Laboratory 1: Finding minima of functions

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1 Introduction

This report investigates the use of numerical methods in finding the minima of quadratic functions, with two real roots. The utility of these methods was compared and the most efficient method was used to determine the minimum of the ionic potential of sodium chloride. The investigation was split into three sections. In sections one and two, the bisection and the Newton-Raphson (NR) methods of numerical approximation were examined. Bisection made use of repeatedly decreasing the interval between two points wheres NR repeatedly estimated the location of a root using the function's derivative, each repeated until the estimated root fell within an acceptable tolerance. The number of steps required by each method to reach particular tolerances was also noted. The NR method was found to be the considerably more efficient method. For the final section, the NR method was used to find that the minimum ionic potential energy for sodium chloride will occur at a bond separation of approximately 0.236 nm. Theses tests were run in Python 3, making use of the Numpy and Matplotlib libraries within the Anaconda Spyder environment.

2 Methodology

The first two parts of the experiment compared the effectiveness of the two numerical methods in finding the roots of a given function. The same, arbitrary, quadratic equation, with two real roots, was used in both parts, which ensured a one to one comparison.

$$f(x) = 3x^2 + 7x - 9 \tag{2.1}$$

The quadratic formula was used to analytically find the roots, allowing for the verification of the numerical results.

$$x = \frac{-7 \pm \sqrt{7^2 - 4(3)(-9)}}{2(3)} \tag{2.2}$$

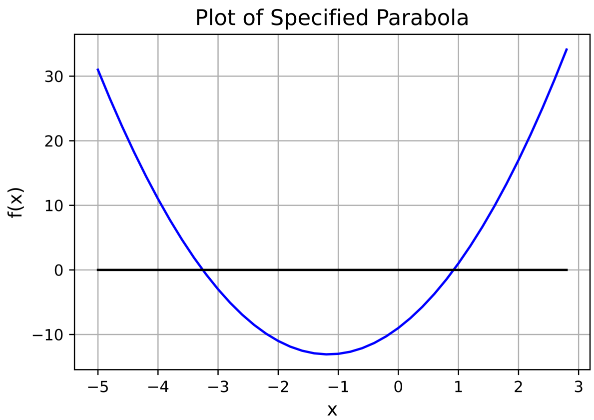


Figure 2.1: Graph of Specified Parabola

2.1 Investigating the Bisection Method

When finding the root of a function the bisection method requires an interval which contains the root. This interval was defined by selecting two points $x_1 = -3.1$ and $x_3 = 7.6$ such that $f(x_1) < 0$ and $f(x_3) > 0$ were both true, else the code would refuse to run. A third point $x_2 = \frac{x_1+x_3}{2}$ signified the midpoint of the interval. An acceptable tolerance was defined; generally between 10^{-4} and 10^{-9} based on desired accuracy. If the absolute value of $f(x_2)$ were greater than the chosen tolerance then the interval would be reduced by replacing either x_1 or x_3 with the current value of x_2, with x_1 being replaced if $f(x_2) < 0$ and x_3 being replaced if $f(x_2) > 0$. This sequence was repeated, using while loops, until $|f(x_2)| <$ tolerance. The initial points were then redefined such that the interval instead contained the second root which was also found. These roots were each plotted graphically confirming the results. Each root was also checked against the analytic solution to check the deviation.

To gauge the efficiency of the bisection method it was necessary to observe the steps required to find a root for a range of tolerances. This was achieved by iterating the root finding process over a range of tolerances from 10^{-3} to 10^{-7}. A log plot was then generated; plotting the relationship between tolerance and the number of steps required to achieve it.

