Senior Fresh Computational Physics Laboratory Report

Laboratory 1: Finding Roots and Minima of Functions

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1 Introduction

Often in physics and mathematics there are problems which are impossible to / are very difficult to solve analytically. Fortunately, it is possible to solve many of these problems computationally through estimation. Two such methods of estimation which exist are the bisection method and the Newton-Raphson method.

The initial aim of these exercises is to compare estimates the roots of a polynomial function with known roots using these two methods. The bisection method **(Fig 2.1)** involves varying an input generated to be the mean average of the sum of two modified values until the function of the input is within a tolerance of the required value. The Newton-Raphson method **(Fig 2.2)** involves adjusting the input of the function by the ratio of the function of that input and the derivative of the function of that input iteratively until it is within the desired tolerance of the required value.

Following from this; an additional aim is to apply the Newton-Raphson method to find the the minimum of a potential energy function in order to determine the bond length of Sodium Chloride (NaCl). The initial aim was met through applying the two methods of root estimation to the polynomial: $\mathrm{x}^{\mathbf{2}} + \pi \mathrm{x} - 2\pi^{\mathbf{2}}$. The additional aim was met through applying the Newton-Raphson method to the negative of the derivative of the the potential energy function in order the find its minimum and thus the associated bond length of sodium chloride (NaCl).

2 Methodology

2.1 Exercise 1:

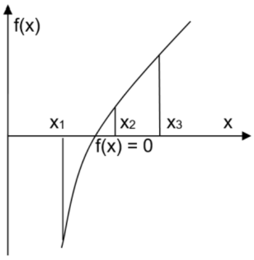

Figure 2.1: **The Bisection Method**

In exercise 1: the bisection method was used to estimate the roots of a parabola. The bisection method involves bisecting two initial values:

$$x_2 = \frac{x_1 + x_3}{2}$$

The mean average of the value of these initial figures are adjusted incrementally until the value of the function of their bisection is within the desired tolerance of the intended output value **(Fig 2.1)**.

This was performed with a for loop which included if-else statements which determined whether the function of the bisection was posive or negative and adjusted initial values until the function of the bisection was within the tolerance. This could have been performed with a while loop but the use of the for loop functioned as intended albeit less efficiently. The function to be estimated was arbitrary and therefore a parabola was selected with the roots π and -2π as the accuracy of the root estimation could be evaluated based on the amount of 'numbers of digits π' which were correct. Both roots were found with this method and the desired tolerance was plotted in a log-log plot against the number of steps required to be within it.

2.2 Exercise 2:

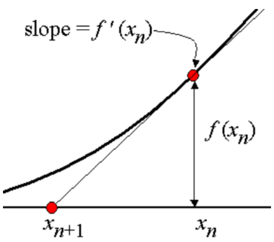

Figure 2.2: **The Newton-Raphson Method**

In exercise 2: the Newton-Raphson method was used to estimate the roots of a parabola. The Newton-Raphson Method involves amending the initial estimate by the ratio of the function of that input and the derivative of the function of that input:

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

This was performed with a while loop which was much more efficient than the for loop employed in exercise 1. The same parabola as exercise 1 was used in order to make comparison between the two methods feasible. Both roots were found with this method and the desired tolerance was plotted in a log plot against the number of steps required to be within it. The maximum accuracy of the method was found and the maximum associated tolerance was noted. This information was used to compare the accuracy and efficiency of the two methods.

2.3 Exercise 3:

In exercise 3: the Newton-Raphson method was used to find the minimum of a potential energy function in order to determine the bond length of Sodium Chloride (NaCl). The function v(x) where x is the separation in nanometers between the sodium and chlorine ions within the influence the pauli repulsion and electrostatic attraction between them.

$$v(x) = Ae^{-\frac{x}{p}} - \frac{e^2}{4\pi\varepsilon_0 x}$$

In order to find the minimum of this function and thus the equilibrium bond length of Sodium Chloride (NaCl), the negative of the derivative of v(x) was found named f(x). The root of f(x) nearest to an appropriate guess of the minimum of v(x) (0.2 nm) was found. The function v(x) was taken of the estimated root of f(x) which corresponded to the associated bond energy in eV of the bond length of Sodium Chloride (NaCl).

