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Computational Physics Lab Report-5

Aim:

Q1.

***Numerical integration 1:** Plot and integrate the tabulated data given below by a suitable method. Take the end points of the table as integration limits.

x	1.34	1.46	1.52	1.6	1.87	2.03	2.18	2.8	3.2	3.8	4.15
$f(x)$	1.5	2.3	2.3	2.4	2.5	3.2	4.9	4.7	3.4	7.8	17.1

Q2.

***Numerical integration 2:** Write a function in python *trap* (f, a, b, N) which will evaluate the integral $\int_a^b f(x)dx$ using the trapezoidal rule with N steps. Also develop a similar function *simp* (f, a, b, N) for the Simpson's rule. Use these functions to evaluate the numerical integrals in the subsequent problems, wherever applicable.

Use these functions to evaluate the following integrals in limits a to b for $[a,b]$ interval divided into N ($=2^n$, n=1, 2, 3, ...10) **intervals** with:

1) trapezoidal rules
2) Simpson's rule

$f(x)$	x^2	$sin(x)$	$\left(\frac{Sinx}{x}\right)^2$
a	-1	0	0
b	1	π	∞
Analytical value	2/3	2	π/2

Let y_N be the numerical result for N number of intervals used. Let y_{AN} be the analytic result. We define the relative error as

$$e(N) = \left|\frac{y_N - y_{AN}}{y_{AN}}\right|$$

where the error depends on N. Show plot of *log e(N)* with varying *log N* for all the integrals. Are these results keeping with how you expect the error to scale with N?

Q3.

***Numerical integration 4:** We consider the bound 1-D motion of a particle of mass *m* in a time independent potential *V(x)*. The fact that the energy *E* will be conserved allows us to integrate the equation of motion and obtain a solution in closed form. The time period of the oscillation *T* is given by:

$$T = \int_a^b \frac{\sqrt{2m}}{\sqrt{E - V(x)}} dx$$

Where the limits a and *b* are obtained by solving $V(x)=E$, $a<x<b$.

a) Consider a simple harmonic oscillator with potential $\frac{1}{2}m\omega_0{}^2x^2$ for a particle with m = 1Kg and $\omega_0 = 2\pi$ sec^{-1}. Express this integral in terms of dimensionless variables.

a) Numerically calculate the time period of oscillation by integrating the equation with Trapezoidal method and check this against the expected value. Note that the integrand will diverge at the limits. So the limits has to be redefined *i.e.* $b(1\text{-}\varepsilon)$ in place of *b*. Numerically obtained values of *T* will also diverge for very low values of ε. Make a log-log plot of ε vs. *T*. Then choose a suitable value of ε that will provide a reasonably accurate value of *T*. Verify that *T* does not depend on the amplitude of oscillation.

b) Solve for the time period for the potential $V(x) = \frac{m\omega_0{}^2L^2}{2}\left[\exp\left(\frac{x^2}{L^2}\right) - 1\right]$. Plot time period as a function of the amplitude of bound motion in the range [-10 to 10] meters with L = 5m. Observe the variation of *T* for small amplitude.

Tools Used: Jupyter Notebook, Python, NumPy, Pandas, Matplotlib.

Theory:

1. In calculus, the trapezoidal rule (also known as the trapezoid rule or trapezium rule) is a technique for approximating the definite integral.
2. For a non-uniform grid, the trapezoidal rule is defined in the following way-

When the grid spacing is non-uniform, one can use the formula

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{N} \frac{f(x_{k-1}) + f(x_k)}{2} \Delta x_k,$$

wherein $\Delta x_k = x_k - x_{k-1}$.

