CHAPTER 4

ROOTS OF EQUATIONS
Chapter 3: TOPIC COVERS
(ROOTS OF EQUATIONS)

Definition of Root of Equations
Bracketing Method
• Graphical Method
• Bisection Method
• False Position Method
Open Method
• One-Point Iteration Method
• Newton-Raphson Iteration Method
• Secant Method
Applications in Chemical Engineering
LEARNING OUTCOMES

INTRODUCTION

*It is expected that students will be able to:*

- Recognize what is the root of equation
- Use bracketing and open methods for root location
- Clarify the concept of convergence/meeting point and divergence/deviation
CHAPTER 3 : ROOTS OF EQUATIONS

3.1 Introduction

Years ago, you learned to use the quadratic formula;

\[ x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (3.1) \]

To solve; \[ f(x) = ax^2 + bx + c = 0 \quad (3.2) \]

The values calculated by equation (3.1) are called the “roots” of equation (3.2). They represent the values of \( x \) that make equation (3.2) equal to zero.

Thus, roots of equations can be defined as “the value of \( x \) that makes \( f(x) = 0 \)” or can be called as the zeros of the equation.

Although the quadratic formula is handy for solving, there are many other functions/formulas which the root cannot be determined. For these cases, NM in this chapter provide the efficient answer.

An example where mathematical function (such as quadratic formula) cannot be used to determine roots of equation is The Newton’s 2\textsuperscript{nd} Law for the parachutist’s velocity:
\[ v = \frac{gm}{c} \left(1 - e^{-(c/m)t}\right) \quad (3.3) \]

If the parameters are known, equation (3.3) can be used to predict the parachutist’s velocity as a function of time.

However, suppose we had to determine the drag coefficient, \( c \) for a parachutist of a given mass to prescribe velocity, \( v \) in a set time period, \( t \).

Although equation (3.3) provides a mathematical representation of the interrelationship among the model variables & parameters, it cannot be solved for the drag coefficient, \( c \).

The solution to the dilemma is provided by NM for roots of equations.

3.2 Methods to Determine Roots of Equations

A. Bracketing Methods

i. Graphical Method
ii. Bisection Method
iii. False-Position Method
B. Open Method
i. Simple Fixed-Point Iteration
ii. Newton-Raphson Method
iii. The Secant Method

C. Engineering Application for Roots of Equations

A. Bracketing Methods
These techniques are called bracketing methods because 2 initial guesses for the root are required and these guesses must be “bracket”.

i. Graphical Method
“Obtaining an estimate of the root of the equation \( f(x) = 0 \) is to make a plot of the function & observe where it crosses the axis. This point, which represents the \( x \) value for which \( f(x) = 0 \), provides a rough approximation of the root.”
Example 3.1 : Graphical Method

Use the graphical method to determine the drag coefficient, $c$ for a parachutist of mass, $m = 68.1 \text{ kg}$, velocity, $v = 40 \text{ m/s}$ after free-falling for time, $t = 10 \text{ s}$. The acceleration due to gravity is $9.8 \text{ m/s}^2$.

Solution:

Given formula: 
$$v = \frac{gm}{c} (1 - e^{-(c/m)t})$$

Then, deducting/subtracting the dependent variable, $v$ from both side of the equation to give:
$$f(c) = \frac{gm}{c} (1 - e^{-(c/m)t}) - v$$

Substitution all given values;
$$f(c) = 9.8 \frac{(68.1)}{c} [1 - e^{-(c/68.1)10}] - 40$$

Simplify the equation;
$$f(c) = \frac{667.38}{c} [1 - e^{-0.146843c}] - 40$$

Then, various values of $c$ can be substituted into right-hand side of this equation to compute:
These points are plotted in Fig. 3.1. The resulting curve crosses the \( c \) axis is between 12 and 16.

Visual inspection (shows in Fig. 3.1) of the plot provides a rough estimate of the root of 14.75. The validity of the graphical estimate can be checked by substituting it into equation (3.4) to yield:

\[
f(14.75) = \frac{9.8(68.1)}{14.75} \left(1 - e^{-\frac{14.75}{68.1}10}\right) - 40
\]

\[
= 0.059 \text{ (which is close to zero)}
\]

It can also be checked by substituting \( c = 14.75 \) into given equation (3.3) to give:

\[
v = \frac{gm}{c} \left(1 - e^{-\frac{c}{m}t}\right) \text{ (given equation)}
\]

\[
v = \frac{9.8(68.1)}{14.75} \left(1 - e^{-\frac{14.75}{68.1}10}\right) = 40.059 \text{ m/s}
\]

which is very close to desire fall velocity of 40 m/s.
Fig. 3.1: Graphical method for determining the roots of an equation.
ii. Bisection Method

When applying graphical method, we observed $f(x)$ has changed sign from +ve to –ve, where;

$$f(x_l).f(x_u) < 0$$

Then there is at least one real root between $x_l$ and $x_u$.

