NUMERICAL ANALYSIS I

Introduction
Numerical analysis is concerned with the process by which mathematical problems are solved by the operations of ordinary arithmetic.

We shall be concerned with fundamental mathematical problems such as solution of equations, the evaluation of functions and integration etc. Although, quite a lot of these problems have exact solutions, the range of problems which can be solved exactly is very limited. Therefore, we require efficient methods of obtaining good approximation.

Computer Arithmetic and Errors
A feature of numerical methods is that they usually provide only approximation solutions: a deliberate error may be made e.g. truncation of a series, so that the problem can be reconstructed to get a stable solution.

Types of Errors
1. **Blunder called Human Error:** This occurs when a different answer is written from what is obtained e.g. writing 0.7951 instead of 0.7591.

2. **Truncation Error:** These arises when an infinite process is replaced by a finite one. For instance, consider a finite number of terms in any infinite series e.g.

   \[
   \sqrt{x + 1} = 1 + x \cdot \frac{1}{2} \cdot x^2 + \ldots \text{ has truncation error of } \frac{1}{16} x^3 + \ldots 
   \]

   \[
   (x + 1)^{1/2} - (1 + x)^{1/2} = 1 + \frac{1}{2} x^2 + \frac{1}{2} \cdot (\frac{1}{2} - 1) x^3 + \ldots 
   \]

   If we consider

   \[
   (x + 1)^{1/2} \sqrt{x + 1} = 1 + x n + \frac{n(n-1)}{2!} x^2 + \frac{n(n-1)(n-2)}{3!} x^3 + \ldots 
   \]

   \[
   = 1 + \frac{x}{2} - \frac{1}{2} \left(\frac{1}{2} - 1\right) x^2 
   \]

   \[
   = 1 + \frac{2}{4} - \frac{1}{2} \cdot 1 
   \]

   \[
   = - \frac{1}{4} + \frac{1}{2} = \frac{1}{8} 
   \]

   Consider the taylor series expansion

   \[
   e^x = 1 + x 
   \]

   If the formula is used to calculate \( f = e^{0.1} \) we get

   \[
   f = 1 + 0.1 + \ldots 
   \]
Where do we stop? Theoretically, the calculation will never stop. There are always more terms to add on. If we do stop after a finite number of terms, we will not get the exact answer.

3. **Round-off Error:** Numbers having decimal or binary representations are often rounded e.g. \(1/3 = 0.3333\). If we multiply by 3 we have 0.9999 which is not exactly 1.

Round-off errors can be avoided by preventing cancellation of large terms.

### 1.2 Notation:
Let \(\Sigma\) (Epsilon) be the error. Let true value and appropriate be \(x\) and \(x^1\) respectively. The absolute error = |\(\Sigma\)| = |\(x - x^1\)| and relative error = \(\frac{|x-x|}{|x|}\) provided \(x \neq 0\).

**Definition:** A number \(x\) is said to be rounded to a \(d\)-decimal place number \(x^{(d)}\) if error \(\Sigma\) is given by \(|\Sigma| = |x - x^{(d)}| \leq \frac{1}{2} 10^{-d}\).

**Example:** Take \(\frac{1}{7} = 0.142857142\).

- Subtract it.
  - 0.002857142 (is the error)
  - 0.002857142 \(\leq \frac{1}{2} 10^{-2} = 0.005\)

Suppose \(x^1 = 0.1429\) (4 dec. place)

\[|\Sigma| = |x - x^1| = 0.000042858 \leq \frac{1}{2} 10^{-4} = 0.00005\]

### 1.3 Arithmetical Errors

Let \(x, y\) be two numbers and let \(x^1, y^1\) be their respective approximation with error \(\Sigma\) and \(\eta\) (eta).

**Solution:**
\[
x_1 + y_1 = (x - \Sigma) + (y - \eta) \\
(x + y) - (y - \eta) \\
(x + y) - (x^1 + y^1) = \Sigma + \eta
\]

Error in sum is sum of errors.

**Subtraction:**
\[
x_1 - y_1 = (x - \Sigma) - (y - \eta) \\
(x - y) - (x^1 - y^1) = \Sigma - \eta
\]

Error in difference is difference in errors.

**Assignment**
Compute the multiplication and division.

### 2.0 Condit and Stability

The condition of a function is a measure of the sensitivity of that function to small changes in its parameters.

If small change in the parameters induce only a small change in the behaviour of the function the function is well-conditioned otherwise it is ill-conditioned.

A numerical method is said to be stable, if small changes in the data induce only small changes in the solution of the process otherwise, the process is unstable. It is therefore clear that the stability of a numerical process is related to its conditioning.

Let the error, \(\Sigma_n\), at the \(n^{th}\) iteration be such that \(|\Sigma_n| a_n\), then the growth in error is called linear whereas if \(|\Sigma_n| a < n\) \((n > 1)\), the growth is exponential and if \(K < 1\), the error decreases exponentially.

