a program to calculate $E(x)$ for values of x from 0 to 3 in steps of 0.1. Choose for yourself what method you will use for performing the integral and a suitable number of slices.
2. When you are convinced your program is working, extend it further to make a graph of $E(x)$ as a function of x.

Note that there is no known way to perform this particular integral analytically, so numerical approaches are the only way forward.

Exercise 3 (part of 5.4 from book)

The Bessel functions $J_m(x)$ are given by

$$J_m(x) = \frac{1}{\pi}\int_0^{\pi} \cos(m\theta - x\sin\theta)\, d\theta,$$

where m is a nonnegative integer and $x \geq 0$.

Write a Python function `J(m,x)` that calculates the value of $J_m(x)$ using Simpson's rule with $N = 1000$ points. Use your function in a program to make a plot, on a single graph, of the Bessel functions J_0, J_1, and J_2 as a function of x from $x = 0$ to $x = 20$.

Exercise 4 (part of 5.7 of the book)

To solve this problem you need to read the Sec.5.3 of the book.

Consider the integral

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

1. Write a program that uses the adaptive trapezoidal rule method of Section 5.3 and Eq. (5.34) to calculate the value of this integral 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. (Hint: You should find the result is around $I = 0.45$.)

Exercise 5 (5.8 of the book)

To solve this problem you need to read the Sec.5.3 of the book.

Consider the integral

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

1. Write a program that uses the adaptive Simpson's rule method of Section 5.3 and Eqs. (5.35) to (5.39) to calculate the same integral as in Exercise 5.7, again to an approximate accuracy of $\epsilon = 10^{-6}$. Starting this time 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. You should find you reach that accuracy for a significantly smaller number of slices than with the trapezoidal rule calculation.

Exercise 6 (5.12 from the book)

The Stefan–Boltzmann constant

The Planck theory of thermal radiation tells us that in the (angular) frequency interval ω to $\omega + \mathrm{d}\omega$, a black body of unit area radiates electromagnetically an amount of thermal energy per second equal to $I(\omega)\,\mathrm{d}\omega$, where

$$I(\omega) = \frac{\hbar}{4\pi^2 c^2} \frac{\omega^3}{(\mathrm{e}^{\hbar\omega/k_B T} - 1)}.$$

Here,

*) $\hbar$ is Planck's constant over 2π, that is $\hbar = 1.054571800 \times 10^{-34}$ J.s

*) $c = 299792458$ m/s is the speed of light,
*) $k_B = 1.38064852 \times 10^{-23}$ m^2.kg.s^{-2}.K^{-1} is Boltzmann's constant,
*) and $\sigma = 5.670367 \times 10^{-8}$ W.m^{-2}.K^{-4} is the Stefan–Boltzmann constant.
The total energy per unit area radiated by a black body is

$$W = \frac{k_B^4 T^4}{4\pi^2 c^2 \hbar^3} \int_0^\infty \frac{x^3}{\mathrm{e}^x - 1}\,\mathrm{d}x.$$

1. Write a program to evaluate the integral in this expression. Explain what method you used, and how accurate you think your answer is.
2. Even before Planck gave his theory of thermal radiation around the turn of the 20th century, it was known that the total energy W given off by a black body per unit area per second followed Stefan's law: $W = \sigma T^4$, where σ is the Stefan–Boltzmann constant. Use your value for the integral above to compute a value for the Stefan–Boltzmann constant (in SI units) to three significant figures. Check your result against the known value written above.

Exercise 7 (5.13 from the book)

Quantum uncertainty in the harmonic oscillator

In units where all the constants are 1, the wavefunction of the nth energy level of the one-dimensional quantum harmonic oscillator—i.e., a spinless point particle in a quadratic potential well—is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\, \mathrm{e}^{-x^2/2}\, H_n(x),$$

for $n = 0 \ldots \infty$, where $H_n(x)$ is the nth Hermite polynomial. Hermite polynomials satisfy a relation somewhat similar to that for the Fibonacci numbers, although more complex:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

The first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$.