2.2 Investigating the Newton-Raphson Method

The NR method is able to be derived from the Taylor expansion of a function $f(x+h) = 0$ up to the first order of 'h' as such the first derivative of f(x) was required.

$$f'(x) = 6x + 7 \tag{2.3}$$

This method required only a single starting point, $x_1 = 2.3$, along with a specified tolerance. While $|x_1| >$ tolerance the value of x_1 was repeatedly adjusted according to the following equation.

$$x_1 = x_1 - \frac{f(x_1)}{f'(x_1)} \tag{2.4}$$

The second root was found by redefining $x_1 = -2.3$. The NR method converges on the root which is on the same side of the turning point as the first point, so ensuring the new point was on the other side of the minimum of f(x) was adequate. As with bisection, the roots were both plotted on the parabola and compared to the analytic solutions.

The efficiency of NR was also checked via graphing a log plot of steps required to reach a root against a large range of tolerances from 10^0 to 10^{-7}. Additionally a number of tolerances were manually checked to gauge how closely this numerical method could approach the analytical solution.

2.3 Finding the Minima of a Potential Energy Function

The comparison of the first two sections demonstrated the supremacy of the NR method for numerical approximation, so only the NR method was used in this part. The equation for Ionic Interaction potential between Na^+ and Cl^- (sodium chloride) was given as:

$$V(x) = Ae^{-\frac{x}{p}} - \frac{e^2}{4\pi\varepsilon_0 x} \tag{2.5}$$

With $A = 1090$ eV, $p = 0.033$ nm, and $\frac{e^2}{4\pi\varepsilon_0} = 1.44$ eV nm.
Where previously the NR method was used to find the roots of a function, in this section the minima of V(x) was required. It is known that at the extrema of a function the first derivative is zero. As such the NR method in equation 2.4 was modified such that it would instead find the roots of V'(x).

$$x_1 = x_1 - \frac{V'(x_1)}{V''(x_1)} \tag{2.6}$$

Note:

$$V'(x) = -\frac{A}{p}e^{-\frac{x}{p}} + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{x^2} \equiv -F(x) \tag{2.7}$$

$$V''(x) = \frac{A}{p^2}e^{-\frac{x}{p}} - \frac{e^2}{4\pi\varepsilon_0}\frac{2}{x^3} \tag{2.8}$$

The value force acting on the particles is directly related to the potential energy via $F(x) = -\frac{dV}{dx}$. As such the net force on the particles should be zero at the minimum of V(x), due to it going to zero when V'(x) goes to zero which, as mentioned, will occur at extrema. Based on the graph of V(x) an x_1 in the range of [0.1, 0.25] appeared most suitable for finding a minima.

3 Results

3.1 Evaluating the Bisection Method

This section presents and discusses the bisection method results.[1]

