COUNCIL OF SCIENTIFIC & INDUSTRIAL RESEARCH

Mathematical Science

8. Numerical Analysis

- 8.1 Errors
- 8.2 Interpolation with Equal and Unequal Intervals
- 8.3 Solution of Algebraic and transcendental Equations
- 8.4 Solution of system of linear equations
- 8.5 Numerical Integration
- 8.6 Numerical solution of Differential equations
- 8.7 Determination of eigenvalues by power method



8. Numerical Analysis

8.1 Errors

8.1.1 Significant figures/digits: The Significant figures/digits are the digits which are used to represent a number.

Examples (8.1):

- (i) $0, 1, 2, \dots 9$ are significant figures.
- (ii) 3.15673, 4.00901 both contain six significant figures.
- (iii) 0.0008 contains only one significant figure which is 8 and all the zeros left to 8 here are used to fix the decimal positions.
- (iv) 6.0001 contain five significant figures.
- **8.1.2 Exact Numbers** (N_E): Exact numbers are those numbers which have no approximation.

Examples (8.2): $3, \frac{1}{7}, e, \sqrt{5}, \pi \text{ etc}$

8.1.3 Approximate Numbers (N_A): Approximate numbers are those numbers which can not be represented by finite numbers of digits.

Examples (8.3):

- (i) 1.732 is the approximation of $\sqrt{3}$.
- (ii) 3.142 is the approximation of π .
- **8.1.4 Error** (E): Error of a number is the differences of the exact value and approximate value of a number.

Error = Exact number - Approximate number

i.e.
$$E = N_E - N_A$$

Examples (8.4): $\sqrt{3}$ -1.732 is the error for $\sqrt{3}$.

Errors are committed two ways: (i) rounding a number to a finite digits (Rounding-off error) (ii) due to calculation (Significant error).

8.1.5 Rounding-off Error: Rounding-off error is the error for discarding all but a predecided number of digits.

Rules for rounding-off a number to n-significant figures:

- (i) If the digit at (n+1)-th place is less than 5, discard all the digits after n-th pace.
- (ii) If the digit at (n+1)-th place is greater than 5, add one to n-th place and discard all the digits after n-th pace.
- (iii) If the digit at (n+1)-th place is exactly 5 and n-th place is even, discard all the digits after n-th pace.

(iv) If the digit at (n+1)-th place is exactly 5 and n-th place is odd, add one to n-th place and discard all the digits after n-th pace.

Examples (8.4):

Correct the following numbers up to 4 significant figures.

- (i) $2.356489 \approx 2.356$ (4< 5, so 6 remains same)
- (ii) $3.78376 \ 3 \approx 3.784 \ (7 > 5$, so add 1 to 3)
- (iii) $5.3485345 \approx 5.348$ (8 is at 4th place even, so 8 remains same)
- (iv) $2.6735674 \approx 2.674$ (3 is at 4th place odd, so add 1 to 3)

8.1.6 Types of Errors: Significant Error (S_a) , Absolute (E_a) , Relative (E_r) and Relative Percentage Errors (E_p)

- (i) Significant Error (S_a) = Exact Numbers (N_E) Approximate Numbers (N_A) i.e. $S_a = N_E N_A$
- (ii) Absolute Error $(E_a) = |$ Exact Numbers (N_E) Approximate Numbers $(N_A)|$ i.e. $E_a = |N_E N_A|$
- i.e. $E_a = |N_E N_A|$ (iii) Relative Error $(E_r) = \frac{\text{Absolute Error }(E_a)}{\text{Exact Numbers }(N_E)}$

i.e.
$$E_r = \frac{E_a}{N_E}$$

(iv) Relative Percentage Error (E_p) = Relative Error $(E_r) \times 100\%$ i.e. $E_p = E_r \times 100\%$

Example (8.5):

Write the approximate representation of $\frac{1}{3}$ correct up to 4 significant figures and also find (i) Significant Error (S_a) , (ii) Absolute Error (E_a) , (iii) Relative Error (E_r) and (iv) Relative Percentage Error (E_n) .

<u>Solution:</u> $\frac{1}{3} = 0.3333$

- (i) $N_E=1.2345627$, $N_A=1.2345584$ Significant Error $(S_a)=N_E-N_A=0.0000043$ (looses 6 significant digits each N_E and N_A)
- (ii) Absolute Error $(E_a) = |N_E N_A| = |\frac{1}{3} 0.3333| = 0.000033$
- (iii) Relative Error $(E_r) = \frac{E_a}{N_E} = \frac{0.000033}{\frac{1}{3}} = 0.000099 \approx 0.0001$
- (iv) Relative Percentage Error $(E_p) = E_r \times 100 = \frac{E_a}{V_T} \times 100 = \frac{|V_T V_A|}{V_T} \times 100$

Remark:

(i) If a number be rounded up to m decimal places the absolute error $E_a \leq \frac{1}{2} 10^{-m}$