3 Results

3.1 Exercise 1:

In exercise 1: the roots of the parabola were calculated to be correct to the fourth decimal place when a tolerance of 0.0001 was utilised:

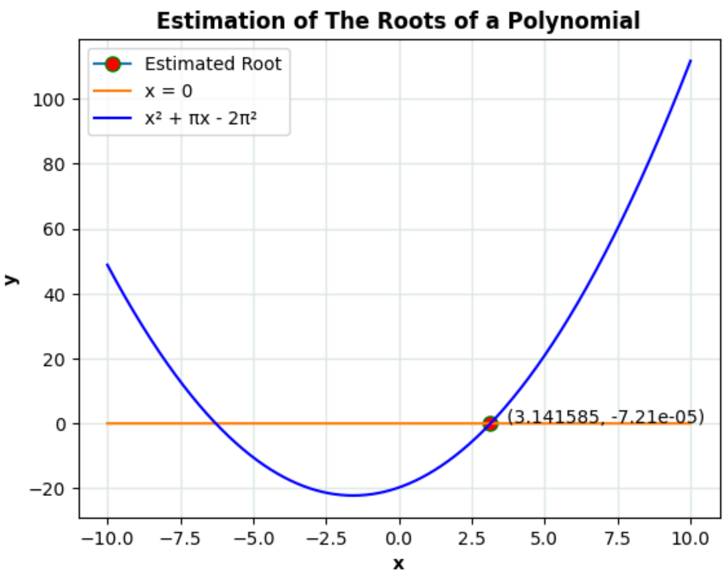

Figure 3.1: **Estimation of the Roots of a Polynomial by Bisection**

3.2 Accuracy and Efficiency of the Bisection Method:

The bisection method required 628318 steps to be within this tolerance which was due part to the less than optimal logic employed within the code. The rate at which the steps required to reach a desired tolerance grew exponentially. Below is a log-log plot of the desired tolerance vs the number of steps required with regard to this method:

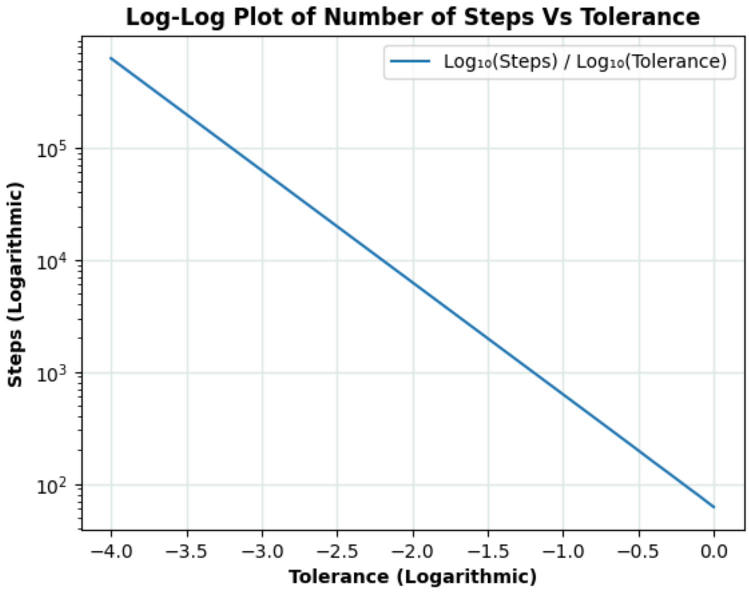

Figure 3.2: **Steps vs Tolerance for Bisection Method**

3.3 Exercise 2:

In exercise 2: the roots of the parabola were calculated to be correct to the fifth decimal place when a tolerance of 0.0001 was utilised which is greater in accuracy than that of the previous method:

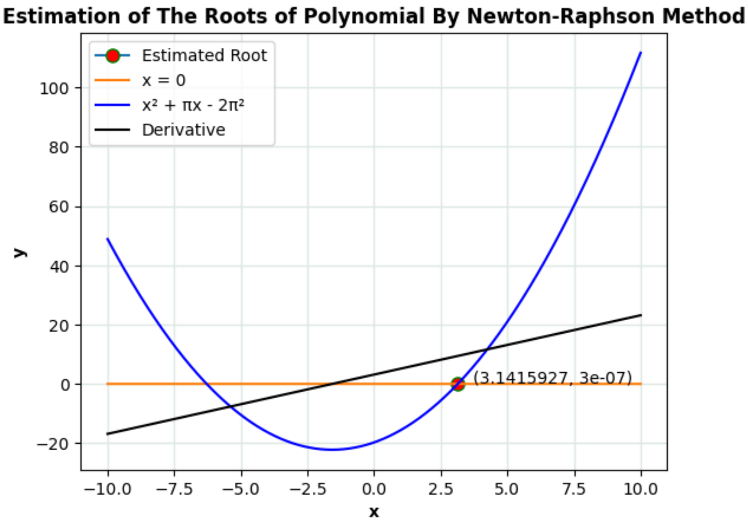

Figure 3.3: **Estimation of the Roots of a Polynomial by Newton-Raphson Method**

3.4 Accuracy and Efficiency of the Newton-Raphson Method:

The Newton-Raphson method required 4 steps to be within this tolerance which is significantly better than the previous method in terms of efficiency by several factors. The Newton Raphson method was able to get the root of the polynomial correct to fifteen decimal places after 6 steps while the bisection method require too much processing time to allow any more than five correct decimal places of accuracy. Below is a log plot of the desired tolerance vs the number of steps required with regard to this method which resembles a step function:

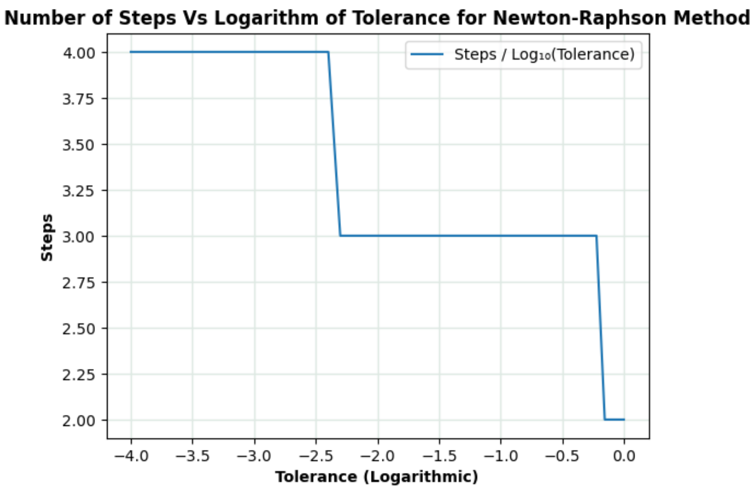

Figure 3.4: **Steps vs Tolerance for Newton-Raphson Method**

3.5 Exercise 3:

In exercise 3: The bond length with minimum bond energy of sodium-chloride (NaCl) was found to be 0.23605384841577942 nm when the tolerance was minimised which is in line with official estimates to at least three decimal places and is also roughly in line with the crude estimation utilised initially which was 0.2nm. Below is a graphical display of the estimation:

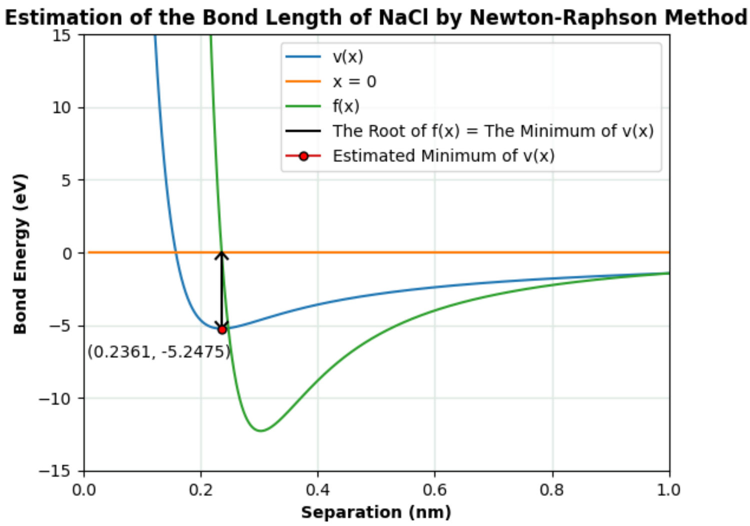

Figure 3.5: **Estimation of Sodium Chloride Bond Length by Newton-Raphson Method**

