CRISTIAN B. JETOMO
MATH 175 - H4L

Exercise 2.1: The Newton-Raphson Method in Root-finding

In this exercise, we wish to use the *Redlich-Kwong equation* given by

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)\sqrt{T}} \tag{2.1.1}$$

where

$$a = 0.42747\left(\frac{R^2T_c^{5/2}}{P_c}\right), b = 0.08664\left(\frac{RT_c}{P_c}\right), \text{ and } R = 0.08206$$

to find the volume V of one mole of ammonia at $T = 450$ Kelvin, $P = 56$ atm and where $T_c = 405.5$ Kelvin and $P_c = 111.3$ atm. We construct the Newton-Raphson iteration formula of the form

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

for $n \geq 0$ to find V. To do this, we define the function

$$f(V) = \frac{RT}{V-b} - \frac{a}{V(V+b)\sqrt{T}} - P \tag{2.1.2}$$

and find V which satisfied $f(V) = 0$. We can do this by determining the root of f. Solving for f and its 1$^{\text{st}}$ order derivative using MATLAB, we have

$$f(V) = \frac{36.93}{V-0.0259} - \frac{4.037}{V^2+0.0259V} - 56 \tag{2.1.3}$$

$$f'(V) = \frac{4.037}{V^3+0.05181V^2+0.000671V} - \frac{36.93}{V^2-0.05181V+0.000671} + \frac{4.037}{V^3+0.0259V^2} \tag{2.1.4}$$

Hence, we derived the Newton-Raphson iteration formula to solve the required root V which is given by

$$V_{n+1} = V_n - \frac{f(V_n)}{f'(V_n)} \tag{2.1.5}$$

for $n \geq 0$ and where f and f' is given in Equations 2.1.3 and 2.1.4.

We run the method in Equation 2.1.5 using a jump-based stopping criterion with $\epsilon = 10^{-8}$ and maximum iteration $N_{\max} = 1000$. Suppose we use the initial value $V_0 = 1$, then we obtain the result in MATLAB as follows:

```
n     V_n          rel jump
1     0.292825     7.071746E-01
2     0.459255     5.683591E-01
3     0.551833     2.015814E-01
4     0.569326     3.170060E-02
5     0.569803     8.383316E-04
6     0.569804     5.925830E-07
7     0.569804     2.961615E-13
Root is 0.5698037041 after 7 iterations.
Note that the function value at the estimate is 1.417064E-11.
```

Figure 2.1.1: Result obtained by implementing the Newton-Raphson Method to find the root of f.

We can observe that using the Newton-Raphson Method, we obtained an estimate of $V \approx 0.5698037041$ after only 7 iterations. We also obtained that $f(0.5698037041) = 1.417064 \times 10^{-11}$ which is very close to 0, hence a good estimate for the required root.

Now, we try to solve the problem using the Secant Method. For this, we use the iteration formula given by

$$V_{n+1} = V_n - f(V_n)\frac{V_n - V_{n-1}}{f(V_n) - f(V_{n-1})} \tag{2.1.6}$$

Note that similarly with the Newton-Raphson method, the functions f and f' used is obtained from Equations 2.1.3 and 2.1.4. We also use the same jump-based stopping criterion of $\epsilon = 10^{-8}$ and $N_{\max} = 1000$. Implementing this in MATLAB with initial guesses of $V_0 = 1$ and $V_1 = 0.5$, we obtain the result below.

```
n     V_n         rel jump
1     0.614430    2.288609E-01
2     0.574411    6.513322E-02
3     0.569499    8.550615E-03
4     0.569806    5.385772E-04
5     0.569804    3.644490E-06
6     0.569804    1.644136E-09
Root is 0.5698037041 after 6 iterations.
Note that the function value at the estimate is 2.395144E-13
```

Figure 2.1.2: Result obtained in MATLAB by implementing the Secant Method to find the root of f.

From these results, we obtain the estimate to be $V \approx 0.5698037041$ after 6 iterations. We can also infer that this is a good estimate since $f(0.5698037041) = 2.395144 \times 10^{-13}$, a value very close to 0.

In summary, the respective approximated volumes of one mole of ammonia using the Newton-Raphson and Secant methods are 0.5698037041 and 0.5698037041. Comparing the results of the two methods used, we can conclude that the Secant method converges faster to the root or the volume required since the value is obtained after a fewer number of iterations than with the Newton-Raphson method. The obtained estimate using the Secant method is also more accurate since its corresponding function value is smaller and closer to 0.

We note however that this difference in rate of convergence is not consistent. We can observe this by using different initial guesses for the Secant method, say $V_0 = 1$ and $V_1 = 0.9$. The result of this is given in Figure 2.1.3. Here, we can see that it took 8 iterations instead to obtain a good estimate of the root. This shows that even a slight change in the initial values makes the method perform slower than the Newton-Raphson method.

```
n     V_n         rel jump
1     0.357375    6.029164E-01
2     0.673364    8.841943E-01
3     0.602183    1.057102E-01
4     0.564827    6.203472E-02
5     0.570042    9.234213E-03
6     0.569805    4.156207E-04
7     0.569804    3.086607E-06
8     0.569804    1.090095E-09
Root is 0.5698037041 after 8 iterations.
Note that the function value at the estimate is -1.334743E-13
```

Figure 2.1.3: Result obtained in MATLAB by implementing the Secant Method using different initial guess.

Remark: *The program used to solve this problem is made in MATLAB and is made solely by the author of this paper.*