In this method, we dividing halve the interval $(x_l$ and $x_u$) into a number of sub-intervals. Each sub-interval is to locate the sign changes.

**Step of Calculation:**

Step 1: Choose lower $x_l$ and upper $x_u$ such that the function changes sign (+ve and –ve) over the interval, where this can be checked by ensuring that $f(x_l).f(x_u) < 0$

Step 2: Estimate the root: $x_r = (x_l + x_u)/2$

Step 3: Make the following evaluations to determine in which subinterval the root lies:

a. If $f(x_l).f(x_r) < 0$, root lies in the lower subinterval. Therefore, set $x_u = x_r$ and return to step 2.

b. If $f(x_l).f(x_r) > 0$, root lies in the upper subinterval. Therefore, set $x_l = x_r$ and return to step 2.

c. If $f(x_l).f(x_r) = 0$, the root equals $x_r$; terminate the computation.
Example 3.2: Bisection Method

Use bisection to solve the same problem approached graphically in Example 3.1. Stopping criterion is given as $\varepsilon_s = 0.5\%$.

Solution:

The first step in bisection is to guess 2 values of the unknown, which in present problem, $c$ that give values for $f(x)$ with different sign.

Therefore, in 2nd step the initial estimate of the root, $x_r$, lies at the midpoint of the interval values of 12 and 16.

$$x_r = \frac{(x_l + x_u)}{2}$$

$$x_r = \frac{(12 + 16)}{2} = 14$$

This estimate represents a true percent relative error of $\varepsilon_t = 5.3\%$ [true value of the root is 14.7802]

Next we compute the function value at the lower bound and at the midpoint (as trial):

$$f(12).f(14) = (6.067)(1.569) = 9.517$$

which is greater than zero, hence no sign change occurs between the lower bound and the midpoint. Consequently, the root must be located between 14 and 16. Therefore, redefining the lower bound as 14 and determining a revised root as:
Fig. 3.2: The Bisection Method for the first three iterations from Example 3.2

Fig. 3.3: True and Approximation Errors of Bisection Method
\[ x_r = \frac{(14 + 16)}{2} = 15 \]

Which represent a true percent error \( \varepsilon_t = 1.5\% \). The process can be repeated to obtain refined estimate, such as:

\[ f(14).f(15) = (1.569)(-0.425) = -0.666 \]

Therefore, the root is between 14 and 15. The upper bound is redefined as 15, and the root estimate for the 3\(^{rd}\) iteration is calculated as:

\[ x_r = \frac{(14 + 15)}{2} = 14.5 \]

Which represent a true percent error \( \varepsilon_t = 1.9\% \). The method can be repeated until the result is accurate enough to satisfy your needs.

Normally the termination of computation can be defined as:

\[ | \varepsilon_a | < \varepsilon_s \]

If \( \varepsilon_s \) is not given, to calculate \( \varepsilon_s = (0.5 \times 10^{2-n})\% \)

(from equation 2.4 in Chapter 2)

\( n = \) number of significant figure
Example 3.2: Continue previous example until $\varepsilon_a$ falls below $\varepsilon_s = 0.5\%$

<table>
<thead>
<tr>
<th>Iteration</th>
<th>$x_l$</th>
<th>$x_u$</th>
<th>$x_r$</th>
<th>$\varepsilon_a$ (%)</th>
<th>$\varepsilon_t$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12</td>
<td>16</td>
<td>14</td>
<td>-</td>
<td>5.279</td>
</tr>
<tr>
<td>2</td>
<td>14</td>
<td>16</td>
<td>15</td>
<td>6.667</td>
<td>1.487</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>15</td>
<td>14.5</td>
<td>3.448</td>
<td>1.896</td>
</tr>
<tr>
<td>4</td>
<td>14.5</td>
<td>15</td>
<td>14.75</td>
<td>1.695</td>
<td>0.204</td>
</tr>
<tr>
<td>5</td>
<td>14.75</td>
<td>15</td>
<td>14.875</td>
<td>0.840</td>
<td>0.641</td>
</tr>
<tr>
<td>6</td>
<td>14.75</td>
<td>14.875</td>
<td>14.8125</td>
<td>0.422</td>
<td>0.219</td>
</tr>
</tbody>
</table>

After six iterations the computation can be terminated with root value of 14.8125.
iii. The False-Position Method  (or linear interpolation Method)

Although bisection method perfectly valid technique for determine roots, but its approach are relatively inefficient.