Example (8.6)

$$V_T = 345.26132$$
, $V_A = 345.261$

$$\therefore E_a = 0.00032 \le \frac{1}{2} \times 10^{-3} = 0.0005$$

(ii) If a number be rounded to n correct significant figures, then the relative error

$$E_r < \frac{1}{k \times 10^{n-1}}$$
, $k: first significant digit in the number.$

Example (8.7)
$$V_T = \frac{2}{3}$$
, $V_A = 0.6667$

(a)
$$E_a = |V_T - V_A| = 0.000033$$

(b)
$$E_r = \frac{E_a}{V_T} = 0.0000495 \approx 0.00005$$

(c)
$$E_p = E_r \times 100 = 0.005\%$$

$$E_p = 0.000033 < 0.00005$$

$$E_r < \frac{1}{k \times 10^{n-1}} = \frac{1}{6 \times 10^3} = 0.00166 \approx 0.0017 \ (k = 6, n = 4)$$

8.2 Interpolation with Equal and Unequal Intervals

Let y = f(x) defined in [a, b]. Let us consider the consecutive value of x, differing by h as $a = x_0$, $x_1 = x_0 + h$,, $x_r = x_0 + rh$,, $x_n = x_0 + h$

$$y_0 = f(x_0), y_1 = f(x_1), \dots, y_n = f(x_n).$$

 x_0, x_1, \ldots, x_n are called nodes and y_1, y_2, \ldots, y_n are called entries.

8.2.1 Forward differences: -

$$\Delta f(x_0) = f(x_0 + h) - f(x_0) = f(x_1) - f(x_0) = y_1 - y_0 = \Delta y_0$$

$$\Delta f(x_1) = f(x_1 + h) - f(x_1) = f(x_2) - f(x_1) = y_2 - y_1 = \Delta y_1$$

$$\Delta f(x_{n-1}) = f(x_{n-1} + h) - f(x_{n-1}) = f(x_n) - f(x_{n-1}) = y_n - y_{n-1} = \Delta y_{n-1}$$

$$\Delta^2 f(x_0) = \Delta^2 y_0 = y_2 - 2y_1 + y_0$$

$$\Delta^3 f(x_0) = \Delta^3 y_0 = y_3 - 3y_2 + 3y_1 - y_0$$

8.2.2 Backward differences: -

$$\nabla f(x_1) = f(x_1) - f(x_1 \cdot h) = f(x_1) - f(x_0) = y_1 - y_0 = \nabla y_1$$

$$\nabla f(x_n) = f(x_n) - f(x_{n-1}) = y_n - y_{n-1} = \nabla y_n$$

$$\Delta \cdot \nabla = \Delta - \nabla$$

Result:
$$\Delta^k f(x) = \sum_{i=0}^k (-1)^i \binom{k}{i} \delta[x + (k-i)\hbar]$$

• Fundamental theorem of difference calculus:-

If f(x) be a polynomial of degree n, then the n^{th} difference of f(x) is constant and (n+1)th difference vanish.

8.2.3 Shift operator E:-

$$E f(x) = f(x + h) \Rightarrow E = \Delta + 1$$
 and $E\Delta = \Delta E$

(i) Relation between Δ (difference operator) and $D \equiv \frac{d}{du}$ (differential operator)

By Taylor's Theorem:-

$$f(x + h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \dots$$

or,
$$E f(x) = f(x) + h D f(x) + \frac{h^2}{2!} D^2 f(x) + \dots \dots$$

or,
$$(\Delta + 1)f(x) = (1 + hD + \frac{h^2}{2!}D^2 + \dots)f(x)$$

or,
$$\Delta + 1 = e^{hD}$$

or,
$$hD = \log(1 + \Delta)$$

or,
$$D = \frac{1}{\hbar} \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots \right]$$

(ii) Expression of any value of a function in terms of the leading term and leading difference of a difference table

By Shift operator E, we have –

$$f(x + xh) = E f(x) = (1 + \Delta)f(x)$$
$$= \left[1 + \binom{n}{1}\Delta + \binom{n}{2}\Delta^2 + \dots + \binom{n}{n-1}\Delta^{n-1} + \Delta^n\right]f(x)$$

$$= \left[f(x_0) + \binom{n}{1} \Delta f(x_0) + \binom{n}{2} \Delta^2 f(x_0) + \dots + \binom{n}{n-1} \Delta^{n-1} f(x_0) + \Delta^n f(x_0) \right] f(x)$$

$$= y_0 + \binom{n}{1} \Delta y_0 + \binom{n}{2} \Delta^2 y_0 + \dots + \binom{n}{n-1} \Delta^{n-1} y_0 + \Delta^n y_0$$

8.2.4 Factorial notation:-

$$x^{(n)} = x(x - h)(x - 2h)....(x - \overline{x - 1}h)$$

(i)
$$\Delta^n x^{(n)} = n! \, h^n$$
 and $\Delta^{n+1} x^{(n)} = 0$

Example (8.8): Find the polynomial f(x), which satisfy the following data and hence find the value of f(1.5).