3. For a uniform grid, the trapezoidal rule is defined in the following way-

For a domain discretized into N equally spaced panels, considerable simplification may occur. Let

$$\Delta x_k = \Delta x = \frac{b-a}{N}$$

the approximation to the integral becomes

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \frac{\Delta x}{2} \sum_{k=1}^{N} (f(x_{k-1}) + f(x_k)) \\ &= \frac{\Delta x}{2}(f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + \cdots + 2f(x_{N-1}) + f(x_N)) \\ &= \Delta x \left(\sum_{k=1}^{N-1} f(x_k) + \frac{f(x_N) + f(x_0)}{2} \right).\end{aligned}$$

4. For Simpson's Rule, the following formula is used -

$$\boxed{\int_a^b f(x)dx \approx \frac{\Delta x}{3} \left[f(x_0) + 4f(x_1) + 2f(x_2) + \ldots.. + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right]}$$

where, $\Delta x = \frac{b-a}{n}$

$x_0 = a$ and $x_n = b$

$x_0, x_0, \ldots\ldots\ldots, x_n$ are the ends of the n sub intervals

$$\boxed{\text{Error bound} = \frac{M(b-a)^5}{180n^4}}$$

where $|f^{(4)}(x)| \leq M$

Observations:

<u>For problem-1:</u>

We made use of the following formula since the given table has non-uniform intervals.

When the grid spacing is non-uniform, one can use the formula

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{N} \frac{f(x_{k-1}) + f(x_k)}{2} \Delta x_k,$$

wherein $\Delta x_k = x_k - x_{k-1}$.

And the value obtained using this is 14.592500000000005 sq. units.

<u>For problem-2:</u>

Yes, the graphs for the first two equations are linear as expected, which are obtained using both methods - Simpson's and Trapezoidal. They have to be linear since the error in the integral obtained using the trapezoidal rule varies in the order of ($1/N^2$), and we are plotting a log-log plot, therefore, the error varies linearly as **-2logN**. For the last function, we do not obtain a completely linear graph as it's not possible to integrate in a definite time from 0 to infinity, hence we are approximating the limiting values to obtain values in finite time.