False-position method is an alternative based on graphical insight.

A shortcoming of the bisection method is that, in dividing the interval from $x_i$ to $x_u$ into equal halves, no account is taken of the magnitudes of $f(x_i)$ and $f(x_u)$.

For example, if $f(x_i)$ is much closer to zero than $f(x_u)$ and it is likely that the root is closer to $x_i$ than to $x_u$ (Fig. 3.4).

Thus, an alternative method that exploits this graphical insight to joint $f(x_i)$ and $f(x_u)$ by a straight line. The intersection of this line with the $x$ axis represents an improved estimate of the root.

The fact that the replacement of the curve by a straight line gives a “false position” of the root.
Fig. 3.4: False Position Method

Fig. 3.5: Comparison of relative error of Bisection and False-Position Method
To determine the formula for the false-position method:

Using similar triangles, (From Fig. 3.4) the intersection of the straight line with the x-axis can be estimated as:

\[
\frac{f(x_l)}{(x_r - x_l)} = \frac{f(x_u)}{(x_r - x_u)} \quad \text{--- (3.5)}
\]

The equation above can be solved:

\[
x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)} \quad \text{--- (3.6)}
\]

Equation (3.6) is called as False-Position Formula.
Example 3.3: False-Position Method

Use the false-position method to determine the root of the same equation investigated in Example 3.1

Solution: As in Example 3.2, the computation guesses of $x_l = 12$ and $x_u = 16$ (true value of the root is 14.7802)

First iteration: $x_l = 12 \quad f(x_l) = 6.0699$

$x_u = 16 \quad f(x_u) = -2.2688$

$x_r = 16 - (-2.2688)(12-16)/(6.0669)\{-2.2688\} 
= 14.9113$ (true relative error 0.89%)

Therefore, the root lies in the first subinterval $[x_l]$, and $x_r$ becomes the upper limit for the next iteration, $x_u = 14.9113$
Second iteration: \( x_l = 12 \quad f(x_l) = 6.0699 \)
\( x_u = 14.9113 \quad f(x_u) = -0.2543 \)
\( x_r = 14.9113 - (-0.2543)(12 - 14.9113)/(6.0669) - (-0.2543) \)
\( = 14.7942 \) (approximate relative error 0.79% and true error 0.09%)

Additional iteration can be performed to refine the estimate of the roots.
**Bisection Algorithm Results**

Example 4.4 with $\varepsilon_s = 0.5\%$

<table>
<thead>
<tr>
<th>Iter</th>
<th>$x_l$</th>
<th>$x_u$</th>
<th>$x_r$</th>
<th>$E_a$</th>
<th>$E_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.00</td>
<td>16.00</td>
<td>14.0000</td>
<td>-</td>
<td>5.279</td>
</tr>
<tr>
<td>2</td>
<td>14.00</td>
<td>16.00</td>
<td>15.0000</td>
<td>6.667</td>
<td>1.487</td>
</tr>
<tr>
<td>3</td>
<td>14.00</td>
<td>15.00</td>
<td>14.5000</td>
<td>3.448</td>
<td>1.896</td>
</tr>
<tr>
<td>4</td>
<td>14.50</td>
<td>15.00</td>
<td>14.7500</td>
<td>1.695</td>
<td>0.205</td>
</tr>
<tr>
<td>5</td>
<td>14.75</td>
<td>15.00</td>
<td>14.8750</td>
<td>0.840</td>
<td>0.641</td>
</tr>
<tr>
<td>6</td>
<td>14.75</td>
<td>14.875</td>
<td>14.8125</td>
<td>0.422</td>
<td>0.218</td>
</tr>
</tbody>
</table>