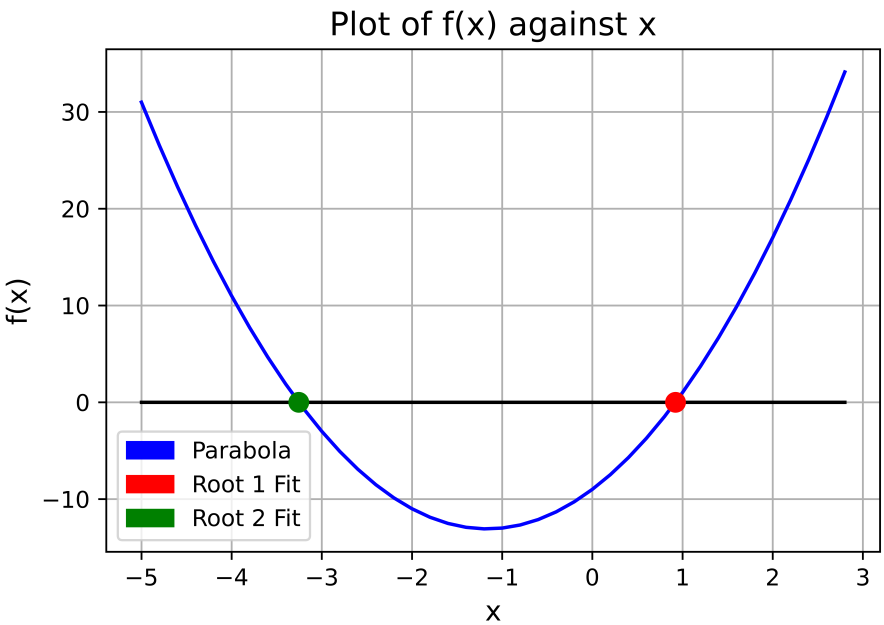


Figure 3.1: Graph of f(x) against x with roots

	Root 1	Root 2
Analytical[2]	0.9216606810236113	-3.2549940143569445
Approximate	0.9216606810572556	-3.254994014310069
Difference	-3.36443$x10^{-11}$	-4.68754$x10^{-11}$
Steps	32	34
$f(x)$ [3]	4.2156$x10^{-10}$	-5.8735$x10^{-10}$
$\|f(x)\|$	4.2156$x10^{-10}$	5.8735$x10^{-10}$

Table 3.1: Table of Bisection Results

An examination of the plot gave an early indication that both roots were found numerically to a good accuracy, with both dots on the x-axis and intersected by the parabola. An analysis of the printed results found that the error in the numerical results of both roots agreed with the analytical solutions up to the order of 10^{-11}; for tolerance of order 10^{-9}. It was interesting that the error improved on the tolerance by two orders of magnitude for both roots. This suggested that each iteration offered a fairly consistent jump in accuracy. Considering the roots differed in total iterations required, it was evident that the initial conditions have a non-negligible effect on the steps required to find a root.

[1] In Figure and Table 3.1, Tolerance = 0.000000001

[2] Printed exactly as Python returned

[3] $f(x) = 3x^2 + 7x - 9$

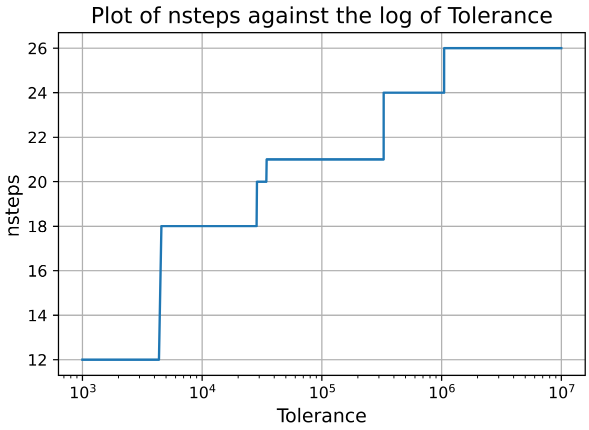


Figure 3.2: Bisection:Steps against log(tol)

Convergence of Bisection	
Tolerance	Steps
10^{-3}	12
10^{-4}	18
10^{-5}	21
10^{-6}	24
[a] 10^{-7}	26

Table 3.2: Bisection:Tolerance to Steps

[a]Plotted against the inverse of tolerance to give a positive slope

The examination of the plot and the table made it clear that that the bisection method tended to scale with the $log_{10}(tolerance)$. This relationship made for a quite computationally intensive program and it was decided to only test as far as 10^{-7}. Accuracy was tested, as shown, at 10^{-9} but running multiple trials above 10^{-7} would cause either unacceptable run-times or a crash which must be considered when assessing this method.

3.2 Evaluating the Newton-Raphson Method

This section presents and discusses results for NR method of numerical approximation.[4]