The error in the Trapezoidal method is given by -

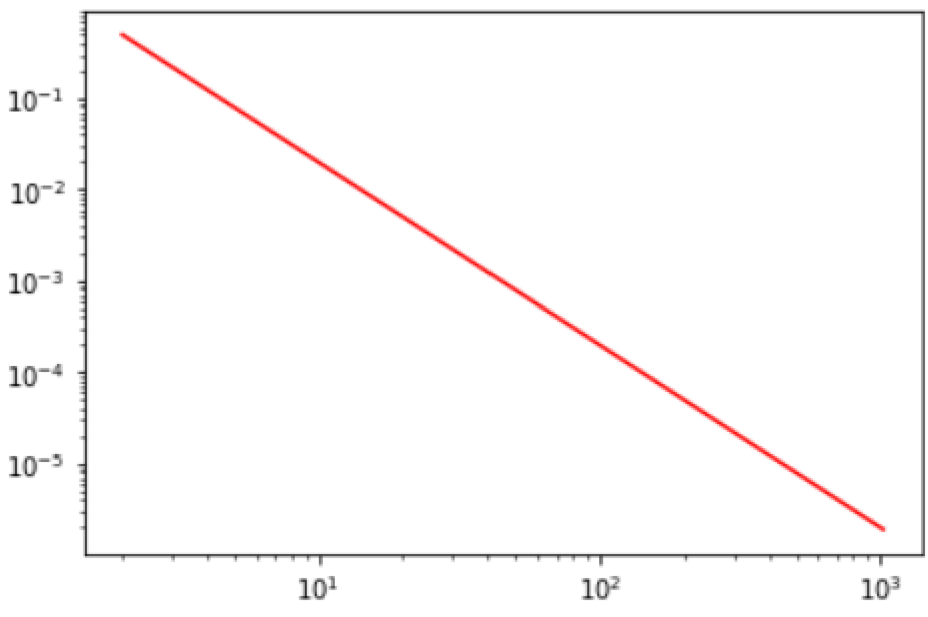
$$E = -\frac{(b-a)^3}{12N^2} f''(\xi)$$

Graphs-

<u>Using Trapezoidal Rule-</u>

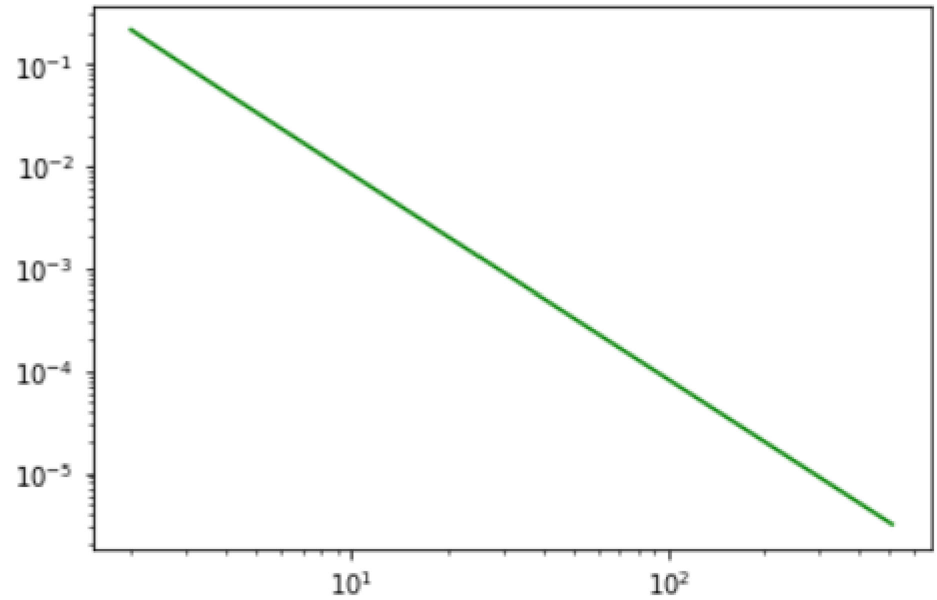
For function-1-

Its value is 0.68



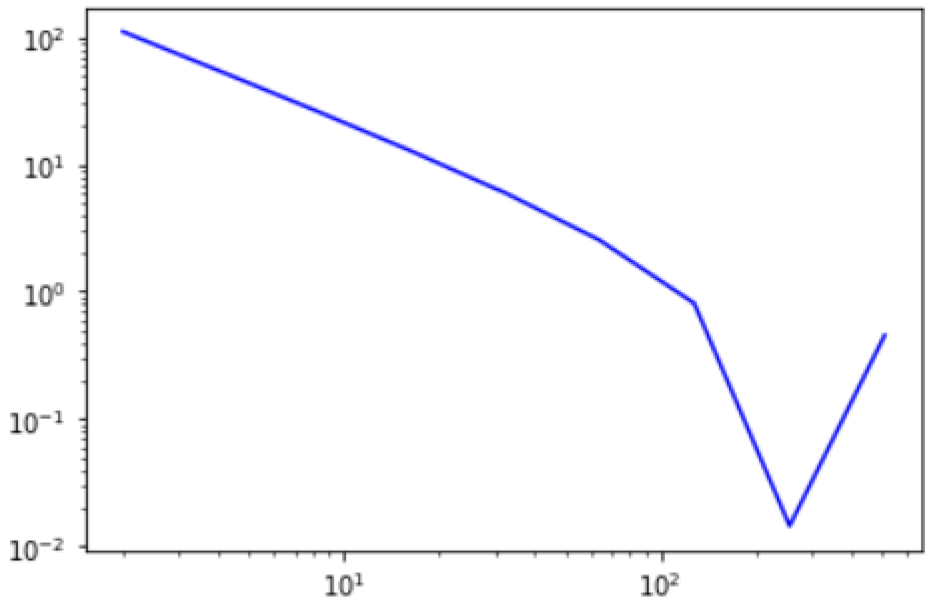
For function-2-

Its value is 1.9835235375094546