x	1	2	3	4	5
f(x)	4	13	34	73	136

Difference table:

x	$\Delta f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	
1	4				
2	13	9	12		(3rd degree polynomial
3	34	21	18	6	as 3rd order difference
4	73	39	24	6	is constant)
5	136	63			

We know that $f(x + nh) = E^n f(x_0) = (1 + \Delta)^n f(x_0)$

Here
$$x = 1, h = 1, x + nh = 1 + n = x$$
 $\therefore x = n - 1$

$$f(x) = (1 + \Delta)^{x-1} f(1)$$

$$= [1 + (x - 1)\Delta f(1) + \frac{(x-1)(x-2)}{2!} \Delta^2 f(1) + \frac{(x-1)(x-2)(x-3)}{3!} \Delta^3 f(1) + \dots$$

$$= 1 + 9(x - 1) + 12 \frac{(x-1)(x-2)}{2} + 6 \frac{(x-1)(x-2)(x-3)}{3}$$

$$= x^3 + 2x + 1$$

$$\therefore f(1.5) = (1.5)^3 + 2 \times (1.5) + 1 = 7.375$$

8.2.5 Newton's Forward Interpolation Formula:-

Let f(x) is known for (n+1) distinct equispaced arguments namely $x_0, x_1, x_2, \ldots, x_{n-1}, x_n$ such that $x_r = x_0 + r \hbar$ $(r = 0, 1, \ldots, n-1), \hbar = setp \ length$.

$$y = f(x) \text{ and } y_j = f(x_j), \ j = 0, 1, \dots, n, \ s = \frac{x - x_0}{\hbar}$$

$$f(x) \simeq y_0 + s \, \Delta y_0 + s \, (s-1) \frac{\Delta^2 y_0}{2!} + s \, (s-1)(s-2) \frac{\Delta^3 y_0}{3!} + \dots + s \, (s-1) \dots (s-1) \frac{\Delta^n y_0}{n!}$$

Which is known as Newton's Forward Interpolation Formula.

Error:-
$$R_{n+1}(x) = \frac{\delta(\delta-1)(\delta-2)....(\delta-n)}{n+1} n^{n+1} f^{n+1}(\xi)$$

Where $\min\{x_1, x_0, x_n\} < \xi < \max\{x_1, x_0, x_n\}$

$$|R_{n+1}(x)| < 1$$
 for $x > 1$ and $0 < s < 1$

8.2.6 Newton's Backward Interpolation Formula: -

$$s = \frac{x - x_n}{h}$$

$$f(x) = y_n + s \, \Delta y_n + s \, (s+1) \frac{\Delta^2 y_n}{2!} + s \, (s+1) \dots (s+n-1) \frac{\Delta^n y_n}{n!}$$

Error:-
$$R_{n+1}(x) = s (s+1)....(s+n) h^{n+1} \frac{f^{n+1}(\xi)}{(n+1)!}$$

Where $\min\{x_0, x, x_n\} < \xi < \max\{x, x_0, x_n\}$

8.2.7 Lagrange's Interpolation Formula: -

Let y = f(x) be defined on [a,b] and is only known for $a = x_0, x_1, \dots, x_n = b$, in general are not equispaced and $y_i = f(x_i)$, $i = 0,1,2,\dots$

$$f(x) \simeq \sum_{i=0}^{n} li(x) f(x_i)$$

Where
$$li(x) = \frac{(x-x_0)(x-x_1)......(x-x_{i-1})(x-x_{i+1}).....(x-x_n)}{(x_i-x_0)(x_i-x_1).....(x_i-x_{i-1})(x_i-x_{i+1}).....(x_i-x_n)}$$
, $i = 0, 1,n$

Error:-
$$R_{n+1}(x) = (x - x_0)(x - x_1)...(x - x_n) \frac{f^{n+1}(\xi)}{(n+1)!}$$
, $(x_0 < \xi < x_n)$

8.2.8 Divided Difference:-

Let y = f(x) is known for $x_j (j = 0, 1, \dots, n)$ are not necessarily equipspaced. Then the first order divided difference for $x_0, x_1, f(x_0, x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{f(x_0) - f(x_1)}{x_0 - x_1} = f(x_1, x_0)$

Second order divided difference for x_0, x_1, x_2

$$f(x_0, x_1, x_2) = \frac{f(x_1, x_2) - f(x_0, x_1)}{x_2 - x_0} = \frac{f(x_0)}{(x_0 - x_1) - (x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0) - (x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0) - (x_2 - x_1)}$$

n th order divided difference for $x_0, x_1, x_2, \ldots, x_n$

$$f(x_0, x_1, x_2, \dots, x_n) = \sum_{i=0}^n \frac{f(x_i)}{(x_i - x_0) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)} = \sum_{j=0}^n \frac{f(x_j)}{\prod_{\substack{i=0 \ i \neq j}}^n (x_j - x_i)}$$