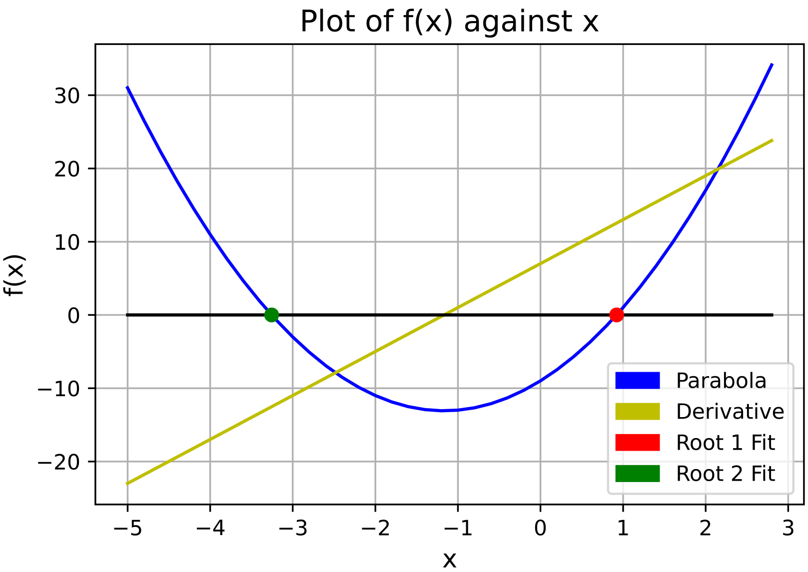


Figure 3.3: Graph of f(x), f'(x) against x with roots

[4]In Figure and Table 3.3, Tolerance = 0.000000001

	Root 1	Root 2
Analytical[5]	0.9216606810236113	-3.2549940143569445
Approximate	0.9216606810236113	-3.254994014356945
Difference	0.0	$4.44089x10^{-16}$
Steps	5	5
$f(x)$ [6]	0.0	$7.1054x10^{-15}$
$\lvert f(x)\rvert$	0.0	$7.1054x10^{-15}$

Table 3.3: Table of NR Results

As with previously the graph immediately demonstrated the success of this numerical method at finding both roots. Examining the table of results provided further insight into the granular results of the NR method. At a tolerance of 10^{-9} the found roots were incredibly accurate, root 2 was correct up to 10^{-15} while root 1 was exactly equal to the analytical solution (at least as far as Python was capable of checking). Each root was found within only five iterations from the starting point[7]. The relative "closeness" of the starting points to each root was undoubtedly an assistance in keeping the number of steps low. Therefore, it is noted that a reasonable guess should be made in order to conserve computing resources on large scales.

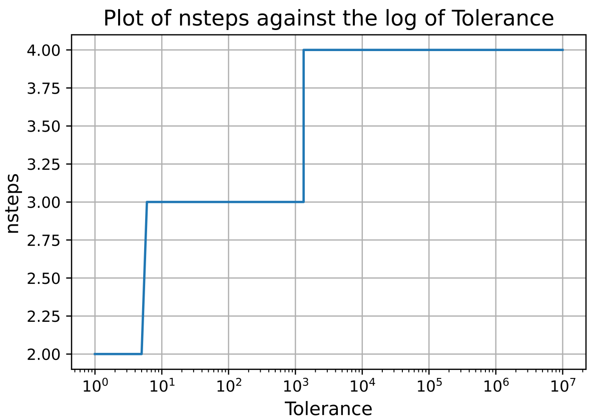


Figure 3.4: NR:Steps against log(tol)

Convergence of NR	
Tolerance	Steps
10^0	2
10^{-1}	3
10^{-4}	4
[a] 10^{-7}	4

Table 3.4: NR:Tolerance to Steps

[a] Plotted against the inverse of tolerance to give a positive slope

There is clearly not a very strong relationship between tolerance and the steps required to reach it using the NR method. Over the period from 1 to 10^{-7} there was only an increase in two steps. The fact that in order to be accurate at to a single unit two steps were required, provided further evidence that the starting point was a relatively significant factor in the number of steps.

