Lab 1: Finding Minima of Functions

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February 1, 2023

1 Introduction

The aim of this lab was to preform an investigation into several numerical methods for the solutions of equations and ultimately find the minimum of a Coulomb potential function. In mathematics it is often found that analytical methods are insufficient in finding solutions to many complex equations and we must instead seek numerical methods of approximation to get results that are extremely close to the actual solution.

The first numerical method that was used was the bisection method, an iterative process of halving an interval until sufficiently close to the know analytical solution. Secondly there was the Newton-Raphson method. Again an iterative process but instead uses derivatives of the function to approach the actual solution. Finally the Newton-Raphson method was used to find the minimum of a Ionic interaction potential function.

This Lab was carried out using python 3 and was written in the Spyder application.

2 Methodology

2.1 Exercise 1: Bisection method

The Bisection method, is a mechanism for solving for the roots of some arbitrary equation (in this case a simple parabola was used). To start two variables x_1 and x_3 were used to define a range over which the bisection method would be starting. Code was also added to detect (and if needed warn the user) weather or not this range contained a root of the equation as with out this the bisection process does not work

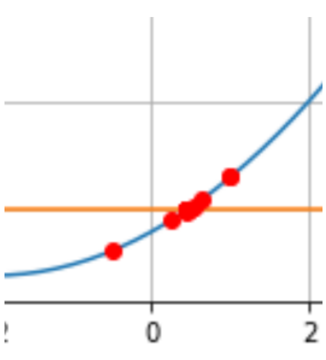

Figure 1: *example of successive bisection steps*

Next came the method of bisection , which involved splitting the interval in question into two and determining which of the two new sections now contained the root. This step was then repeated with the new interval that contains the root and the process was repeated as many times as it was needed using a while loop to continue until a pre-described condition of accuracy was met.

Plots of the function itself and of the approximation results were made, to visually show the effectiveness of the method. Also in a more deeper analysis of the process, plots of the number of steps required to meet a certain tolerance (i.e. accuracy) were made using a logarithmic graph scale.

2.2 Exercise 2: Newton-Raphson method

The Newton-Raphson method was carried out on the same parabola as the bisection method as this allowed an easy comparison of each methods effectiveness. Instead of picking a range, this method picks a point. Evaluating the function and its derivative at that point allows through calculation arrive at a point that is guaranteed to be closer to the root of this equation.

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

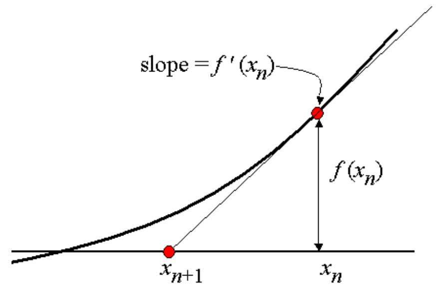

Figure 2: *Newton-Raphson method*

This new point can then be carried through to the next calculation and the process was iterated in a while loop until a certain accuracy was achieved. Once again plots of the function itself and the final approximations were made. To present the exactitude of this method, in a more in-depth analysis (same as bisection method) plots of the number of steps required to meet a certain accuracy were made using a logarithmic graph scale. To calculate the number of steps for each tolerance the while loop was iterated over with a for loop and the number of steps (*nsteps*) was recorded each.

2.3 Exercise 3: Ionic interaction potentials

The task here was to find the minimum of the given ionic potential function $V(x)$. This was an equivalent problem to finding where the Force acting on the particles was zero, seeing as $F = -V'(x)$. To do this the previously explored Newton-Raphson method was employed, modified however, as it was now being used to calculate the zeros of $V'(x)$ using itself and its derivative $V''(x)$ as shown below. This was then iterated in a while loop until the desired accuracy had been met. The equations that were used in the code to carry out these approximations are shown below.

$$V(x) = Ae^{-\frac{x}{p}} - \frac{e^2}{4\pi\epsilon_0 x}, \qquad F(x) = \frac{A}{p}e^{-\frac{x}{p}} - \frac{e^2}{4\pi\epsilon_0 x^2},$$

$$V''(x) = \frac{A}{p^2}e^{-\frac{x}{p}} - \frac{e^2}{2\pi\epsilon_0 x^3}, \qquad x_{n+1} = x_n - \frac{V'(x_n)}{V''(x_n)}.$$

3 Results

3.1 Exercise 1: Bisection method

The Bisection method was quite effective in calculating a point x_3 that was extremely close to the actual value of the root R_1. Shown below is the graph of $f(x)$ with the final approximation point being picked as the first one with an accuracy of less than $1 \cdot 10^{-9}$. Visually this is indistinguishable from the real root.