Some Remarks: -

- (i) The nth order divided difference of a polynomial of degree n is constant.
- (ii) Divided difference for equispaced arguments:-

$$f(x_0, x_1, x_2, \dots, x_n) = \frac{\Delta^n y_0}{n! \hbar^n}$$
Since $f(x_0, x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{y_1 - y_0}{\hbar} = \frac{\Delta y_0}{\hbar}$

$$f(x_0, x_1, x_2) = \frac{f(x_1, x_2) - f(x_0, x_1)}{x_2 - x_0} = \frac{\frac{\Delta y_1}{\hbar} - \frac{\Delta y_0}{\hbar}}{2\hbar} = \frac{\Delta (y_1 - y_0)}{2\hbar^2} = \frac{\Delta y_0}{2\hbar^2}$$

(iii) Newton's general divided difference formula:-

Let y = f(x) be known for $x_0, x_1, x_2, \ldots, x_n$ not necessarily equispaced. Then the polynomial of degree n through $(x_0, y_0), \ldots, (x_n, y_n), y_i = f(x_i), i = 0, 1, \ldots, n$ is given by –

$$f(x) \simeq f(x_0) + f(x - x_0)f(x_0, x_1) + (x - x_0)(x - x_1)f(x_0, x_1, x_2) + \dots + (x - x_0)\dots + (x - x_{n-1})f(x_0, x_1, \dots, x_n)$$

Error:-

$$R_{n+1}(x) = (x - x_0)(x - x_1)... (x - x_n) f(x_0, x_1, x_2, ... x_n)$$
$$= (x - x_0)(x - x_1)... (x - x_n) \frac{f^{n+1}(\xi)}{(n+1)!}$$

8.3 Solution of Algebraic and transcendental Equations: -

Algebraic Equation: (i) If f(x) = 0 is a purely polynomial in x.

Transcendental Equation: If f(x) = 0 contains trigonometric exponential logarithmic function etc.

Assumptions:

- (i) f(x) is continuous and continuously differentiable upto sufficient x_0 of times.
- (ii) f(x) = 0 has no multiple root, i.e., if $f(\alpha) = 0$, then in a neighbourhood of α either f'(x) > 0 or f'(x) < 0.

8.3.1 Method to find the location of roots:

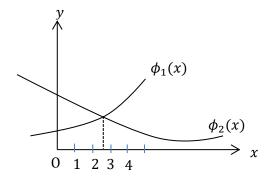
(a) Method of tabulation:

x	x_0	x_1	x_2	x_3
f(x)	$f(x_0)$	$f(x_1)$	$f(x_2)$	$f(x_3)$
Sign	1	-	5 †	+

$$\Rightarrow f(\alpha) = 0$$
 and $x_1 < \alpha < x_2$

(b) Graphical method:

Write
$$f(x) = 0$$
 as $\phi(x) = \phi(x)$. Draw $y = \phi_1(x)$ and $y = \frac{\phi_2(x)}{\phi_2(x)}$



$$\Rightarrow 2 < \alpha < 3$$

8.3.2 Bisection Method

We first find an interval [a_0 , b_0] such that the given function f: [a_0 , b_0] \rightarrow **R** (set of real numbers) is (i) continuous on [a_0 , b_0] (ii) f'(x) keeps the same sign in [a_0 , b_0] and (iii) $f(a_0)f(b_0) < 0$. (These three conditions ensure that the function f in [a_0 , b_0] has a unique root). Consider $x_0 = \frac{a_0 + b_0}{2}$.

- (i) If $f(x_0) = 0$ then x_0 is the root of f.
- (ii) If $f(x_0) \neq 0$ then either $f(a_0)f(x_0) < 0$ or $f(x_0)f(b_0) < 0$. If $f(a_0)f(x_0) < 0$,
- (iii) then the root lies in $[a_0, x_0]$ and we rename $[a_0, x_0]$ as $[a_1, b_1]$ or if $f(x_0)$ 0 then the root lies in $[x_0, b_0]$ and we rename $[x_0, b_0]$ as $[a_1, b_1]$

and consider a point $x_1 = \frac{a_1 + b_1}{2}$.

- (i) If $f(x_1) = 0$ then x_1 is the root of f.
- (ii) If $f(x_1) \neq 0$ then either $f(a_1)f(x_1) < 0$ or $f(x_1)f(b_1) < 0$. If $f(a_1)f(x_1) < 0$,

then the root lies in $[a_1, x_1]$ and we rename $[a_1, x_1]$ as $[a_2, b_2]$ or if $f(x_1)f(b_1) < 0$ then the root lies in $[x_1, b_1]$ and we rename $[x_1, b_1]$ as $[a_2, b_2]$

and consider a point $x_2 = \frac{a_2 + b_2}{1}$.
Text with Technological Text.

Continuing in this process we get a sequence $\{x_n\}$ of points in $[a_0, b_0]$. Now if

 $|x_n - x_{n-1}| < \varepsilon$ (a pre-assigned error) then the root of f will be x_n in $[a_0, b_0]$.