**False Position Algorithm Results**

Example 4.4 with $\varepsilon_s = 0.5\%$

<table>
<thead>
<tr>
<th>Iter</th>
<th>$x_l$</th>
<th>$x_r$</th>
<th>$x$</th>
<th>$E_a$</th>
<th>$E_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.00</td>
<td>14.9113</td>
<td>-</td>
<td>0.887</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>12.00</td>
<td>14.7942</td>
<td>14.7942</td>
<td>0.792</td>
<td>0.094</td>
</tr>
<tr>
<td>3</td>
<td>12.00</td>
<td>14.7817</td>
<td>14.7817</td>
<td>0.085</td>
<td>0.010</td>
</tr>
</tbody>
</table>
B. Open Method

For the bracketing methods, the root is located within an interval prescribed by a lower and an upper bound. Repeated application of these methods always results in closer estimates of the true value of the root (*convergent*: move closer to the truth as the computation progresses)

In contrast, the **open methods** are based on formulas that require only a single starting value of $x$ or 2 starting values that do not necessarily bracket the root.

However, when the open methods converge they usually do so much quickly than the bracketing method.

i. Simple Fixed-Point Iteration

Rearranging the function $f(x) = 0$ so that $x$ is on the left-hand side of the equation:

$$x = g(x) \quad (3.7)$$

This transformation can be accomplished either by algebraic manipulation or by simply adding $x$ to both sides of the original equation. For example;

$$x^2 - 2x + 3 = 0$$
Can be simply manipulated to yield:

\[ x = \frac{x^2 + 3}{2} \]

Another example: \( \sin x = 0 \)

Could be put into the form of equation (3.7) by adding \( x \) to both sides to yield:

\[ x = \sin x + x \]

The utility of equation (3.7) is that provides a formula to predict a new value of \( x \) as a function of an old value of \( x \). Thus, given an initial guess at the root \( x_i \), equation (3.7) can be used to compute a new estimate \( x_{i+1} \) as expressed by the iterative formula;

\[ x_{i+1} = g(x_i) \] \quad (3.8)

The approximate error for this equation can be determined using the error estimator as discussed in previous Chapter 2, which is;

\[ \varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \times 100\% \]
Example 3.4: Simple Fixed-Point Iteration

Use simple fixed-point iteration to locate the root of \( f(x) = e^{-x} - x \)

Solution:

The function can be separated directly and expressed in the form of equation (3.8) as;

\[
x_{i+1} = e^{-x_i}
\]

Starting with an initial guess of \( x_0 = 0 \), this iterative equation can be applied to compute:

<table>
<thead>
<tr>
<th>( i )</th>
<th>( x_i )</th>
<th>( \varepsilon_a(%) )</th>
<th>( \varepsilon_d(%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>100.0</td>
<td>100.0</td>
</tr>
<tr>
<td>1</td>
<td>1.000000</td>
<td>100.0</td>
<td>76.3</td>
</tr>
<tr>
<td>2</td>
<td>0.367879</td>
<td>171.8</td>
<td>35.1</td>
</tr>
<tr>
<td>8</td>
<td>0.560115</td>
<td>3.48</td>
<td>1.24</td>
</tr>
<tr>
<td>9</td>
<td>0.571143</td>
<td>1.93</td>
<td>0.705</td>
</tr>
<tr>
<td>10</td>
<td>0.564879</td>
<td>1.11</td>
<td>0.399</td>
</tr>
</tbody>
</table>

Thus, each iteration brings the estimate closer to the true value of the root: \( 0.56714329 \)
ii. Newton-Raphson Method

Perhaps the most widely used of all root-locating formulas.

As shown by the Fig.3.6, the initial guess at the root is $x_i$, a tangent can be extended from the point $[x_i, f(x_i)]$.

The point where this tangent crosses the x axis usually represents an improved estimate of the root.

The Newton-Raphson method can be derive on the basis of this geometrical interpretation (an alternative method based on the Taylor series).

As in Fig.3.6, the first derivative at $x$ is equivalent to the slope:

$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}} \quad \text{- - - - - (3.9)}$$

Which can be arranged to yield:
\[ x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \quad \ldots \quad 3.10 \]

which is called the Newton-Raphson formula

Fig. 3.6: The Newton-Raphson method
Example 3.5

Use the Newton-Raphson method to estimate the root of \( f(x) = e^x - x \) employing an initial guess of \( x_0 = 0 \).