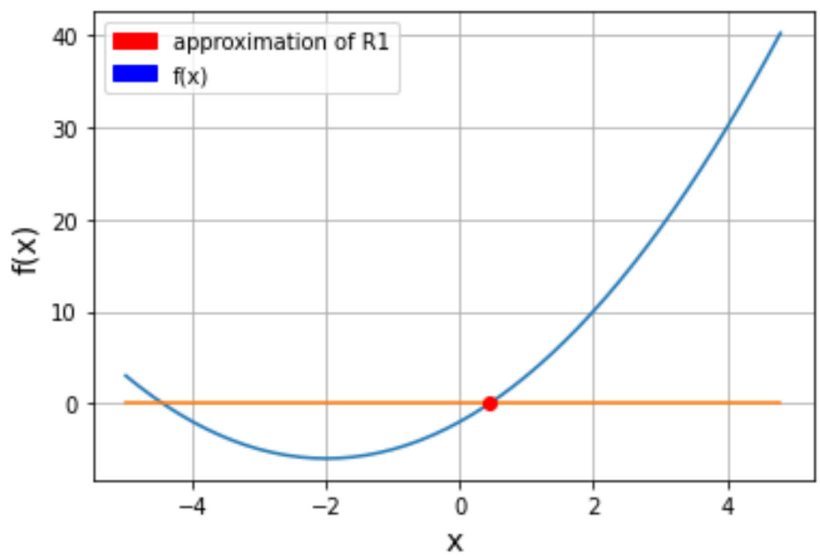

Figure 3: *Bisection approximation graph*

To analyse just how efficient the bisection method is, the number of iterations needed to reach a certain tolerance was recorded. This was then plotted on a logarithmic graph scale so as to precisely show the relationship between *nsteps* and *tolerance*. The relationship can be seen as linear on the log scale graph. Each approximation was over the same sensible range.

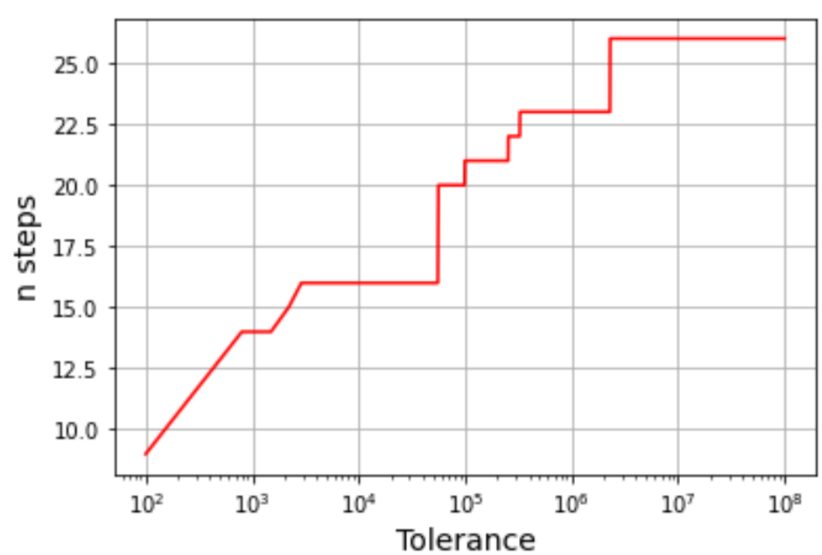

Figure 4: *Bisection graph of nsteps vs tolerance*

3.2 Exercise 2: Newton-Raphson method

The Newton-Raphson method was found to be even more effective at approximating the roots of this parabola. Shown below is the graph of the $f(x)$ with the final approximation point being picked as the first one with an accuracy of less than $1 \cdot 10^{-8}$. Visually this is again indistinguishable from the real root.

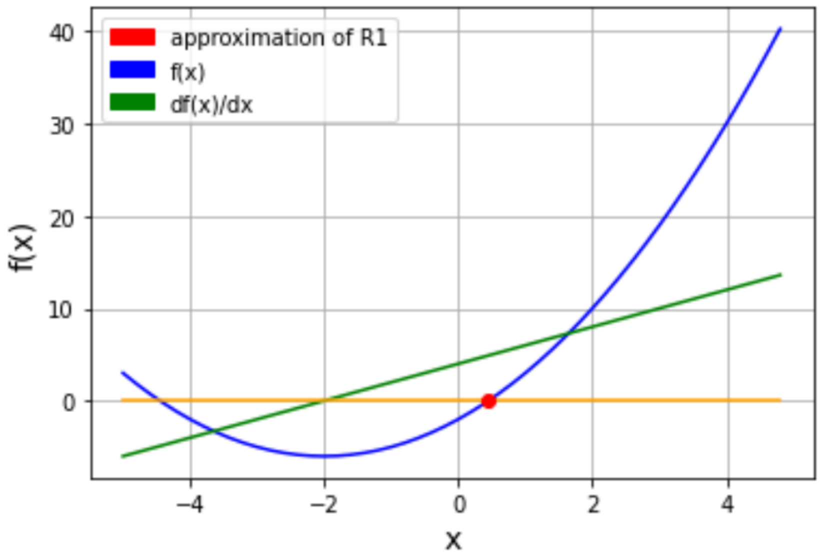

Figure 5: *Newton-Raphson approximation graph*

To analyse the efficiency of the Newton-Raphson approximation, a graph of *nsteps* vs *tolerance* was made once again. This when plotted on a logarithmic scale produced the below graph. This relationship is again roughly linear, though this is not as clear from the graph as due to the accuracy of the Newton-Raphson method. The maximum number of steps before the error was too small for the computer to handle was 4. Thus there was not a great range of values that *nsteps* could take to produce a nice straight figure.