It is desirable to aim at linear error growth and try as much as possible to avoid exponentially error growth.

If we consider a sequence
\[
1, \frac{1}{3}, \frac{1}{9}, \frac{1}{27}, \ldots, \frac{1}{3^n}.
\]

Our \(x_0 = 1\) and \(x_1 = \frac{1}{3}\).

We can have a relation \(A\) the form
\[
x_n = \alpha \left(\frac{1}{3}\right)^n + \beta (3)^n \ldots
\]
where \(\alpha = 1\) and \(\beta = 0\), so that the correct value of \(x_n = (1/3)n\). if we now compute our \(x_n\) (in 4 decimal places) the errors rapidly increase.

<table>
<thead>
<tr>
<th>(n)</th>
<th>(x_n) = ((\frac{1}{3})^n)</th>
<th>(1/3^n -)</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>1</td>
<td>0.3333</td>
<td>0.3333</td>
</tr>
<tr>
<td>2</td>
<td>0.1111</td>
<td>0.1111</td>
</tr>
</tbody>
</table>
At the sixth iteration, the solution \( x_6 \) is significantly different from the correct value.

Error = i.e. 0.0057 – 0.00141 = 0.0043

Thus, this is an exponential error growth and such should be avoided.

**Disadvantages**

1. Only one value of \( x \) can be derived
2. Least value of \( x \) can only be derived through one point formula.

**3.0 Polynomials and their zeros**

This section is concerned with solution of non-linear algebraic equation.

**3.1 Iterative method without derivatives**

A problem which frequently occurs in scientific works is finding roots of equation of the type.

\[ F(x) = 0 \quad (3.1) \]

For example

\[ 5x^3 + 3x^2 - 17x + 1 = 0 \]
\[ e^x \sin x = 0 \]

sometimes it may be possible to get exact root of 3.1 as in the case of factorisable polynomials such as

\[ x^2 + 3x + 2 = 0 \]

which roots are \( x = \frac{1}{2}, \frac{2}{2} \).

In general, we have to get approximate solutions by applying some computational procedure, usually iterative. We carefully choose some initial estimates of a root and improve on it by an iterative formula.

**3.1.1 Fixed Point Formula:** (One point formula)

This formula is also known as successive substitution or one point formula.

To find a root \( \alpha \) of equation (3.1), we write the equation in the form.

\[ x = f(x) \quad (3.2) \]

and given an initial estimate \( x_0 \), we improve by the scheme

\[ x_1 = f(x_0) \]
\[ x_2 = f(x_1) \]
\[ x_3 = f(x_2) \]
\[ \vdots \]
\[ x_{n+1} = f(x_n) \]

where \( x_0, x_1, \ldots x_n \) are successive approximations to the root.

For example

\[ F(x) = x^2 - 4x + 2 = 0 \quad (3.3) \]

We can write (3.3) in the form (3.2) as follows

\[ x = \sqrt{4x - 2} \quad \text{or} \quad x = \frac{4x - 2}{x} \]

but in this case, let us use

\[ x = \frac{1}{4} (x^2 + 2) \]

This suggests a scheme

\[ x_{n+1} = \frac{1}{4} (x_n^2 + 2) \]

Choose \( x_0 \) as 0, 3, and 4.

<table>
<thead>
<tr>
<th>( x_0 )</th>
<th>0</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_1 )</td>
<td>0.5000</td>
<td>2.75</td>
<td>4.5000</td>
</tr>
<tr>
<td>( x_2 )</td>
<td>0.5625</td>
<td>2.3906</td>
<td>5.5628</td>
</tr>
<tr>
<td>( x_3 )</td>
<td>0.5791</td>
<td>1.9287</td>
<td>8.2354</td>
</tr>
<tr>
<td>( x_4 )</td>
<td>0.5838</td>
<td>1.4300</td>
<td>17.4554</td>
</tr>
<tr>
<td>( x_5 )</td>
<td>0.5852</td>
<td>1.0112</td>
<td>76.6715</td>
</tr>
<tr>
<td>( x_6 )</td>
<td>0.5856</td>
<td>0.7556</td>
<td></td>
</tr>
<tr>
<td>( x_7 )</td>
<td>0.5857</td>
<td>0.6427</td>
<td></td>
</tr>
<tr>
<td>( x_8 )</td>
<td>0.5858</td>
<td>0.6033</td>
<td></td>
</tr>
<tr>
<td>( x_9 )</td>
<td>0.5858</td>
<td>0.5910</td>
<td></td>
</tr>
</tbody>
</table>

\( x = 0.5858 \) which is given by initial estimates 0, 3, 4 is obviously a bad initial value. The actual root are \( x^2 - 4x + 2 = 0 \).
1. \[ x = \frac{4 \pm \sqrt{16 - 4(1)^2}}{2} = 2 \pm \sqrt{2} \]

\[ x = 0.586 \text{ or } 3.414 \]

The actual root are 0.586 and 3.414. The other root 3.414 cannot be obtained by this method. The case can be illustrated below.

