1 Introduction

The aim of this project was to implement a Python script to compile, run, and plot the results of the FORTRAN routine "Newton's method to find a root" (which was previously implemented in Homework 4). The Python script allows us to complete the compiling and running steps, having a previously written user-defined runtime parameters file. The script as well as some test applications are described and studied below.

2 Code Description

Since the FORTRAN module has been described earlier in detailed, we will focus on the explanation of the Python module. Given below is the brief understanding of the various functions present in the script.

2.1 A Make function for compilation

This is the function in charge of compiling the complete application including the FORTRAN files. Depending on the situation, it either calls make or make clean.

2.2 Function to write

The part of script which writes the *.init file containing the runtime parameters is done by this function. It takes as input all the parameters, as well as a file name, opens the file and writes the parameters to it. In the current working directory, it creates a file named rootFinder.init, then calls the parameter writing function runtimeParameters.write to complete the task. It also updates the names as per which run and results are going on.

2.3 Function to run the application

This simply runs the application when called. It has no input parameters as well.

2.4 Plotting the Function

This plots the selected function of the user so that the user can make a informed decision while giving the input guesses. It helps the user to select appropriate guesses to the function.

2.5 Plotting the results

We need to plot 2 results at the end of each run. First, the solution as a function of the number of iterations and errors (residuals) as a function of the number of the iterations. This shows the user the plot on the screen as well as saves it as png files. Also, the resulting data points are stored in the .dat files.

2.6 Additional Plots

There is a final plotting function whose idea is to enable us to compare different threshold value having the same x and y scale throughout. It does so by going through the .dat files and finding the maximum value of the x and y points. These values then become the limits of the new plot.
2.7 Main function

This asks for user input and then calls the above function accordingly to give user the appropriate outputs and plots.

3 Test case example

A sample test case is as shown below in Figure 1. The function 1 plot is as shown in Figure 2.
Figure 2: Function Type 1 Plot for reference

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Solution Convergence Summary
Your converged solution x = -6.9045625890752076396
Solution converged in Nstep= 5
Threshold value = 1.000000000000000E-004

Threshold: 0.0001 and initial guess: -4.99
first if
Solution Convergence Summary
Your converged solution x = -6.90456258901151259
Solution converged in Nstep= 8
Threshold value = 1.000000000000000E-004

Threshold: 1e-06 and initial guess: -0.1
first if
Solution Convergence Summary
Your converged solution x = -6.9045625927253433
Solution converged in Nstep= 6
Threshold value = 9.999999999999995E-007

Threshold: 1e-06 and initial guess: -4.99
first if
Solution Convergence Summary
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Figure 3: Runs-1
Figure 4: Runs-2
Figure 5: Output Plots
Figure 6: Output Plots using same scales