Minimisation Problems

David-Alexander Robinson
08332461

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1 Abstract

In this experiment the common functions of C programing were investigated. A per-programed C program was edited and used to to find the roots of real valued polynomial functions, and state the unmber of steps required to compute these roots. The Gnuplot terminal was then used to plot these polynomials. The C program was then improved upon to use the Newton-Raphson method to find the roots of the functions.

The Lennard-Jones potential was then investigated for a Sodium-Chloride molecule. The C program was edited further to to find the minima of functions representing potential scaler fields, ie. to find the positions of equilibrium, and state weather they are stable or unstable positions of equilibrium. The Bond Length of an NaCl molecule was found to be 0.2360538442nm. Finally, Gnuplot was again used to plot the potential.

2 Introduction and Theory

2.1 C programing

C is a relativly simple, yet powerful computer programing language. It can be used to write adn compute mathamatical algorithms which would be far to tedious to do by hand, with great accuracy. Our program uses **do-while**, **if-else**, **if** and **for** statements to compute the roots of the functions.

We also use *Gnuplot* to plot graphs of our functions. It is another simple terminal based prompt that can be used to accurately plot functions with great spefication.

2.2 The Newton-Raphson Method

The *Newton-Raphson Method* is an algorithm which can be used to find increasingly accurate values for the roots of polynomial functions. It uses the formula

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

where x_n is the first approximation of the root, which can be guessed by plotting the function.

2.3 The Sodium-Chloride Molecule

Sodium-Chloride, *NaCl*, is a diatomic moleucle which has polar bonding. The potential between the Na^+ and Cl^- ions can be apporximated by

$$U(x) = -\frac{e^2}{r} + \alpha \exp\left(\frac{-e}{\rho}\right)$$

, the *Lennard-Jones Potential*.

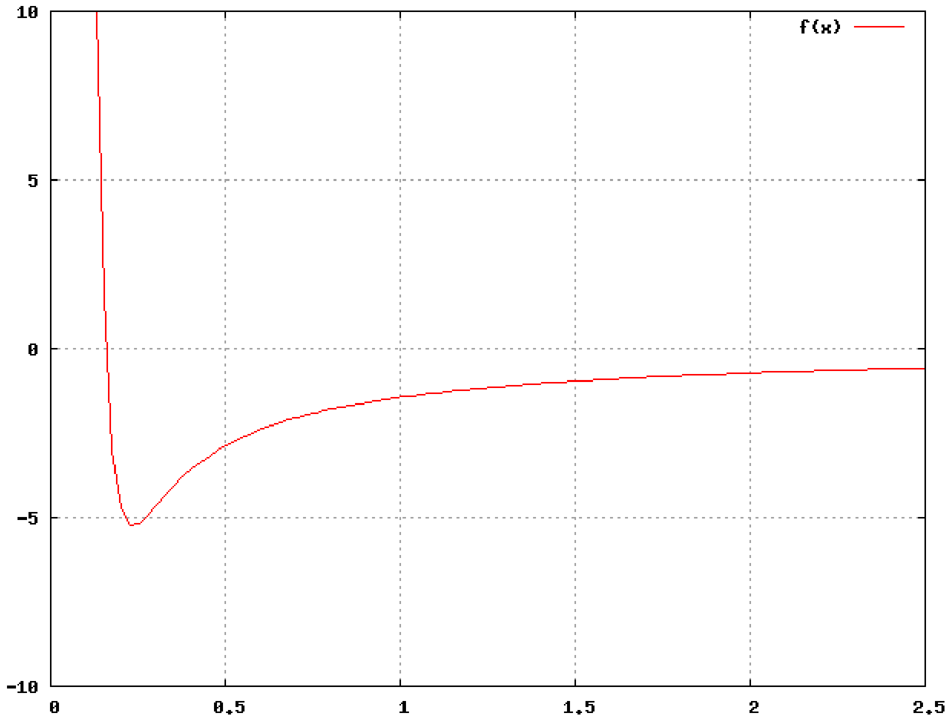

Figure 1: A typical Lennard-Jones Potential Well

The molecule is at a stable equilibrium when it sits at the bottom of the *Potential Well*. Typical values of the parameters for an NaCl molecule are; $\alpha = 1.09 * 10^3 eV$, $\rho = 0.033nm$, $e^2 = 1.44eV$.

3 Experimental Method

3.1 Quadratic Functions

The program was run for a set of values a,b and c, of the quadratic function

$$f(x) = ax^2 + bx + c$$

which give real valued roots.

A graph of the polynomial was then plotted using Gnuplot. It was used to find an estimate for a second root for our quadratic function, which was then used in the program to find an exact second root.

The C program was edited to require a better approximation to the root of the quadratic by increasing the number of decimal places which must match. It was also set to desplay the value of the root to a large number of decmial places.