For function-3-

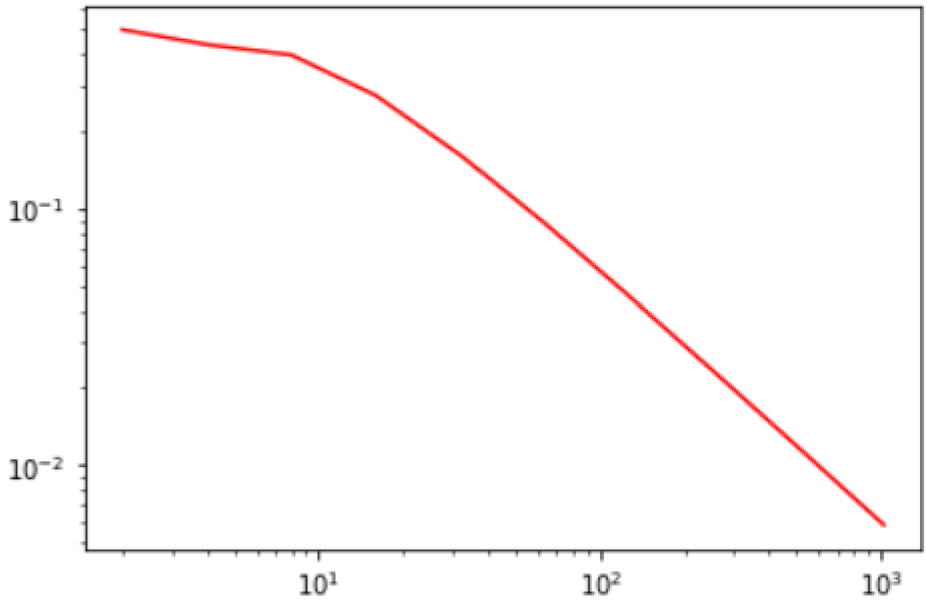
Its value is 500000000.0



<u>Using Simpson's Rule-</u>

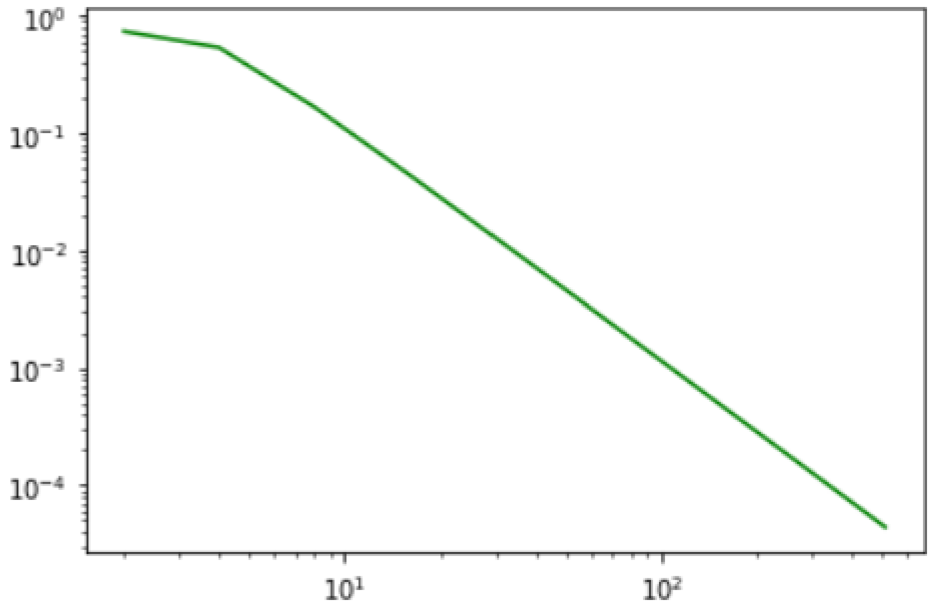
For function-1-

Its value is 0.42399999999999993



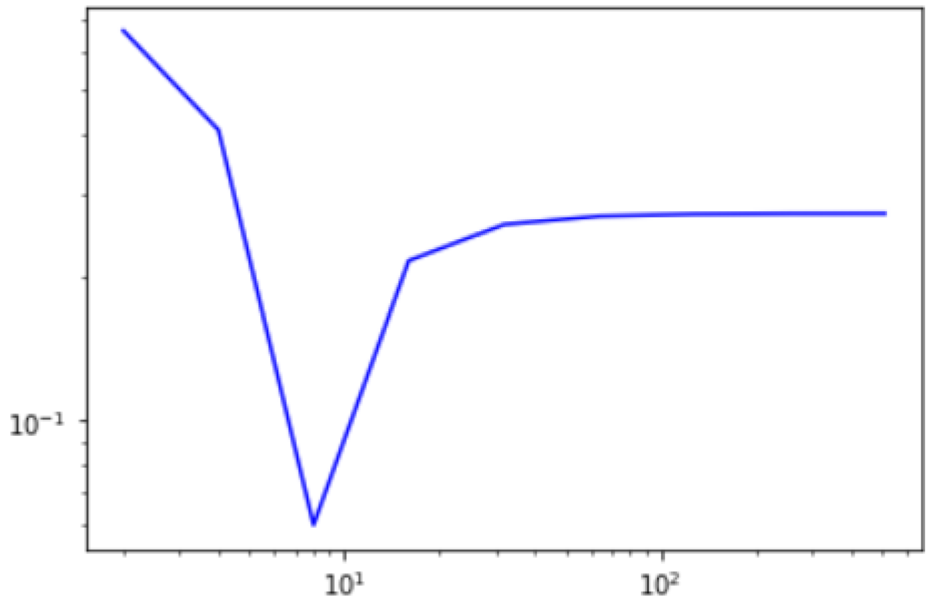
For function-2-

Its value is 1.7799235100127004



For function-3-

Its value is 333333333.3333333



