Comp. Laboratory #1: Minima of Functions

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1 Introduction

I investigate different methods for numerical approximations of finding roots or minima of various functions. The bisection method is first used on a quadratic function with two roots, and then compared in efficacy to the Newton-Raphson method. I find that the number of steps in both methods appears to follow a negative-logarithmic relationship with the precision, however the latter method to perform significantly better on average. I also find that the Newton-Raphson method is very sensitive to the choice of starting values and tends to require many more steps for starting points near extrema of the given function.

Finally, the Newton-Raphson method is used to find the minimum of the interaction potential between two ions using analytic function definitions of the function of potential against distance, as well as its two derivatives. For the given numerical values, the value of the distance found is $x_{min} = (0.2361 \pm 0.0001)$nm.

2 Methodology

2.1 Exercise 1: Finding the roots of a parabolic function

For this exercise, the bisection method was used to find roots of a given function. The method works in the following way: first, two initial points, x_1 and x_3 are chosen such that $f(x_1) > f(x_3)$. The midpoint $x_2 = \frac{x_1+x_3}{2}$ is then calculated. If $f(x_2) > 0$, the value of x_1 is set to x_2, and in the opposite case, the value of x_3 is set to x_2. A new midpoint is then calculated and the procedure continues until a desired tolerance is met i.e. $|f(x_2)| < tol$ for some given tol.

2.2 Exercise 2: Finding the roots of a function using the Newton-Raphson method

Here, the Newton-Raphson method was used to find roots of a function. This method works by using the Taylor expansion to approximate the slope of the function and iteratively approach roots, similarly to the bisection method. An initial point, x_1 is chosen and its value is repeatedly updated to $x_1 = x_1 - \frac{f(x_1)}{f'(x_1)}$. This continues until, again, the desired tolerance is met.

2.3 Exercise 3: Finding the minima roots of a potential energy function

In this exercise, the same method was used as in **2.2**, however it was the derivative of the given function that was examined. This is because of the fact that at local extrema (such as a local minimum) of a given $V(x)$, $V'(x)$ is equal zero and so one can use the Newton-Raphson method to find them. This requires computing the second derivative of the initial function.

3 Results

3.1 Exercise 1

The function chosen for examination with the previously described bisection method was the parabola $f(x) = (x-5)^2 - 4$.

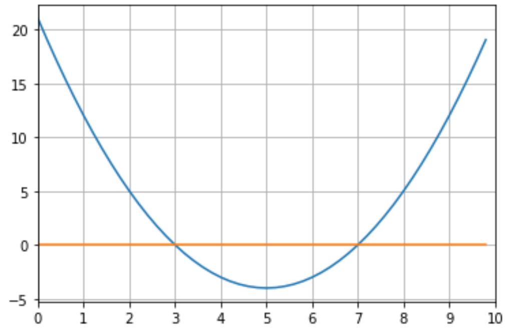

Figure 1: Plot of parabola $y = (x-5)^2 - 4$

The successive points x_2, given the bisection method for initial points $x_1 = 1.0$, $x_3 = 6.0$ and tolerance $tol = 0.0001$, were plotted over the parabola, with the color saturation increasing with each iteration. It can be observed that the guesses converge quite quickly to the root. The final values found were $x_2 = 3.000$ and $f(x_2) = 0.00003$.

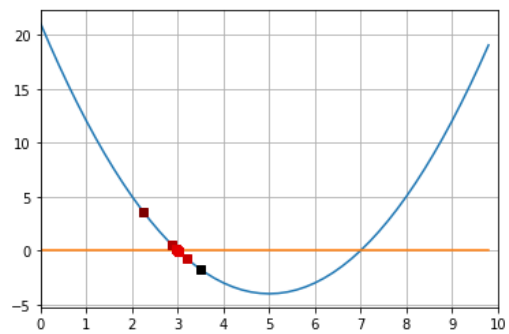

Figure 2: Plot of $f(x)$ and the sequence of points $(x_2, f(x_2))$

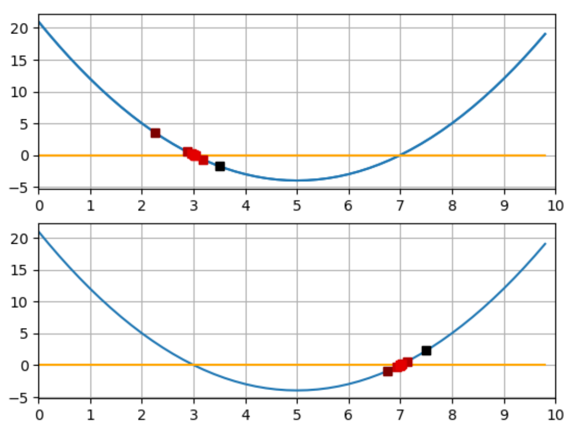

Figure 3: Plot of $f(x)$ and the sequences $(x_2, f(x_2))$ approaching two different roots

