## Minimisation of Functions

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## Introduction

The aim of this experiment is to evaluate methods of finding the roots of a quadratic function to within an accepted margin of error.

A C script which uses a simple method of finding the roots of a function is provided at the beginning of the lab. This method’s accuracy will be evaluated for a quadratic function by calculating the roots of a known function analytically using traditional methods and comparing the values attained with those attained by the script. The number of steps taken by the script to attain answers to particular accuracies will also be scrutinised.

The script finds roots of a function as follows:

Two values for x are required, x1, for which f(x) is less than 0 and x2, for which f(x) is larger than 0.Then an approximation x­3 is calculated according to the relation:

$$x\_{3}=\frac{x\_{1}+x\_{2}}{2}$$

If f(x3)>0 then the above equation is repeated, having replaced x2 with x3­.

 If f(x3)<0 then the above equation is repeated, having replaced x1 with x3­.

This will be repeated until the magnitude of f(x) is sufficiently close to zero, i.e, when f(x)<min.

A more efficient method is the Newton-Raphson method of approximation. For a function f(x), an initial value of x is chosen, x1. A second approximation is calculated from the relation:

$$x\_{n+1}=x\_{n}-\frac{f(x\_{n})}{f'(x\_{n})}$$

This relation is repeated by the script until f(x)<min, where min is a value chosen to define the accuracy of the result.

### Exercise 1

The first method of finding the roots of a function was applied to the function f(x)= x2+2x-2. The function was also plotted in Gnuplot. The roots of the function were calculated manually to be $-1+\sqrt{3}$ and $-1-\sqrt{3}$. The script calculated each of the roots respectivlely by ensuring that the initial values of x1 and x2 were on different sides of the root to be calculated, along the x-axis.

The series of approximations of the above root was calculated manually using this method and the tending of the approximation to the true value is plotted:

The value of min was made smaller and the number of steps required to reach the required accuracy was recorded. The results are tabulated below.

|  |  |
| --- | --- |
| Min Value | Number of Steps |
| 0.001 | 13 |
| 0.0001 | 16 |
| 0.00001 | 20 |
| 0.000001 | 23 |
|  |

### Exercise 2 The Newton Raphson Method

The program provided root.c was edited to calculate the root of a function using the Newton Raphson method. A second function, funcderiv was added to the script, which was the first derivative with respect to x of the previous function.

A flaw in the newton raphson method is that if the initial approximation chosen, x1 , lies on the other side of a local minimum or maximum to the root which is being calculated, then f’(x) will approach zero and the relation $x\_{n+1}=x\_{n}-\frac{f(x\_{n})}{f'(x\_{n})}$ will no longer continue to provide further approximations.

A condition was added to the script to address this issue. A Do/While loop was added whereby after each new approximation of x, the script checked that f’(X) was not equal to zero. Had the first derivative tended to zero( when approaching a max/min point) the script stopped further calculations and displayed a message explaining that the inital value of x provided was unsuitable.

An initial value of x=-5 was chosen for the function f(x)=x2+2x-2 and the number of steps for different levels of accuracy are recorded below.

|  |  |
| --- | --- |
| min | Number of Steps |
| 0.001 | 27 |
| 0.0001 | 33 |
| 0.00001 | 39 |
| 0.000001 | 45 |

### Discussion and Conclusions

The methods for finding the minima of functions were successfully evaluated. However, a third exercise to calculate the bond length of NaCl from the equation of the potential of it;s electric field was not completed.