<u>For problem-3:</u>

a) $$T = \sqrt{\frac{2m}{E}} \int_a^b \sqrt{\frac{1}{1-(\frac{V(x)}{E})}}, \; where\, m = 1kg$$

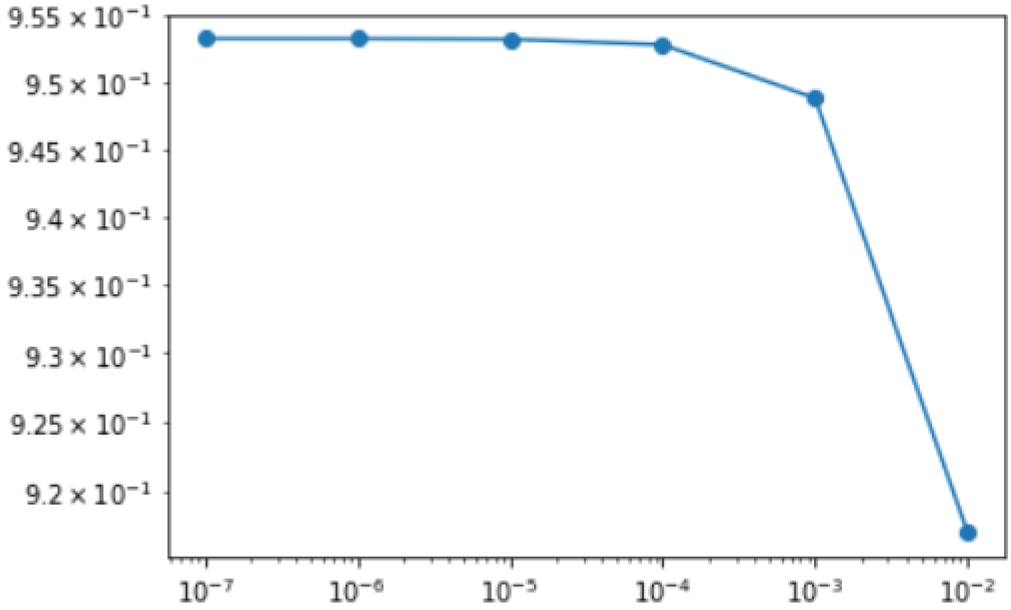
Where a and b are obtained by solving V(x)=E and are expressed in terms of E. Since the integrand will diverge at the limits, redefine the limits as a+e and b-e, where e can be 0.001.