This method is surely convergent.

Tabulation of the bisection method

Suppose $f(a_0) > 0$ and $f(b_0) < 0$

x	$a_n(+ve)$	$b_n(-ve)$	$x_{n+1} = \left(\frac{a_n + b_n}{2}\right)$	$f(x_{n+1})$
0	a_0	b_0	$x_1 \left(= \frac{a_0 + b_0}{2} \right)$	$f(x_1) > 0 $ (suppose)
1	$a_1(=x_1)$	$b_1(=b_0)$	x_2	$f(x_2) > 0$ (suppose)
2	$a_2(=x_2)$	$b_2(=b_0)$	<i>x</i> ₃	$f(x_3) > 0$ (suppose)
3	$a_3(=a_2)$	$b_3(=x_3)$	x_4	$f(x_3) > 0$ (suppose)

8.3.3 Method of iteration or fixed point iteration:

This method is based on the principle of finding a sequence $\{x\}$ each elements of which successively approximates to a real root α so f(x) = 0 in [a, b]. We rewrite f(x) = 0

as
$$x = \phi(x)$$
.

Let $x = x_0 \in [a, b]$ be the initial approximation of α , then we set its first approximation as $x_1 = \phi(x_0)$ and then the successive approximations are $x_{n+1} = \phi(x_n)$, $x = 0, 1, \dots$ (iteration formula.)

Convergence of the method of iteration:

 $x = \phi(x)$ is not unique.

By MVT,

$$|\alpha - x_1| = |\phi(\alpha) - \phi(x_0)| = |\alpha - x_0||\phi'(\xi_1)|$$
 for $x_0 < \xi_1 < \alpha$

$$|\alpha - x_2| = |\phi(\alpha) - \phi(x_1)| = |\alpha - x_1| |\phi'(\xi_2)|$$
 for $x_1 < \xi_2 < \alpha$

.

$$|\alpha - x_{n+1}| = |\phi(\alpha) - \phi(x_n)| = |\alpha - x_n||\phi'(\xi_{n+1})| \text{ for } x_n < \xi_{n+1} < \alpha$$

Thus
$$|\alpha - x_{n+1}| = |\alpha \cdot x_0| |\phi'(\xi_1)| \dots |\phi'(\xi_{n+1})|$$

Assuming
$$|\phi'(x)| \le \rho$$
 in $(a \le x \le b)$, $|\alpha - x_{n+1}| \le |\alpha - x_0| \rho^{n+1}$

Estimation of error:

$$|\varepsilon_{n+1}| \leq \frac{\rho}{1-\rho} |h_n|$$

$$\begin{aligned}
Order &= 1 \\
\downarrow \\
[|\varepsilon_{n+1}| &\leq \rho |\alpha - x_n|]
\end{aligned}$$

8.3.4 Newton - Raphson Method: -

This is also an iterative method and it is used to find isolated roots of an equation f(x) = 0.

We first find an interval [a_0 , b_0] such that

- (i) the given function $f: [a_0, b_0] \rightarrow \mathbf{R}$ (set of real numbers) satisfies the condition,
- $f(a_0)f(b_0) < 0$ and $f'(x) \neq 0$ in $[a_0, b_0]$ with f'(x) is not very small in $[a_0, b_0]$
- (ii) the interval [$a_{0,}\ b_{0}$] should be very close to the root desire root
- (iii) $|f(x)\cdot f''(x)| < \{f'(x)\}^2$.

Then we find a sequence $\{x_n\}$ of points in $[a_0, b_0]$ such that $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$. If

 $|x_{n+1} - x_n| < \varepsilon$ (a pre-assigned error) then the root of f will be x_{n+1} in $[a_0, b_0]$.

Convergence of this method:

Comparing with the iteration method

$$\phi(x) = x - \frac{f(x)}{f'(x)}$$
 and

$$|\phi'(x)| < 1 \Rightarrow |f(x) f'(x)| < |\{f'(x)\}^2|$$

Let x be an approximation of α . Then $x_1 = x_0 + \hbar$

is correct root

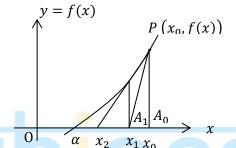
$$\Rightarrow f(x_0 + h) = f(x_1) = 0 \Rightarrow f(x_0) + h$$

$$h f'(x_0) + \frac{h}{2} f''(x_0) + \dots = 0$$

$$\Rightarrow h = -\frac{f(x_n)}{f(x_n)} (\because h \to 0, h^n = 0, n \ge 2)$$

$$\therefore x_1 = x_0 - \frac{f(x_0)}{f(x_0)}$$

$$\therefore x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$



Estimation of error:-

$$|\varepsilon_{n+1}| = |\alpha - x_n + 1| = \frac{1}{2} \left| \frac{f''(\alpha)}{f'(\alpha)} \right| |\alpha - x_n|^2$$

Definition (Order of a method):- A method is said to be of order P. If P is the largest number for which \exists a finite number C such that $|x_{n+1} - \alpha| \le C |x_n - \alpha|^p$ i.e.,

$$|\varepsilon_{n+1}| \le C|\varepsilon_n|^p, n \to \alpha.$$

So, the order of Newton – Raphson method is 2.