The code was then modified to find the second root of the parabola, using $x_1 = 9.0$, $x_3 = 6.0$ and the same tolerance. The values found were $x_2 = 7.000$ and $f(x_2) = -0.00006$.

In the next part, the steps required to reach a given accuracy were counted for different values of *tol*, in the range of 10^{-4} to 5.0. The following graph was produced:

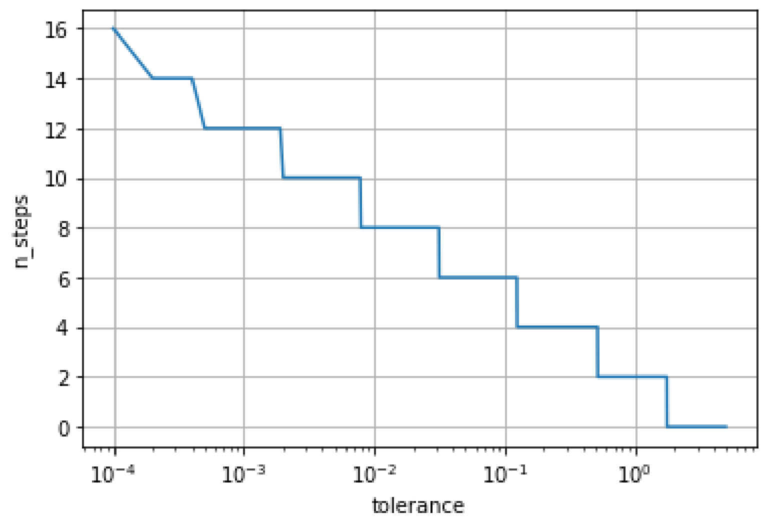

Figure 4: Number of steps required by the bisection method vs. tolerance

3.2 Exercise 2

Here, the same function was used and its derivative calculated:

$$f'(x) = \frac{d}{dx}\left[(x-5)^2 - 4\right] = 2(x-5)$$

The Newton-Raphson method was used as explained above, to find consecutively better approximations of the roots, using the derivative definition.

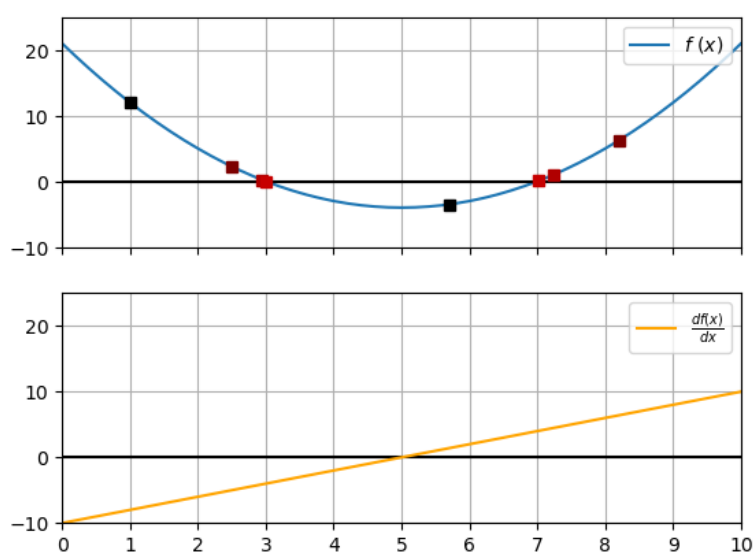

Figure 5: Plots of $f(x)$ and $f'(x)$, with sequences of points $(x_2, f(x_2))$ overlaid

Here, the successive points of approximation were plotted, again with the color saturation increasing with step number. To find the first root, the starting point of $x_1 = 1.0$ was chosen, and for the second, the starting point $x_1 = 8.0$. In both cases, the tolerance was set to $tol = 0.0001$. The final values returned were: $x_1 = 3.000$ and $f(x_1) = 3.717 \times 10^{-7}$ for the first root, and $x_1 = 7.000$ and $f(x_1) = 4.096 \times 10^{-5}$ for the second.