The time period is 0.9867665659584414 s at e=0.01

b) The time period for the second case is 0.6718245425314862 s for E = 2 x $(0.4\Pi)^2$ and L = 5m.

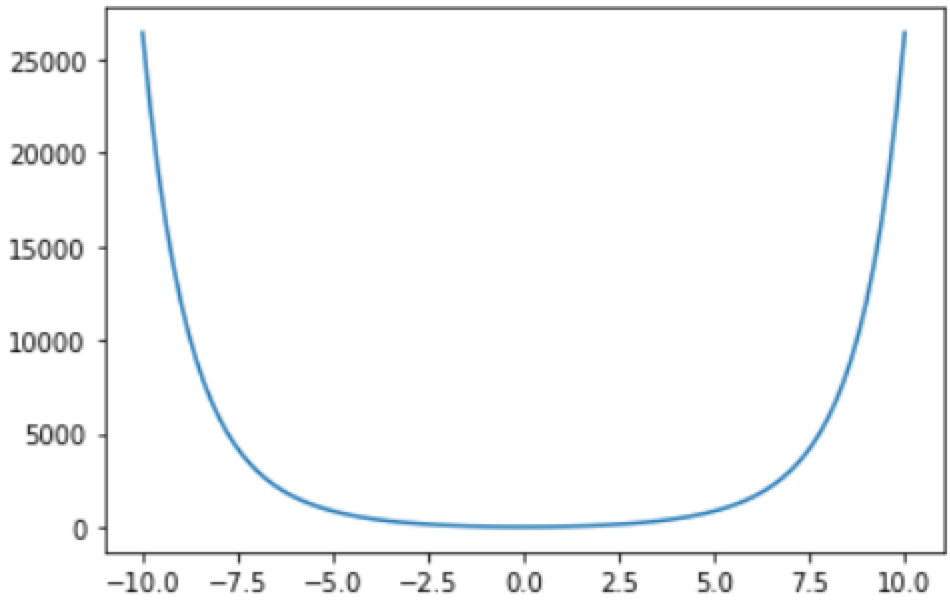
Graphs-

a) Plot of log-log for e vs T

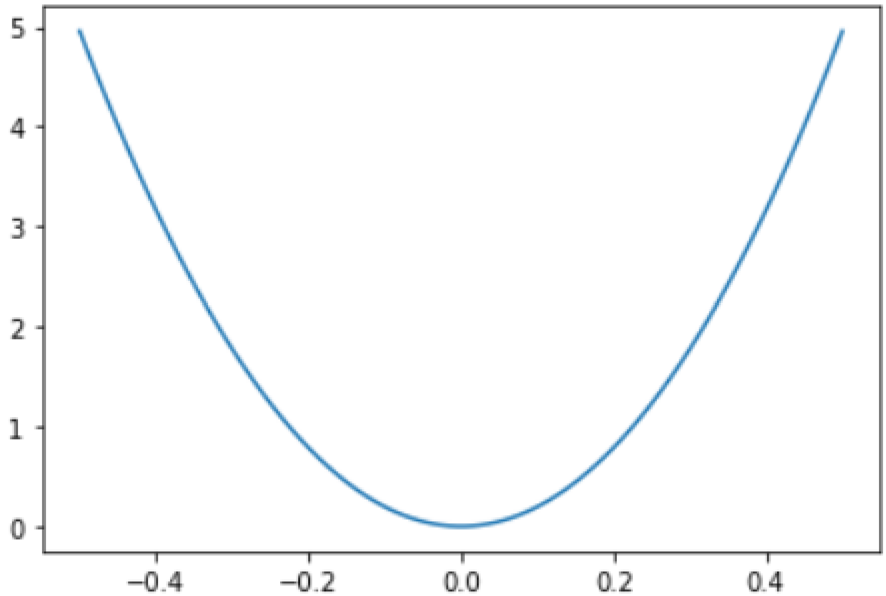


b) Plot of the time period as a function of the amplitude

i) For the range (-10,10)



ii) For very small amplitude whose range lies from -0.5 to 0.5


5
4
3
2
1
0
−0.4
−0.2
0.0
0.2
0.4