1. Write a user-defined function `H(n,x)` that calculates $H_n(x)$ for given x and any integer $n \geq 0$. Use your function to make a plot that shows the harmonic oscillator wavefunctions for $n = 1$, 2, 3, and 4, all on the same graph, in the range $x = -4$ to $x = 4$. Use a legend.
2. Make a separate plot of the wavefunction for $n = 30$ from $x = -10$ to $x = 10$.
3. The quantum uncertainty of a particle in the nth level of a quantum harmonic oscillator can be quantified by its root-mean-square position $\sqrt{\langle x^2 \rangle}$, where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2\,\mathrm{d}x.$$

   Write a program that evaluates this integral and then calculates the uncertainty (i.e., the root-mean-square position of the particle) for a given value of n. Use your program to calculate the uncertainty for $n = 5$. You should get an answer in the vicinity of $\sqrt{\langle x^2 \rangle} = 2.3$.

Exercise 8 (5.15 from the book)

Create a user-defined function `f(x)` that returns the value $1 + \frac{1}{2}\tanh 2x$, then use a central difference to calculate the derivative of the function in the range $-2 \le x \le 2$. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots. (Hint: In Python the tanh function is found in the `math` package, and it's called simply `tanh`.)

Exercise 9 (part of 5.17 from the book)

The gamma function

A commonly occurring function in physics calculations is the gamma function $\Gamma(a)$, which is defined by the integral

$$\Gamma(a) = \int_0^\infty x^{a-1} \mathrm{e}^{-x} \, \mathrm{d}x.$$

There is no closed-form expression for the gamma function, but one can calculate its value for given a by performing the integral above numerically. You have to be careful how you do it, however, if you wish to get an accurate answer.

1. Write a program to make a graph of the value of the integrand $x^{a-1}\mathrm{e}^{-x}$ as a function of x from $x = 0$ to $x = 5$, with three separate curves for $a = 2$, 3, and 4, all on the same axes. You should find that the integrand starts at zero, rises to a maximum, and then decays again for each curve.

2. Most of the area under the integrand falls near the maximum, so to get an accurate value of the gamma function we need to do a good job of this part of the integral. We can change the integral from 0 to ∞ to one over a finite range from 0 to 1 using the change of variables in Eq. (5.67), but this tends to squash the peak towards the edge of the $[0, 1]$ range and does a poor job of evaluating the integral accurately. We can do a better job by making a different change of variables that puts the peak in the middle of the integration range, around $\frac{1}{2}$. We will use the change of variables given in Eq. (5.69), which we repeat here for convenience:

$$z = \frac{x}{c + x}.$$

   For what value of x does this change of variables give $z = \frac{1}{2}$? Hence what is the appropriate choice of the parameter c that puts the peak of the integrand for the gamma function at $z = \frac{1}{2}$?

3. Before we can calculate the gamma function, there is another detail we need to attend to. The integrand $x^{a-1}\mathrm{e}^{-x}$ can be difficult to evaluate because the factor x^{a-1} can become very large and the factor e^{-x} very small, causing numerical overflow or underflow, or both, for some values of x. Write $x^{a-1} = \mathrm{e}^{(a-1)\ln x}$ to derive an alternative expression for the integrand that does not suffer from these problems (or at least not so much).

4. Now, using the change of variables above and the value of c you have chosen, write a user-defined function `gamma(a)` to calculate the gamma function for arbitrary argument a.

Use whatever integration method you feel is appropriate. Test your function by using it to calculate and print the value of $\Gamma(\frac{3}{2})$, which is known to be equal to $\frac{1}{2}\sqrt{\pi} \simeq 0.886$.

Exercise 10 (part of 5.17 from the book)

For integer values of a it can be shown that $\Gamma(a)$ is equal to the factorial of $a - 1$. Use your Python function from Exercise 9 to calculate $\Gamma(3)$, $\Gamma(6)$, and $\Gamma(10)$. You should get answers closely equal to $2! = 2$, $5! = 120$, and $9! = 362\,880$.