**Assignment**

1. Find an approximation to the smallest positive root of \( F(x) = 8x^4 - 8x^2 + 1 = 0 \) (Take \( x_0 = 0.3 \)).
2. Draw a flow chart illustrating the use of fixed point formula to solve \( x^2 - 4x + 2 = 0 \)
   Hence, write a FORTRAN program to solve the equation.

### 3.1.2 Bisection Rule

Using the formula, too initial estimates \( x_0 \) and \( x_1 \) are needed so that \( F(x_0) \) and \( F(x_1) \) are of opposite signs. A new estimate is

\[ X_2 = \frac{1}{2} (x_0 + x_1) \]

generally \( C_n = (a_n + b_n)/2 \)

\( X_2 \) is used to replace which ever of \( x_0 \) or \( x_1 \) has the same sign in \( F(x) \)

The process is repeated

For example

\[
\begin{array}{c|c|c|c}
 a_n & b_n & C_n(a_n + b_n)/2 & F(c_n) \\
 0.0 & 1.5 & 0.75 & + \\
 0.0 & 0.75 & 0.375 & - \\
 0.375 & 0.75 & 0.5625 & - \\
 0.5625 & 0.75 & 0.65625 & - \\
 0.65625 & 0.75 & 0.70313 & - \\
 0.70313 & 0.75 & 0.72656 & - \\
 0.72565 & 0.75 & 0.73828 & - \\
 0.73828 & 0.74414 & 0.74414 & + \\
 0.73728 & 0.74121 & 0.74121 & + \\
\end{array}
\]

Once an interval has been located, the method is very easy to implement, very reliable and has good error bounds. The only disadvantage is that the method is slow.

The interval ‘halving’ or ‘bisection’ method can be *speed* up by making better use of the information computed. The method only uses the sign of the function \( f \) and not its value. Thus, if the absolute value of the function is much smaller at one end than at the other it is likely that the root will be closed to the end where the function is smaller. The idea is exploited in the **Regula falsi** method.

### 3.1.3 Regular Falsi

Consider two initial estimates \( x_0 \) and \( x_i \)

\[ y_0 = F(x_0) \text{ and } y_1 = F(x_1) \]

It is possible to express the equation of a straight line through \( (x_0, y_0), (x_1, y_1) \) as

\[ x = y - y_1 \]

\[ x = \frac{y_0 - y}{y_1 - y_0} \]

It is possible to express the equation as a linear interpolation in the form of

\[ \frac{x_0 F(x_1) - x_1 F(x_0)}{F(x_1) - F(x_0)} \]

**Bisection Rule**

Example \( F(x) = x^2 - 3x + 1 = 0 \)

\[ x_0 = 0 \]

So that \( F(x_0) = 1 \) +ve
Choose

\[ x_1 = 1 \quad \text{F}(x_1) = -1 - \text{ve} \]

\[ x_2 = \frac{1}{2} (x_0 + x_1) = \frac{1}{2} (0 + 1) = 0.5 \]

\[ \text{F}(0.5) = -0.25 \text{ is } -\text{ve} \]

We neglect \( x_1 \) and we have

\[ X_3 = \frac{1}{2} (x_0 + x_2) = \frac{1}{2} (0 + 0.5) = 0.25 \]

\[ \text{F}(0.25) = 0.3125 \text{ +ve} \]

We neglect \( x_0 \) and we have

\[ x_4 = \frac{1}{2} (x_2 + x_3) = \frac{1}{2} (0.5 + 0.25) = 0.375 \]

\[ \text{F}(0.375) \text{ is +ve} \]

We reject \( x_3 \) and we have

\[ x_5 = \frac{1}{2} (x_2 + x_4) = \frac{1}{2} (0.5 + 0.375) = 0.4375 \]

\[ \text{F}(0.4375) \text{ is } -\text{ve} \]

We reject \( x_2 \), and have

\[ x_6 = \frac{1}{2} (x_4 + x_5) = \frac{1}{2} (0.375 + 0.4375) \]

\[ \text{F}(x_6) = \frac{1}{2} (\text{F}(x_4) - \text{F}(x_5)) \]

This is linear function \( x(y) \) with \( x(y_0) = x_0 \) and \( x(y_1) = x_1 \)

The line intersects the \( x - \) axis at the point obtained by putting \( y = 0 \) in (3.4)

\[ x_2 = \frac{y_1}{y_1 - y_0} x_0 + \frac{-y_0}{y_1 - y_0} x_1 \]

\[ = x_0 y_1 - x_1 y_0 \]

This may be re-written on a linear interpolation form as

\[ x_0 \frac{\text{F}(x_1) - x_1 \text{F}(x_0)}{\text{F}(x_1) - \text{F}(x_0)} \]

This can also be written as

\[ x_2 = x_1 - (x_1 - x_0) \frac{\text{F}(x_1)}{\text{F}(x_1) - \text{F}(x_0)} \]

It may be repeated such that an iterative scheme results. As in the case of binary search (bisection rule) the two estimates slide give opposite signs in \( \text{F}(x) \).