Note:

- (i) N-R method fails if f'(x) = 0 or very small in a neighbourhood of the root.
- (ii) N-R method id faster than iteration method.
- (iii) The initial guess (approximation) must be taken very close to the root other wise it may diverge.
- (iv) To find q-th root of R > 0. Let $x = \sqrt[q]{R} \Rightarrow x^q R = 0$

but
$$f(x) = x^q - R = 0$$
 then $f'(x) = q x^{q-1}$, $x_{n+1} = \frac{(q-1)x_n^q + R}{qx_n^{q-1}}$ $(n = 0, 1, 2, ...)$

8.3.5 Regula - Falsi Method:

We first find an interval $[x_0, x_1]$ such that the given function $f: [x_0, x_1] \to \mathbf{R}$ (set of real numbers) satisfies $f(x_0)f(x_1) < 0$. We find a point $x_2 = x_1 - \frac{x_1 - x_0}{f(x_1) - f(x_0)}$ $f(x_0)$.

- (i) If $f(x_2) = 0$ then x_2 is the root of f.
- (ii) If $f(x_2) \neq 0$ then either $f(x_0)f(x_2) < 0$ or $f(x_1)f(x_2) < 0$. If $f(x_0)f(x_2) < 0$ then the root lies in $[x_0, x_2]$ and we rename $[x_0, x_2]$ as $[x_1, x_2]$ or if $f(x_1) = 0$ then the root lies in $[x_1, x_2]$ and we keep the interval $[x_1, x_2]$ as same name $[x_1, x_2]$ and find a point

$$x_3 = x_2 - \frac{x_2 - x_1}{f(x_2) - f(x_1)} f(x_1)$$

- (iii) If $f(x_3) = 0$ then x_3 is the root of f.
 - If $f(x_3) \neq 0$ then either $f(x_1)f(x_3) < 0$ or $f(x_2)f(x_3) < 0$. If $f(x_1)f(x_3) < 0$, then the root lies in $[x_1, x_3]$ and we rename $[x_1, x_3]$ as $[x_2, x_3]$ or if $f(x_2)f(x_3) = 0$ then

the root lies in $[x_2, x_3]$ and we keep the interval $[x_2, x_3]$ as same name $[x_2, x_3]$

and find a point
$$x_4 = x_3 - \frac{x_3 - x_2}{f(x_3) - f(x_2)} f(x_2)$$

Continuing in this process we get a sequence $\{x_n\}$ of points in $[x_0, x_1]$. Now if

 $|x_n-x_{n-1}|<\varepsilon$ (a pre-assigned error) then the root of f will be x_n in [x_0 , x_1].

Graphically,

(iv)

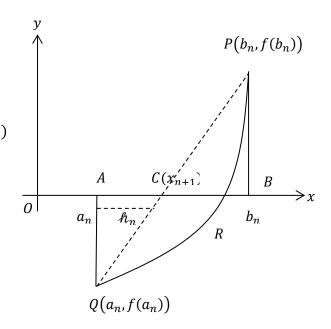
$$\frac{AC}{AQ} = \frac{CB}{BP}$$

$$\Rightarrow AC = \frac{AQ}{BP} \cdot CB = \frac{AQ}{BP} (AB - AC)$$

$$\Rightarrow x_{n+1} - a_n = \frac{|f(a_n)|}{|f(b_n)|} (b_n - a_n - (x_{n+1} - a_n))$$

$$\Rightarrow (x_{n+1} - a_n) \left[1 + \frac{|f(a_n)|}{|f(b_n)|} \right]$$

$$= \frac{|f(a_n)|}{|f(b_n)|} (b_n - a_n)$$



$$= x_{n+1} = a_n + \frac{|f(a_n)|}{|f(a_n)| + |f(b_n)|} (b_n - a_n)$$

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

8.4 Solution of system of linear equations: -

8.4.1 Gauss-Elimination Method

Let us consider a system of linear algebraic equation in n unknown.

The above system can be written as AX = b, where

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ a_{31} & a_{32} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}, \quad X = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} \text{ and } b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}$$

Now making the augmented matrix (A|b) in the following form by elementary row operations, we will get the solutions by back substitution.

$$(A|b) \approx \begin{pmatrix} a'_{11} & a'_{12} & \cdots & a'_{1n} & b'_{1} \\ 0 & a'_{22} & \cdots & a'_{2n} & b'_{2} \\ 0 & 0 & a'_{3n} & \cdots & a'_{3n} & b'_{3} \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a'_{nn} & b'_{n} \end{pmatrix}$$

$$x_n = \frac{b'_n}{a'_{nn}}$$

$$a'_{nn-2}$$
 x_{n-1} + a'_{nn-1} x_n = b'_{n-1} gives x_{n-1} etc.