3.2 The Newton-Raphson Method

The program was edited to use the Newton-Raphson Method to find the roots of quadratic functions. Another function was created within the program to represent $f'(x)$, the first derivative. Then, using the formula above and repeating for a specified number of decimal places accuracy, the root was calculated. An **if-else** statement was added to warn the user and close the program if $f'(x) = 0$ for some x to avoid looping infinities using the **exit(1)** statement.

3.3 The Sodium-Chloride Molecule

The program was again altered to solve for the turning points of the Lennard-Jones potential for a NaCl molecule, that is positions where $f'(x) = 0$. A statement was included to tell the user weather the turning point found is a minimum or a maximum.

The program was then used to find the value of r_0, the bond length of the NaCl molecule.
Finally, the potential was plotted using Gnuplot and the minimum identified.

4 Experimental Results

4.1 Quadratic Functions

The values of a, b and c used were 2, -21 and 7 respectivly. This gave roots of 0.3446 and 10.1554, which took 24 adn 25 steps respectivly for an accuracy of 3 decimal places. The number of steps required to get the roots depending on the accuracy required was as follows

value of 'min'	number of steps
0.0001	18 and 20
0.000001	24 and 25
0.00000001	32 and 33

and the graph obtained using Gnuplot was

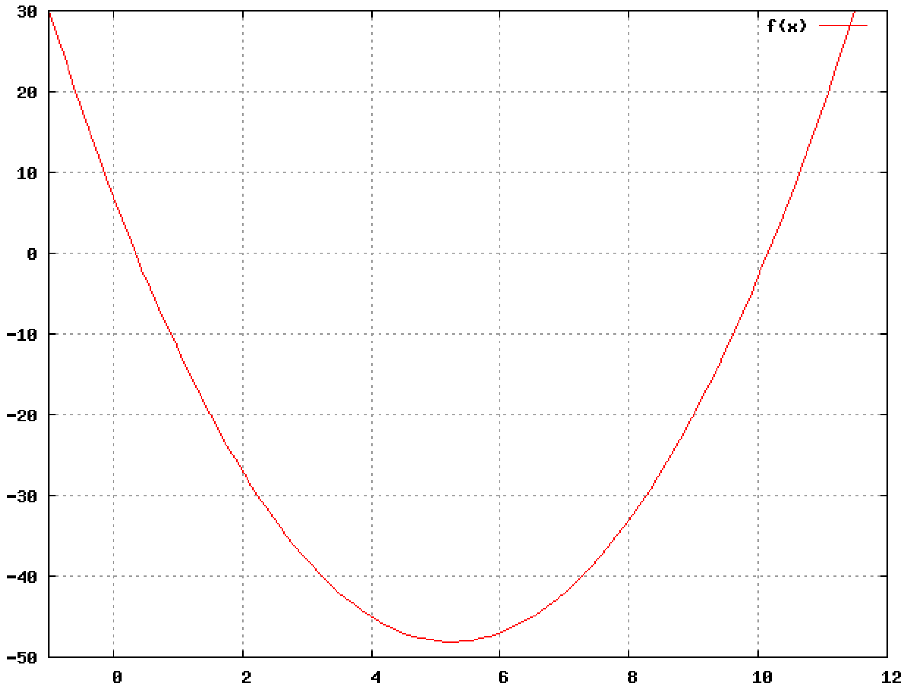

Figure 2: Graph of a Quadratic Function

4.2 The Newton-Raphson Method

The roots obtained using the Newton Raphson Method were 0.3447 and 10.1554, which took 6 and 6 steps respectivly. This was much less than the original *Average Value* algorithm used for the same degree of accuracy.

4.3 The Sodium-Chloride Molecule

The positions where the potential had a minimum was found to be 0.2360538442nm. This corresponds to r_0, the Bond Length of NaCl.

5 Error Analysis

There are errors in our calculations due to the rounding that we allow the computer to do. In the above, we saw that it took more steps to get a solution to the quadratic equation to increasing dergees of accuracy, but this will inhearently have a larger error due to the extra number of times that a number was rounded. In general we have

$$\Delta x \propto N$$

where N is the number of steps taken.

6 Conclusions

In this experiment we learnt of the ease of programing in C. We conclude that it is an easy programing language to work with. Also, We used two different algorithims to find the roots of equations. It was found that the newton Raphson method is much better, as it took far less itterations to get a solution to the same degree of accuracy. Finally, we learnt that computer modeling is very usefull for solving real life problems, for example that of the Bond Length of a Sodium Chloride molecule. By simply altering the function in our program, we were able to get the computer to give us a value for the bond length to a very high degree of accuracy, of 0.2360538442nm, without having to do any tedious calculations by hand.