Roll No: 20PH20014
Name: Jessica John Britto

Computational Physics Lab Report-3

Aim:

1. Root finding 2: Solve the equation $f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4}$ using Newton-Raphson method for a given error limit of e = 0.0001.
   1. With initial guess of x(0) = 0.05.
   2. With initial guess of x(0)=0.11,

   Why does the 2nd case does not offer any solution? You may start off by plotting the function.
   3. Can you find another initial guess which will lead to no solution? Explain why.
   4. Now take e = [0.1 0.01 0.001 0.0001 0.00001 0.000001 ...] and plot e vs the number of steps needed for convergence (N).

2. Newton-Raphson for finding reciprocal of a number: The reciprocal of a real number a is defined as a zero of the function: $f(x) = x - \frac{1}{a}$.
   The function converges for an initial estimate in the range $0 < x_0 < \frac{2}{a}$.
   a. Write a matlab code that will be able to find the reciprocal of any real number using Newton-Raphson method. Do not set an error limit. Rather let the code run for a fixed number of 50 iterations.
   b. Plot the error propagation (by comparing the outcome of the code and $\frac{1}{a}$) and plot is as a function of the iteration.

3. Diagonal dominance of matrix: Consider the square matrices:

A =[-6 2 1 2 1;
3 8 -4 1 0;
-1 1 4 10 1;
3 -4 1 9 2;
2 0 1 3 10]

B=[18 3 6 -3;
9 13 -5 2;
-3 -2 4 9;
6 0 11 3]

Write a code to see is the matrices A and B are diagonally dominant. In case if they are not, make the code display a message like “Not strictly diagonally dominant on row (row number)”

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

Theory:

1. Newton–Raphson method is a root-finding algorithm that produces successively better approximations of the roots of a real-valued function.
2. In mathematics, a square matrix is said to be diagonally dominant if, for every row of the matrix, the magnitude of the diagonal entry in a row is larger than or equal to the sum of the magnitudes of all the other (non-diagonal) entries in that row. More precisely, the matrix A is diagonally dominant if -

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}| \quad \text{for all } i$$

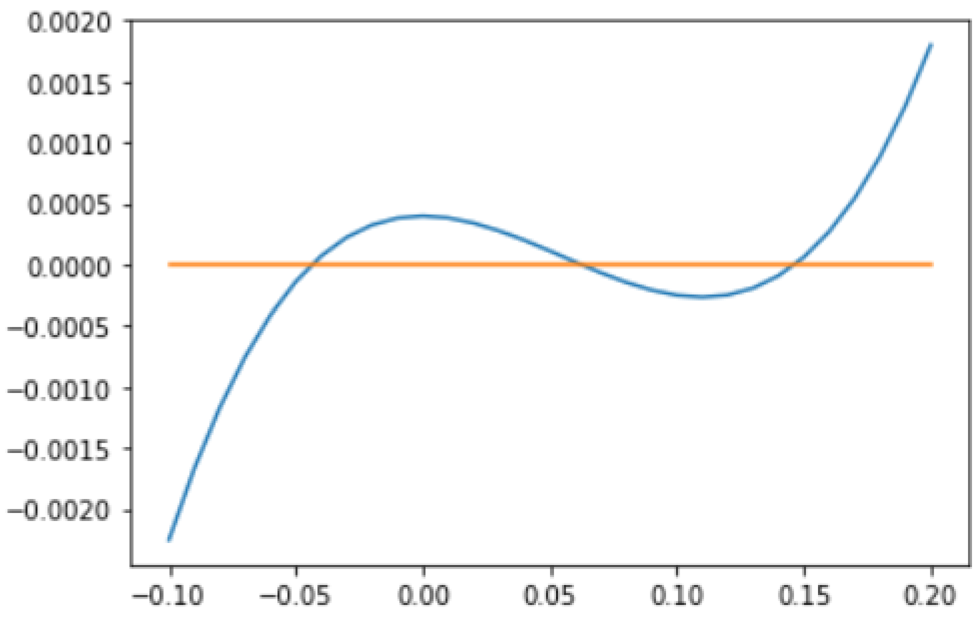
where a_{ij} denotes the entry in the ith row and jth column. If a strict inequality (>) is used, this is called strict diagonal dominance.