Solution:

The first derivative of the function can be evaluated as:

\[
f'(x) = e^x - 1
\]

Which can be substituted along with the original function equation (3.10) to give:

\[
x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{e^{-x_i} - 1}
\]

Starting with an initial guess of \( x_0 = 0 \), this iterative equation can be applied to compute:

<table>
<thead>
<tr>
<th>( i )</th>
<th>( x_i )</th>
<th>( \varepsilon_i(%) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>0.50000000000</td>
<td>11.8</td>
</tr>
<tr>
<td>2</td>
<td>0.566311003</td>
<td>0.147</td>
</tr>
<tr>
<td>3</td>
<td>0.567143165</td>
<td>0.0000220</td>
</tr>
<tr>
<td>4</td>
<td>0.567143290</td>
<td>&lt; 10^{-8}</td>
</tr>
</tbody>
</table>
The approach rapidly converges on the true root. Notice that the true percent relative error at each iteration decreases much faster (required only 3 iterations) that it does in Simple Fixed-Point Iteration (Compare with Example 3.4; required more than 10 iterations)

### iii. The Secant Method

A potential problem in implementing the Newton-Raphson method is the evaluation of the derivative.

Although this is convenient for polynomials and many other functions, there are certain functions whose derivatives may be extremely difficult or inconvenient to evaluate. For these cases, the derivatives can be approximated by a backward finite divided difference, as in Fig.3.7.

\[
f'(x_i) \approx \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}
\]
From the backward finite divided difference substituted into equation (3.10)- The Newton-Raphson Method equation: To yield the following iterative equation:

\[ x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)} \]  

This formula is for the Secant Method.
Notice that the Scant Method requires two initial estimates of $x$. However, because $f(x)$ is not required to change signs between the estimates, it is not classified as a bracketing method.

**Example 3.6: The Scant Method**

Use the scant method to estimate the root of $f(x) = e^x - x$. Start with initial estimates of $x_1 = 0$ and $x_0 = 1.0$.

**Solution:**

Recall that the true root is 0.56714329.....

**First iteration:**

$x_1 = 0 \quad f(x_1) = 1.00000$

$x_0 = 1 \quad f(x_0) = -0.63212$

$x_1 = 1 - [-0.63212(0 - 1)] / (1 - [-0.63212]) = 0.61270$

$\varepsilon_t = 8.0\%$
Second iteration:

\[ x_o = 1 \quad f(x_o) = -0.63212 \]
\[ x_1 = 0.61270 \quad f(x_1) = -0.07081 \]

(Note that both estimates are now on the same side of the root.)

\[ x_2 = 0.61270 - \frac{-0.07081(1 - 0.61270)}{-0.63212 - (-0.07081)} \]
\[ = 0.56384 \]
\[ \varepsilon_t = 0.58\% \]

Third iteration:

\[ x_1 = 0.61270 \quad f(x_o) = -0.07081 \]
\[ x_2 = 0.56384 \quad f(x_1) = 0.00518 \]
\[ x_3 = 0.56384 - \frac{0.00518(0.61270 - 0.56384)}{-0.07081 - (0.00518)} \]
\[ = 0.56717 \]
\[ \varepsilon_t = 0.0048\% \]
Problems (Bracketing Method)

5.1 Determine the real roots of \( f(x) = -0.4x^2 + 2.2x + 4.7 \);

a. Graphically

b. Using the quadratic formula

c. Using three iterations of Bisection Method to determine the highest root. Employ guesses of \( x_l = 5 \) and \( x_u = 10 \). Compute the estimated error \( \varepsilon_a \) and the true error \( \varepsilon_t \) after each iteration.

5.4 Determine the real roots of;

\[ f(x) = -11 - 22x + 17x^2 - 2.5x^3: \]

a. Graphically.

b. Using the False-Position Method with a value of \( \varepsilon_s \) corresponding to three significant figures to determine the lowest root.
5.6 Determine the real root of $\ln x^2 = 0.7$:

a. Graphically.

b. Using three iterations of the Bisection Method, with initial guesses of $x_l = 0.5$ and $x_u = 2$.

c. Using three iterations of the False-Position Method, with the same initial guesses as in (b).

5.7 Determine the real root of $f(x) = (0.9 – 0.4x)/x$:

a. Analytically.

b. Graphically.

c. Using three iterations of the False-Position Method and initial guesses of 1 and 3. Compute the approximate error $\varepsilon_a$ and the true error $\varepsilon_t$ after each iteration.