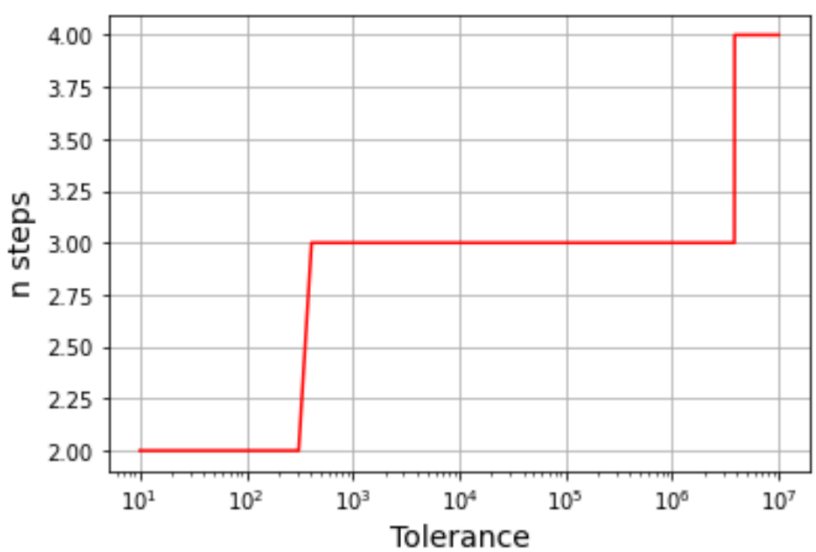

Figure 6: *Newton-Raphson graph of nsteps vs tolerance*

3.3 Exercise 3: Ionic interaction potentials

To examine and find the minimum of this Ionic interaction potential the Newton-Raphson method was used. This cannot directly find the minima of a function but since the function $V(x)$ must have a slope of 0 at the minimum, one can look at the derivative of the function (in this case $F(x) = -V'(x)$) and calculate its zeros to get the value of x for which $V(x)$ is a minimum.

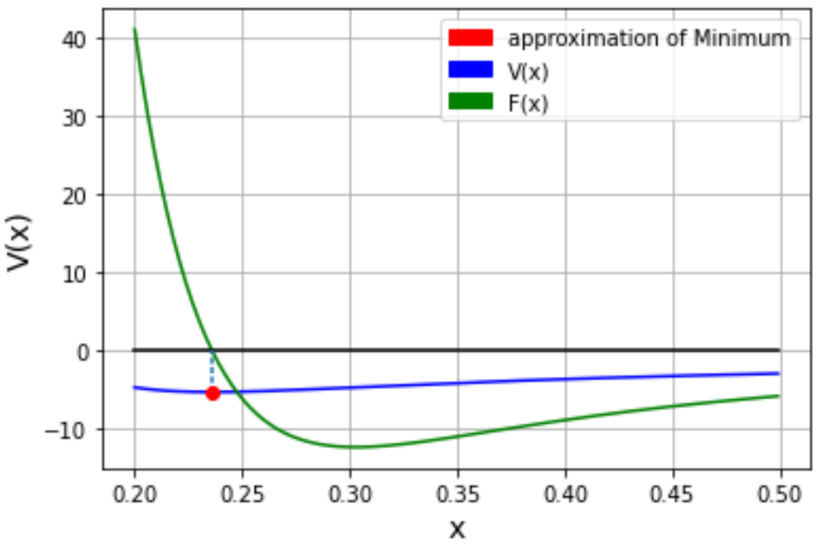

Figure 7: *Graph showing minimum of Ionic potential*

With the previous analysis of the Newton-Raphson method, it is clear that for a sensible starting point this approximation method converges to the zero point with an accuracy greater than the computers in less than 5 steps. So running this approximation 10 times was more than enough to say with confidence that the result accurately represents the minimum of the Ionic interaction potential. This is also quite clear from the above graph

4 Conclusion

The aim of this lab was to preform an investigation into several numerical methods for the solutions of equations. The two numerical methods used were the Bisection method and the Newton-Raphson method. The Newton-Raphson method is clearly by far the superior method. Looking at the graphs for Bisection 3 and Newton-Raphson 5 it is evident that for the same tolerances the Bisection method can take up to 27 steps where as the Newton-Raphson had a maximum of 4 steps. This may not be useful for these simple approximations of parabolas but when applied to more complex functions where more computation is needed it is important that one is using the most efficient approximation method to minimise the time and resources needed. From these results one can conclude that a through study was made into these two numerical methods resulting in the successful approximation for the minimum of the Ionic potential and the conclusion that the Newton-Raphson method is by far the more efficient method.