4 Conclusions

The aim of these exercises was to estimate roots of a polynomial function using the bisection method and the Newton-Raphson method and then apply the Newton-Raphson method to find the minimum of a potential energy function between two ions and thus the associated bond length of sodium chloride (NaCl) The results above indicate that the number of steps and accuracy of each method indicate the Newton-Raphson method is significantly more efficient than the bisection method in estimating the roots of the polynomial due to the decrease in computational time and steps required but unfortunately this was due in part to inefficient logic being employed in the code of the bisection method. The Newton Raphson-Method was shown to accurately estimate the bond length of sodium chloride in line with official estimates using roots of minima. Overall the goals of each exercise were met to sufficient levels of successs.

5 Additional Information

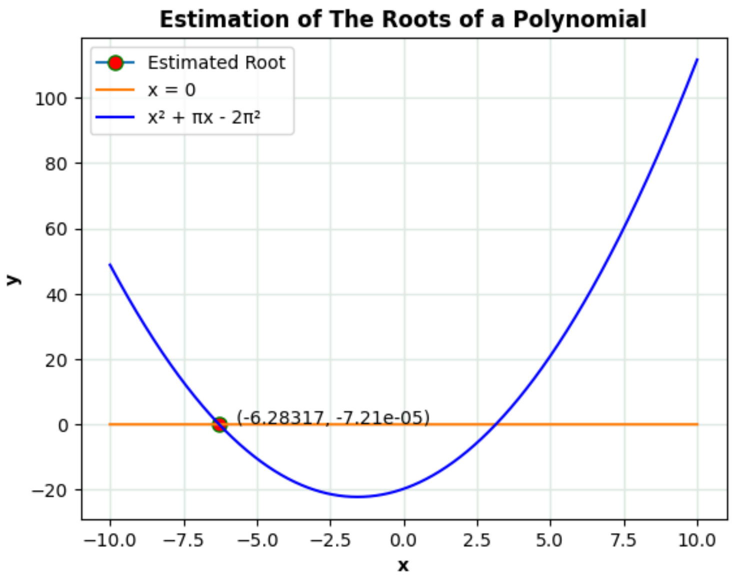

Figure 5.1: **Estimation of the other Root of the Polynomial by Bisection**

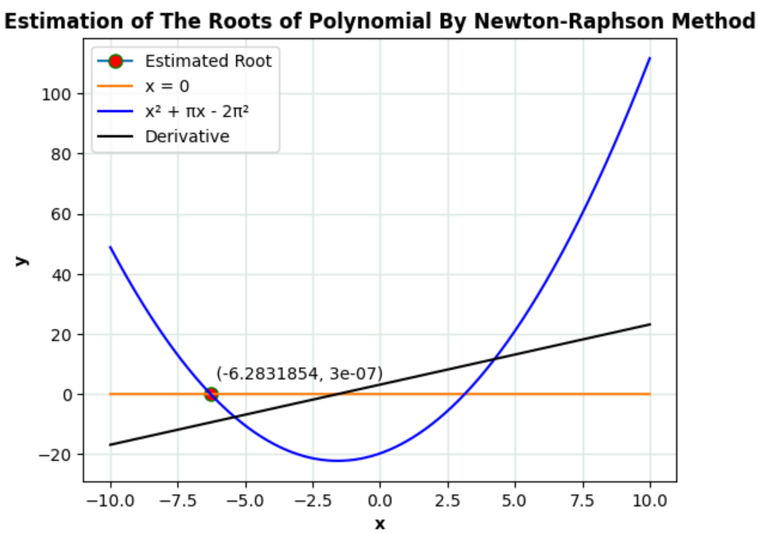

Figure 5.2: **Estimation of the other Root of the Polynomial by Newton-Raphson Method**