5.12 The velocity $v$ of a falling parachutist with a drag coefficient $c = 14\text{kg/s}$, compute the mass $m$ so that the velocity is $v = 35\text{m/s}$ at $t = 7\text{s}$. Use the False-Position Method to determine $m$ to a level of $\varepsilon_s = 0.1\%$. 

Problems (Open Method)

6.1 Use simple Fixed-Point iteration to locate the root of:

\[ f(x) = \sin(\sqrt{x}) - x \]

Use an initial guess of \( x_0 = 0.5 \) and iterate until \( \varepsilon_a \leq 0.01\% \)

6.3 determine the real roots of ;

\[ f(x) = -2.0 + 6x - 4x^2 + 0.5x^3 : \]

a. Graphically.

b. Using the Newton-Raphson Method to within \( \varepsilon_a = 0.01\% \)

6.5 Determine the lowest real root of ;

\[ f(x) = -11 - 22x + 17x^2 - 2.5x^3 : \]

a. Graphically.

b. Using the Secant Method to a value of \( \varepsilon_s \) corresponding to three significant figures.
Solution

5.1 (a) Given equation: \( f(x) = -0.4x^2 + 2.2x + 4.7 \)

Guess the \( x \) values so, give \( f(x) = 0 \):

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2</td>
<td>-1.3</td>
</tr>
<tr>
<td>-1</td>
<td>2.1</td>
</tr>
<tr>
<td>0</td>
<td>4.7</td>
</tr>
<tr>
<td>1</td>
<td>6.5</td>
</tr>
<tr>
<td>2</td>
<td>7.5</td>
</tr>
<tr>
<td>4</td>
<td>7.1</td>
</tr>
<tr>
<td>6</td>
<td>3.5</td>
</tr>
<tr>
<td>8</td>
<td>-3.3</td>
</tr>
<tr>
<td>10</td>
<td>-13.3</td>
</tr>
</tbody>
</table>
5.1 (b) Quadratic formula:

\[ x = \frac{-b \pm \sqrt{b^2 + 4ac}}{2a} \]

Thus;

\[ x = \frac{-2.2 \pm \sqrt{(2.2)^2 + 4(0.4)(4.7)}}{2(0.4)} \]

\[ = 7.1446 \text{ or }\]

\[ = -1.6446 \]
5.1 (c) Bisection Method:

To determine the highest root:

Given initial guesses $x_l = 5$ and $x_u = 10$

1st iteration:

$$x_r = \frac{(5 + 10)}{2} = 7.5$$

Thus;

$$\varepsilon_t = \frac{7.1446 - 7.5}{7.1446} \times 100\% = -4.97\%$$

$$\varepsilon_a = \frac{|x_u - x_l|}{x_u + x_l} \times 100\% = \frac{10 - 5}{10 + 5} \times 100\% = \frac{5}{15} \times 100\% = 33.3\%$$

Since $f(x_l)f(x_r) < 0$, set $x_u = x_r$

Thus for 2nd iteration:

$$x_r = \frac{(5 + 7.5)}{2} = 6.25$$

Thus;

$$\varepsilon_t = \frac{7.1446 - 6.25}{7.1446} \times 100\% = 12.5\%$$

$$\varepsilon_a = \frac{|7.5 - 5|}{7.5 + 5} \times 100\% = \frac{2.5}{12.5} \times 100\% = 20\%$$
Since \( f(x_l)f(x_r) > 0 \), set \( x_l = x_r \).

Thus for 2\(^{nd}\) iteration:

\[
x_r = (6.25 + 7.5) / 2 = 6.875
\]

Thus;

\[
\varepsilon_t = 7.1446 - 6.875 / 7.1446 \times 100\% = 3.77\%
\]

\[
\varepsilon_a = \left| \frac{7.5 - 6.25}{7.5 + 6.25} \right| \times 100\% = \left| \frac{1.25}{13.75} \right| \times 100\% = 9.1\%
\]
C. Engineering Applications: Roots of Equations

The purpose of this chapter is to use the numerical procedure as discussed previously to solve actual engineering problems.

Numerical techniques are important for practical applications because engineers frequently encounter problems that cannot be approached using analytical techniques.

In the example below is taken from chemical engineering, provides an excellent example of how root-location method allow you to use realistic formulas in engineering practice.