8.4.2 Gauss-Jacobi Iteration Method

Let us consider a system of linear algebraic equation in *n* unknown.

Where the system is diagonally dominating i.e. $\sum_{\substack{i=1\\i\neq j}}^{n} |a_{ij}| \leq |a_{ii}|$.

The above system can be written as

This method is an iteration method with some initial guess $x_i^{(0)}$ (i= 1, 2, ...n) and the k+1-th (k is a natural number) iteration is given by

$$x_{1}^{(k+1)} = \frac{1}{a_{11}} [b_{1} - (a_{12} x_{2}^{(k)} + a_{13} x_{3}^{(k)} + \cdots + a_{1n} x_{n}^{(k)})]$$

$$x_{2}^{(k+1)} = \frac{1}{a_{22}} [b_{2} - (a_{21} x_{1}^{(k)} + a_{23} x_{3}^{(k)} + \cdots + a_{2n} x_{n}^{(k)})]$$

$$x_{3}^{(k+1)} = \frac{1}{a_{33}} [b_{3} - (a_{31} x_{1}^{(k)} + a_{32} x_{2}^{(k)} + \cdots + a_{3n} x_{n}^{(k)})]$$

$$x_{n}^{(k+1)} = \frac{1}{a_{nn}} [(b_{n} - (a_{n1} x_{1}^{(k)} + a_{n2} x_{2}^{(k)} + \cdots + a_{nn-1} x_{n-1}^{(k)})]$$

Here the iteration depends on given error ($\varepsilon > 0$). We stop the iteration if $|x_i^{(k+1)} - x_i^{(k)}| < \varepsilon$ (i= 1, 2, ...n) and the solution will be $x_i^{(k+1)}$ (i= 1, 2, ...n).

8.4.3 Gauss-Seidel Iteration Method

Consider a system of linear algebraic equation in *n* unknown.

Where the system is diagonally dominating i.e. $\sum_{\substack{i=1\\i\neq j}}^{n} |a_{ij}| \leq |a_{ii}|$.

The above system can be written as

$$x_{1} = \frac{1}{a_{11}} [b_{1} - (a_{12} x_{2} + a_{13} x_{3} + \dots + a_{1n} x_{n})]$$

$$x_{2} = \frac{1}{a_{22}} [b_{2} - (a_{21} x_{1} + a_{23} x_{3} + \dots + a_{2n} x_{n})]$$

$$x_{3} = \frac{1}{a_{33}} [b_{3} - (a_{31} x_{1} + a_{32} x_{2} + \dots + a_{3n} x_{n})]$$

$$x_n = \frac{1}{a_{nn}} \left[(b_n - (a_{n1} \ x_1 + a_{n2} \ x_2 + \cdots + a_{nn-1} \ x_{n-1}) \right]$$

This method is an iteration method with some initial guess $x_i^{(0)}$ (i= 1, 2, ...n) and the k+1-th (k is a natural number) iteration is given by

$$x_{1}^{(k+1)} = \frac{1}{a_{11}} [b_{1} - (a_{12} x_{2}^{(k)} + a_{13} x_{3}^{(k)} + \dots + a_{1n} x_{n}^{(k)})]$$

$$x_{2}^{(k+1)} = \frac{1}{a_{22}} [b_{2} - (a_{21} x_{1}^{(k+1)} + a_{23} x_{3}^{(k)} + \dots + a_{2n} x_{n}^{(k)})]$$

$$x_{3}^{(k+1)} = \frac{1}{a_{33}} [b_{3} - (a_{31} x_{1}^{(k+1)} + a_{32} x_{2}^{(k+1)} + a_{34} x_{4}^{(k)} + \dots + a_{3n} x_{n}^{(k)})]$$

$$x_n^{(k+1)} = \frac{1}{a_{nn}} \left[(b_n - (a_{n1} x_1^{(k+1)} + a_{n2} x_2^{(k+1)} + \dots + a_{nn-1} x_{n-1}^{(k+1)}) \right]$$

Here the iteration depends on given error ($\varepsilon > 0$). We stop the iteration if $|x_i^{(k+1)} - x_i^{(k)}| < \varepsilon$ (i = 1, 2, ...n) and the solution will be $x_i^{(k+1)}$ (i = 1, 2, ...n).

The convergence of both Gauss-Jacobi and Gauss-Seidel is

 $|a_{ji}| > \sum_{\substack{i=0 \ i \neq i}}^{n} |a_{ji}|$ for all i i.e., the coefficient matrix is diagonally dominating.

8.5 Numerical Integration

8.5.1 Trapezoidal Rule:

Let f be integrable over the interval [a, b]. We divide the interval into n equal subintervals by the points $a = x_0$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h$,..... $x_0 + (n-1)h$, $x_0 + nh = x_n = b$ where h is the step length.