Next, the steps required to reach the condition $|f(x_1)| < tol$ were counted for a set value of tol. It could be quickly noticed, however, that the starting point played a very significant role in the achieved number of steps. Thus, the relationship between this number and the tolerance was examined for two different starting points: $x_0 = 1.0$, a 'generic' point of the parabola; and $x_0 = 5.01$, a value of x very close to the minimum of the function. Because of the very low value of the derivative (f' is 0 at local extrema), the increment $\frac{f(x)}{f'(x)}$ became quite large, which led to guesses falling far from the root and a higher number of steps required.

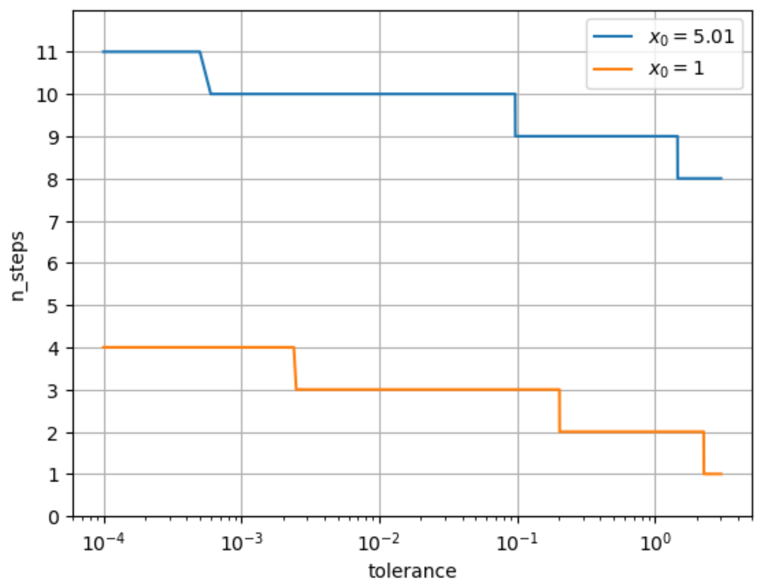

Figure 6: Newton method: number of steps vs. tolerance for different starting points

It did not, however, seem to affect the strength of the relation between the plotted values and only shifted the results 'up' by a constant.

Upon further experimentation, the Newton method does not appear to have a limit on the accuracy that it can achieve, with it being constrained more by the precision limits of a floating point variable in python. This is as expected, since the value of $\frac{f(x)}{f'(x)}$ gets proportionally smaller as x approaches the root, and so the increment becomes more and more precise.

3.3 Exercise 3

The implementation of the Newton-Raphson method was shown, on an example of a potential energy function:

$$V(x) = Ae^{-x/p} - \frac{c}{x} \qquad \text{with } c = \frac{e^2}{4\pi\epsilon_0}$$

The numerical values used to evaluate it were $c = 1.44$ eV nm, $A = 1090$ eV and $p = 0.033$ nm. First, the first derivative of the function was calculated by hand, giving the result:

$$V'(x) = -\frac{A}{p}e^{-x/p} + \frac{c}{x^2}$$

Since the minimum of the potential energy function was to be found, the Newton method was used on its derivative, requiring the caluculation of the second derivative:

$$V''(x) = \frac{A}{p^2}e^{-x/p} - \frac{c}{2x^3}$$

Such usage of the method was possible due to the fact that at minima of $V(x)$, $V'(x)$ vanishes i.e. $V'(x) = 0$, meaning a root of the derivative corresponds to a minimum (or other extremum) of the original function:

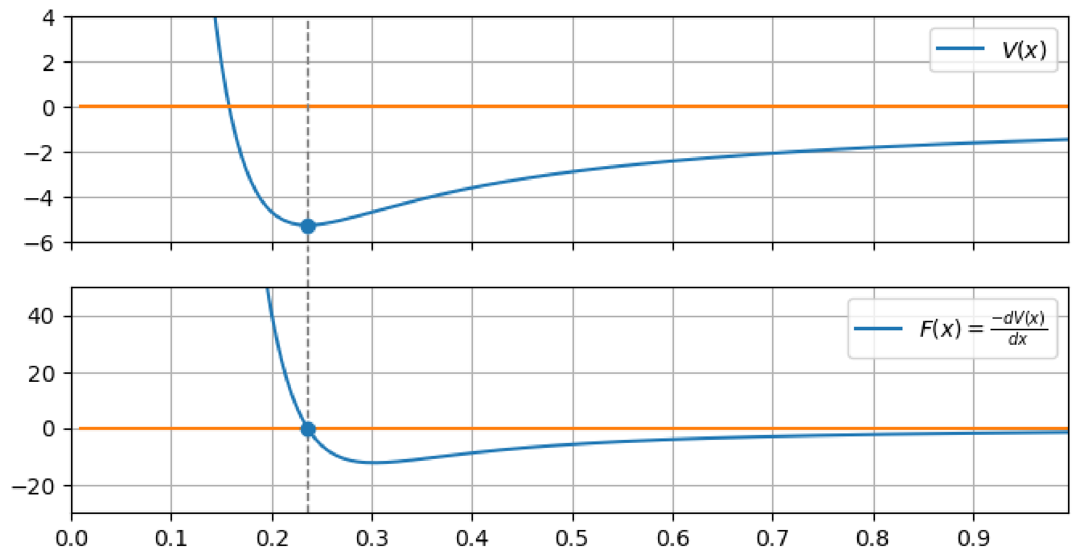

Figure 7: Plots of $V(x)$ and $-V'(x)$

The Newton-Raphson method was implemented with the starting coordinate of $x_1 = 0.2$ and a tolerance $tol = 0.0001$. This generated the following points (coloured as in previous graphs):

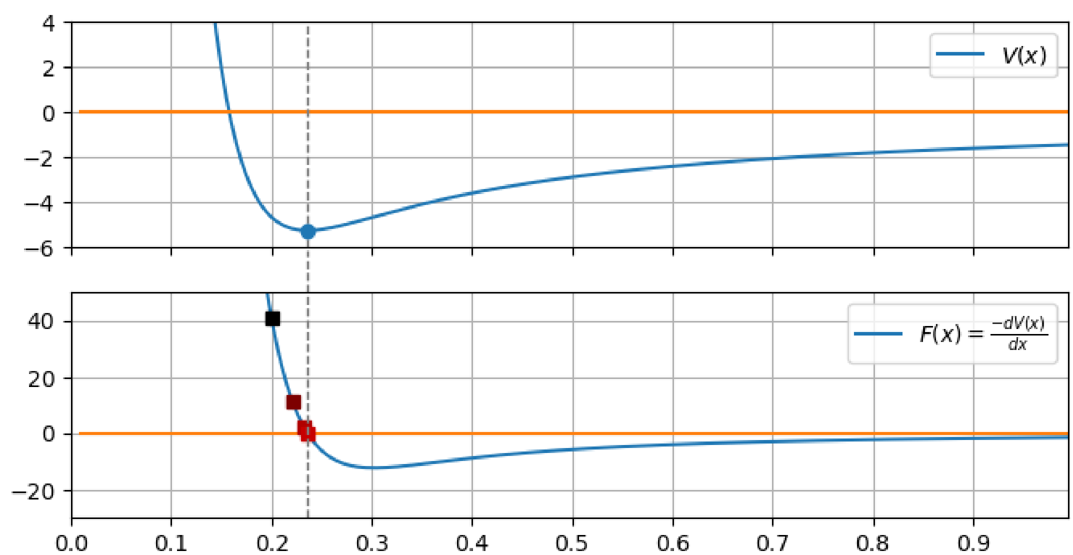

Figure 8: Successive approximations of the Newton method

The values approached at the end were $x_1 = 0.2361$, $-V'(x_1) = 7.421\times10^{-9}$ and $V(x_1) = -5.247$.

4 Conclusions

It is easily noticed that for a 'generic' starting point, the Newton-Raphson method performs significantly better than the bisection method, requiring on average 2-3 times fewer steps. Both appear to have time complexity proportional to the negative logarithm of tolerance, but the former having a significantly better (lower) constant of proportionality. However, both methods have their downsides, with the bisection requiring root in between the starting points, and the Newton method being particularly sensitive to values of the derivative close (or equal) to zero.

The usage of the Newton-Raphson procedure in the case of the potential energy function yielded the result $x = (0.2361 \pm 0.0001)$nm at a low computational cost and in negligible time, proving the usefulness of the method.