Example 3.7: Ideal and Non-Ideal Gas Law

Background: The ideal gas law is given by

\[ pV = nRT \]  \hspace{1cm} (3.12)

where; \( p \) = absolute pressure \( V \) = volume
\( n \) = number of moles \( T \) = temperature
\( R \) = universal gas constant
Although this equation is widely used by engineers and scientists, it is accurate over only a limited ranges of pressure and temperature. Furthermore the equation is more appropriate for some gases than for others. An alternative equation of state for gases is given by:

\[
\left( p + \frac{a}{v^2} \right) (v - b) = RT \quad \text{(3.13)}
\]

known as the \textit{van der Walls equation}.

where;

- \( v = V/n \) is the molal volume
- \( a \) and \( b \) = empirical constants that depend on the particular gas

\textbf{Situation/Problem Given:}

A chemical engineering design project requires that you accurately estimate the molal volume \( v \) of both carbon dioxide and oxygen for a number of different temperature and pressure combinations so that appropriate containment vessels can be selected.
It is also of interest to examine how well each gas conforms to the ideal gas law by comparing the molal volume as calculated by equation (3.12) and (3.13).

The following data are provided:

\[ R = 0.082054 \text{ L atm/(mol K)} \]

For carbon dioxide: \( a = 3.592; b = 0.04267 \)

For oxygen: \( a = 1.360; b = 0.03183 \)

The design pressure of interest are 1, 10, and 100 atm for temperature combinations of 300, 500, and 700 K.

**Solutions:**

Molal volumes for both gases are calculated using the ideal gas law, with \( n=1 \).

Then, if \( p=1 \text{ atm} \) and \( T=300K \),

\[
\nu = \frac{V}{n} = \frac{RT}{p} = 0.082054 \frac{\text{L atm}}{\text{mol K}} \frac{300 \text{K}}{1 \text{ atm}} = 24.6162 \text{L/mol}
\]

These calculations are repeated for all \( T \) and \( p \) combinations as presented in Table 3.1.
**Table 3.1: Computations of molal volume, \( v \)**

<table>
<thead>
<tr>
<th>Temperature ( K )</th>
<th>Pressure ( atm )</th>
<th>molal volume ideal gas law (L/mol)</th>
<th>molal volume ( CO_2 ) (L/mol)</th>
<th>molal volume ( O_2 ) (L/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1</td>
<td>24.6162</td>
<td>24.5126</td>
<td>24.5928</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2.4616</td>
<td>2.3545</td>
<td>2.4384</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.2462</td>
<td>0.0795</td>
<td>0.2264</td>
</tr>
<tr>
<td>500</td>
<td>1</td>
<td>41.0270</td>
<td>40.9821</td>
<td>41.0259</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>4.1027</td>
<td>4.0578</td>
<td>4.1016</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.4103</td>
<td>0.3663</td>
<td>0.4116</td>
</tr>
<tr>
<td>700</td>
<td>1</td>
<td>57.4378</td>
<td>57.4179</td>
<td>57.4460</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>5.7438</td>
<td>5.7242</td>
<td>5.7521</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.5744</td>
<td>0.5575</td>
<td>0.5842</td>
</tr>
</tbody>
</table>
While, the computation of molal volume, $v$ from the van der Waals equation can be accomplished using any the NM for finding roots of equations discussed in Chapter 3;

Thus, the equation (3.13) becomes;

$$f(v) = \left(p + \frac{a}{v^2}\right)(v - b) - RT$$  \hspace{1cm} (3.14)

In this case, the derivative of $f(v)$ is easy to determine and the Newton-Raphson method is convenient and efficient to implement.

The derivative of $f(v)$ with respect to $v$ is given by:

$$f'(v) = \frac{dp}{dv} - \frac{a}{v^3} + \frac{2ab}{v^3}$$

The Newton-Raphson method is described by equation (3.10):

$$v_{i+1} = v_i - \frac{f(v_i)}{f'(v_i)}$$
From this equation, root of equation can be estimated.

For example, using the initial guess of 24.6162, the molal volume of CO$_2$ at 300K and 1 atm is computed as 24.5126 L.mol.

This result was obtained after just 2 iterations and has an $\varepsilon_a$ less than 0.001 %.

The rest of computations can be estimated by using similar method and all results are presented in Table 3.1.

PLEASE DO YOUR HOMEWORK TO PRODUCE ALL RESULTS AS PRESENTED IN TABLE 3.1.

YOU ARE SUGGESTED TO TRY OTHER METHODS AS WELL TO DETERMINE THE ROOTS OF EQUATIONS !!!!!
END OF CHAPTER 3