Assignment 3

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1 Finding roots

This program computes the root of the equation

$$f(x) = x^2 - 7x - ln(x) \tag{1}$$

using bisection and secant method.

1.1 Bisection Method

1.1.1 first root

The source code is:
assign3/qn1/bisection.f90

to comile and run this code for the first root:

f90 bisection.f90 && ./a.out > bisection1.dat
then, we can see output file in the path:
assign3/qn1/bisection1.dat

note that: at the line 14, the code fragment looks like

```
!! initial range (x0,x1) to find the root within it

 x0 = 0.1d0   !! for first root
 x1 = 1.0d0
 !x0 = 5.1d0   !! for second root
 !x1 = 10.0d0
```

1.1.2 second root

The source code is:
assign3/qn1/bisection.f90

to comile and run this code for the second root:

f90 bisection.f90 && ./a.out > bisection2.dat
then, we can see output file in the path:
assign3/qn1/bisection2.dat

note that: at the line 14, the code fragment looks like

```
!! initial range (x0,x1) to find the root within it
```

```
!x0 = 0.1d0   !! for first root
!x1 = 1.0d0
x0 = 5.1d0   !! for second root
x1 = 10.0d0
```

1.2 Newton-Raphson Secant Method

1.2.1 first root

The source code is:
assign3/qn1/secant.f90

to comile and run this code for the first root:

f90 secant.f90 && ./a.out > secant1.dat
then, we can see output file in the path:
assign3/qn1/secant1.dat

note that: at the line 33, the code fragment looks like

```
!FIRST ROOT
      xinitial = 0.1d0
      xfinal   = 1.0d0

      ! SECOND ROOT
      !xinitial = 5.1d0
      !xfinal   = 10.0d0
```

1.2.2 second root

The source code is:
assign3/qn1/secant.f90

to comile and run this code for the second root:

f90 secant.f90 && ./a.out > secant2.dat
then, we can see output file in the path:
assign3/qn1/secant2.dat

note that: at the line 33, the code fragment looks like

```
!FIRST ROOT
      !xinitial = 0.1d0
      !xfinal   = 1.0d0

      ! SECOND ROOT
```

```
xinitial = 5.1d0
xfinal   = 10.0d0
```

1.3 Comparison

– The positive roots of the equation was found upto five significant figures.

– In comparison to secant method the bisection method is slower.
For example:
To find the the first root 0.22203, bisection method required 18 iterations and secant method needed 6 iterations. We can see that difference in:
assign3/qn1/bisection1.dat
assign3/qn1/secant1.dat

– While using these Bisection and Secant method we need prior approximate position of zero.

2 Bond Length of the NaCl Molecule

2.1 Plot of V(r)

In this question I wrote a code to plot r vs. V(r).
The source code and outputs are:
assign3/qn2/ass3qn2.f90
assign3/qn2/potentialplot.dat
assign3/qn2/potential.eps

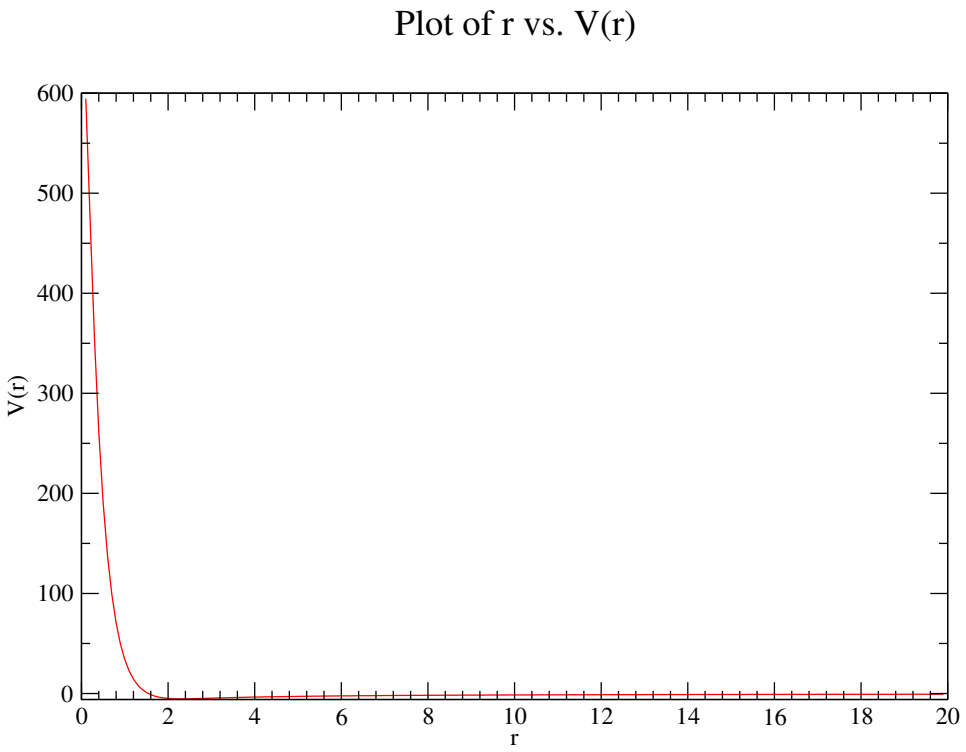

Figure 1: Plot of r vs. V(r)

2.2 Minimum of V(r) and roots

In this question I wrote a code to find roots when V(r) is minimum.
The source code and outputs are:
assign3/qn2/ass3qn2.f90
assign3/qn2/findroot.dat

In the problem we are asked to find equilibrium distance between Na and Cl ions. After finding the root upto 3 significant figures, I found that

$$r_{eq} = 2.32 \tag{2}$$

To find the root I used secant method, because it is faster than bisection method. To find root we have also to guess the approximate position of root. First I plotted the graph in the website Wolfram Alpha and saw the nature of the graph. Then I wrote the code. The constant values were provided in the question.