[5] Printed exactly as Python returned

[6] $f(x) = 3x^2 + 7x - 9$

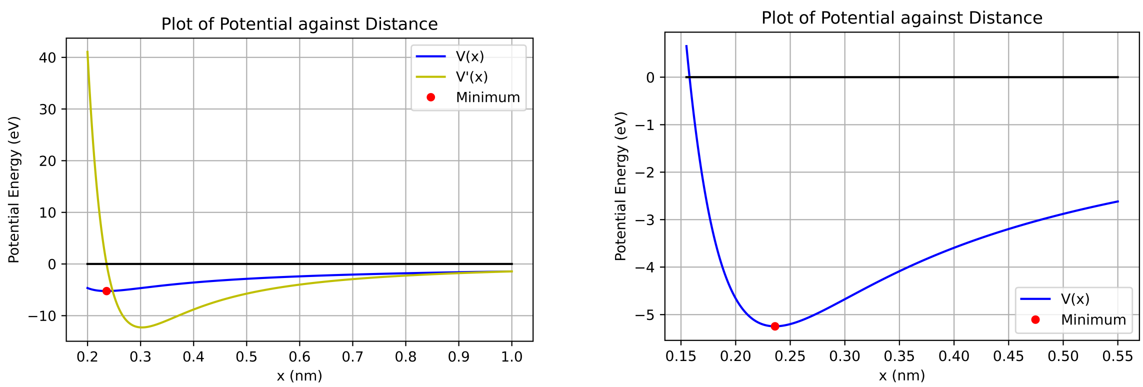
[7] $x_1 = \pm 2.3$

3.3 Comparison between Bisection and NR

The results of sections one and two made a very convincing case for the use of NR over bisection. At the same tolerance level NR found more accurate roots in less steps.
NR also had the advantage that only a single starting point was required, as opposed to two for bisection. With generally less restriction on the point in NR.
There was no question of efficiency with NR clearly requiring less steps in relation to tolerance, as can be immediately seen when comparing Figures 3.2 and 3.4. NR was also able to reach much greater tolerances in much less time than bisection.
Under the circumstances that a function shoots off to infinity there may be advantages to choosing bisection as NR might shoot past the roots in such cases. Also, if a function were continuous but not differentiable then NR would not be possible and bisection would be a reasonable solution. In most other circumstances however the NR method is clearly the more suitable choice.

3.4 Finding the Minima of a Potential Energy Function

As the NR method was seen as more suitable it was used exclusively in this section.[8]



(a) V(x), V'(x)

(b) V(x)

Figure 3.5: Plots of Potential with Minimum Found

The NR root-finder with adjustments[9] found the minimum ionic potential energy within sodium chloride to occur at a separation of $x = 0.23605384841577937$ nm. This value was in agreement with sources online[10] which cited the minimum to occur at "$x = 0.236$ nm".
These sources also stated the potential energy at these points to be "$|V| = 4.26$ eV" which was different to the value $|V(x)| = 5.247489118540433$ eV which was given by our equation. This discrepancy may be due do the numerical values which were used for the constants or perhaps the sources included internal energies which were not relevant for the goal of finding the point of minimum potential which was achieved.

[8] Tolerance = 0.000000001
[9] Equation 2.6
[10] http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/NaCl.html

4 Conclusions

This report was written with the goal of investigating the utility of the bisection and Newton-Raphson methods with regards to their use in numerically finding the roots of functions which could not necessarily be solved analytically. With the ultimate goal of using one such method to find the minimum ionic potential between Na^+ and Cl^-. These goals can be said to have been achieved.
The report described the use of both methods in finding the roots of a quadratic function[11] and compared the results against the analytic solution. Each method was shown to be clearly capable of such a task but the NR method was also seen to have a number of advantages. The NR method was considerably more accurate than the bisection method, even being capable of finding the exact analytical solution; up to the accuracy of python at the least. Efficiency was also considered and once again NR was more subtitle, being capable of great the same accuracy as bisection but within $\frac{1}{6}$ the steps[12]. Due to the mentioned factors the NR method was seen as the clearly best method to achieve the ultimate goal. Using the NR method the minimum ionic potential energy was found to occur at a separation of $x \approx 0.2361$ nm which agreed with online publications. This further supported the accuracy and utility of the Newton-Raphson method.

List of Figures

List of Tables

[11] Equation 2.1
[12] At a tolerance of 10^{-6}