The convergence in this method is faster than that in bisection rule.

Example

\[ \text{F}(x) = x^2 - 3x + 1 = 0 \]

Choose \( x_0 = 0 \)

\[ x_1 = 1 \]

Since \( \text{F}(x_0) \) is +ve = 1

and \( \text{F}(x_1) \) is -ve = -1

\[ x_2 = x_0 \frac{\text{F}(x_1) - x_1 \text{F}(x_0)}{\text{F}(x_1) - \text{F}(x_0)} \]

\[ x_2 = \frac{0 - 1}{1 - 1} = \frac{1}{2} = 0.5 \]

\[ \text{F}(x_2) = \text{F}(0.5) = (0.5)^2 - 3(0.5) + 1 = 0.25 - 1.5 + 1 = -0.25 \text{ +ve} \]

So, we reject \( x_1 \)

\[ x_3 = x_0 \frac{\text{F}(x_2) - x_2 \text{F}(x_0)}{\text{F}(x_2) - \text{F}(x_0)} \]

\[ x_3 = \frac{0 - 0.5 \times 1}{0.25 - 1} = \frac{0.5}{1.25} = 0.4 \]

\[ \text{F}(x_3) = \text{F}(0.4) = 0.4^2 - 3(0.4) + 1 = -0.04 \text{ -ve} \]

So, we reject \( x_2 \)
\[ x_4 = x_0 F(x_1) - x_3 F(x_0) \]
\[ \frac{F(x_4) - F(x_0)}{x_4 - x_0} = 0.3846 \]
\[ F(x_4) = (0.3846)^2 - 3(0.3846) + 1 = -0.154 \]

And so on, we continue until convergence is achieved.

**Assignment**

Write a FORTRAN to illustrate the use of regula falsi to solve \( x^2 - 5x + 1 = 0 \).

### 4.0 ITERATIVE METHODS WITH DERIVATIVES

#### 4.1 Order of Convergence:

Let \( \alpha \) be a root of \( F(\alpha) = 0 \)

\[ \alpha = F(\alpha) \]

suppose the estimate \( \alpha \) has error \( \sum_n \)

**Comments:**

1. Convergence is first order if \( f'(\alpha) \neq 0 \), \( f''(\alpha) =, \ldots, = 0 \)
2. Convergence is second order if
   \[ f'(\alpha) = 0 \text{ and } f''(\alpha) \]
3. Convergence is third order if
   \[ f'(\alpha) = 0 \text{ and } f''(\alpha) \]
   \[ f'''(\alpha) \neq 0 \]

#### 4.2 Newton-Raphson Method

From the figure, \( a \) is the point at which \( f(x) = 0 \) and \( x_0 \) is an estimate of \( a \). The Newton-Raphson method computes a new estimate, \( x_1 \) in the following way:

This is the second order convergence.

Let \( x \) be a root of equation (3.1) \(- \frac{F(x)}{x} = 0 \)

If \( x_n \) is the \( n \)th estimate with error \( \sum_n \),
then \( x = x_n + \sum_n \ldots \)

\[ F(x) = F(x_n + \sum_n) = 0 \]
\[ = F(x_n) + n F'(x_n) + \sum_n^2 F''(x_n) + \ldots + \]
\[ = \frac{\Omega F(x_n) + \sum_n F'(x_n) = 0}{n} \]
\[ = \sum_n = -F(x_n) \]
\[ -F(x_n) \]

The iteration scheme in 4.1 becomes

\[ x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)} \]

- N - R method.

For example

\[ F(x) = x^2 - 4x + 2 = 0 \]
\[ F'(x) = 2x - 4 \]

Therefore \( x_{n+1} = x_n - \frac{(x_n^2 - 4x_n + 2)}{2x_n - 4} \)

Using our former initial estimate

\begin{tabular}{c|c|c}
\( X_0 \) & 0 & 3
\end{tabular}
<table>
<thead>
<tr>
<th>$x_1$</th>
<th>0.5</th>
<th>3.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_2$</td>
<td>0.5833</td>
<td>3.4162</td>
</tr>
<tr>
<td>$x_3$</td>
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<tr>
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<td>0.5858</td>
<td>3.4142</td>
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