Observations:

For problem-1:

For the initial guess of x(0) = 0.05, we get the root of the equation obtained using the Newton-Raphson's method is **0.06242222222222221.**

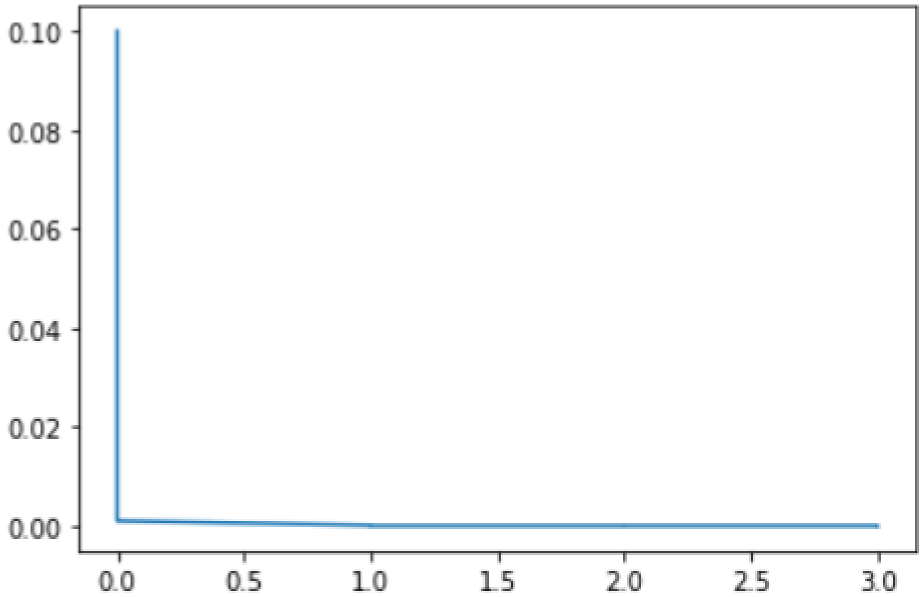
For the initial guess of x(0)=0.11, we cannot find the roots of the function using this initial guess since it is the root of the derivative of the function, and the denominator in Newton–Raphson's method formula, will go to zero at this initial value of x(0), hence x will go to infinity and this initial guess is a point of maxima as can be seen from the graph below. Therefore, this method cannot be used to find the root of the function at the maxima of the function(as initial guess).



Clearly from the plot(of function f(x)) above, the function attains maxima at two points 0 and 0.11. Therefore, the derivative of the function will go to zero at these points of x. Hence, x(0)=0, we cannot Newton-Raphson's method.

Graphs-

Plot of e vs the number of steps needed for convergence (N):



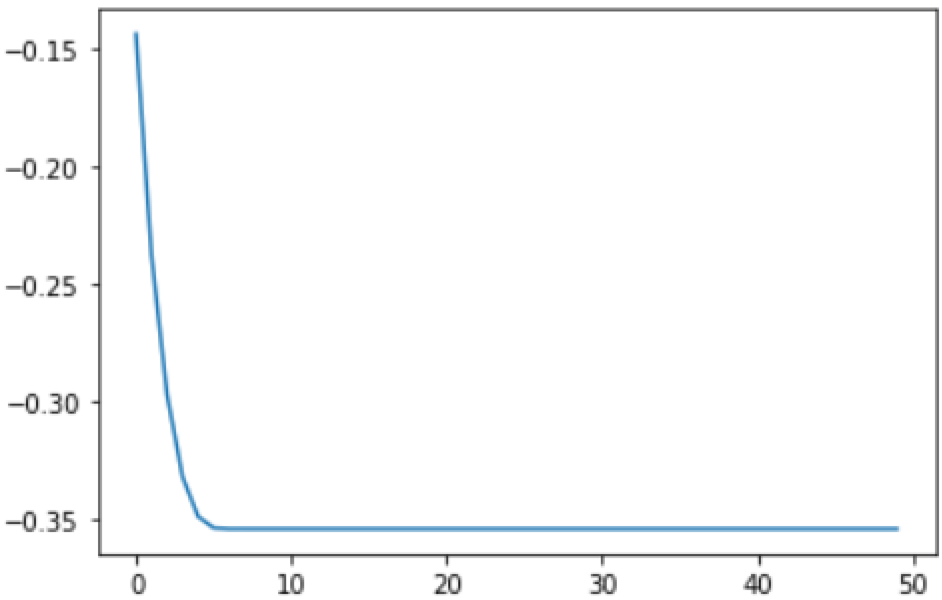
For problem-2:

Clearly, from the graph, we can see that as the number of iterations increases, the error between the calculated value and the actual value decrease and tends to zero.

Graphs-

The following plot is obtained for a value of a = 2 and x = 0.5

Plot of error vs the number of iterations-



For problem-3:

Clearly, the condition below for a square matrix to be diagonally dominant has to be satisfied.

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}| \quad \text{for all } i$$

where a_{ij} denotes the entry in the ith row and jth column. If a strict inequality (>) is used, this is called strict diagonal dominance. This is the condition that has to be satisfied since we are checking if the given matrix is strictly diagonally dominant.

However, as we can see from the output below for A and B, this condition is not satisfied by both of them, we can say that A and B are not strictly diagonally dominant matrices.

```
For A
Not strictly diagonally dominant on row 0
Not strictly diagonally dominant on row 1
Not strictly diagonally dominant on row 2
Not strictly diagonally dominant on row 3


For B
Not strictly diagonally dominant on row 1
Not strictly diagonally dominant on row 2
Not strictly diagonally dominant on row 3
```