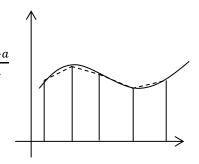
Consider
$$y_r = f(x_r)$$
 for $r = 0, 1, 2, 3,n$.

Then

$$\int_{a}^{b} f(x)dx \simeq \frac{\hbar}{2} \left[(y_0 + y_n) + 2(y_1 + y_2 + \dots + y_{n-1}) \right], \ \hbar = \frac{b-a}{n}$$

$$\text{Error} = -\frac{(b-a)^3}{12n^2} f''(\xi), \ (a = x_0 < \xi < x_n = b)$$

$$= -\frac{n \, \hbar^3}{12} f''(\xi)$$



8.5.2 Simpson's One-third Rule: (n = 2m)

Let f be integrable over the interval [a, b]. We divide the interval into n (even) equal subintervals by the points $a = x_0$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h$,..... $x_0 + (n-1)h$, $x_0 + nh = x_n = b$ where h is the step length.

Consider
$$y_r = f(x_r)$$
 for $r = 0, 1, 2, 3,n$.

Then

$$\int_{a}^{b} f(x)dx \simeq \frac{\hbar}{3} \left[y_0 + y_n + 4 \left(y_1 + y_3 + \dots + y_{n-1} \right) + 2 \left(y_2 + y_4 + \dots + y_{n-2} \right) \right]$$

$$\text{Error} = -\frac{n\hbar^5}{180} f^{iv}(\xi), \quad (a < \xi < b)$$

8.5.3 Simpson's three-eight Rule: (n = 3m)

Let f be integrable over the interval [a, b]. We divide the interval into n (multiple of three) equal subintervals by the points $a = x_0$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h$,..... $x_0 + (n-1)h$, $x_0 + nh = x_n = b$ where h is the step length.

Consider
$$y_r = f(x_r)$$
 for $r = 0, 1, 2, 3,n$.

Then

$$\int_a^b f(x)dx \simeq \frac{3h}{8} \left[y_0 + y_n + 2 \left(y_3 + y_6 + y_9 \dots \right) + 3 \left(y_1 + y_2 + y_4 + y_5 \dots \right) \right]$$

8.5.4 Weddle's Rule: (n = 6m)

Let f be integrable over the interval [a, b]. We divide the interval into n (multiple of six) equal subintervals by the points $a = x_0$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h$,..... $x_0 + (n-1)h$, $x_0 + nh = x_n = b$ where h is the step length.

Consider
$$y_r = f(x_r)$$
 for $r = 0, 1, 2, 3,n$.
Then
$$\int_a^b f(x)dx = \frac{3h}{10}[(y_0 + y_n) + 5(y_1 + y_5 + y_7 + y_{11} + \cdots + y_{n-5} + y_{n-1}) + (y_2 + y_4 + y_8 + y_{10} + \cdots + y_{n-4} + y_{n-2}) + 6(y_3 + y_9 + y_{15} + \cdots + y_{n-3}) + 2(y_6 + y_{12} + \cdots + y_{n-6})]$$

8.6 Numerical solution of Differential equations

(A) Single step Method:

8.6.1 Euler's method:

$$\frac{dy}{dx} = f(x, y) \text{ with } y(x_0) = y_0$$

$$y_{n+1} = y_n + h f(x_n, y_n), n = 0, 1, 2, \dots$$
 p where $x_r = x_r + rh, r = 1, 2, \dots$ p

8.6.2 Euler's Modified method (Euler-Cauchy Method):

$$y_{n+1}^{(0)} = y_n + h f(x_n, y_n)$$

$$y_{n+1}^{(1)} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(0)})]$$

$$\vdots$$

$$y_{n+1}^{r} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{r-1})]$$

8.6.3 Picard's Method:

$$\frac{dy}{dx} = f(x, y) \text{ with } y(x_0) = y_0$$

Integrating
$$[x_0, x]$$
 we have $\int_{x_0}^x dy = \int_{x_0}^x f(t, y) dt$ or, $y(x) = y(x) + \int_{x_0}^x f(t, y) dt$ $y^{(n+1)}(x) = y_0 + \int_{x_0}^x f(t, y_t^n) dt$ where $y^n(x) = y_0$

8.6.4 Taylor's series method: -

$$y' = \frac{dy}{dx} = f(x, y) \text{ with } y(x_0) = y_0$$

$$y(x) = y(x + h) = y_0 + h y_0' + \frac{h^2}{2!} y_0'' + \frac{h^3}{3!} y_0''' + \dots$$

$$y' = f(x, y)$$

$$y'' = f_x + f_y y' = f_x + f_y f$$

Order =
$$\left|\frac{1}{\hbar} f(\hbar)\right|$$

 $f(\hbar) = error$
Example:
 $y_1 = y_0 + \hbar y_0' + \frac{\hbar^2}{2!} y_0'' + f(\hbar)$
Then
Order = $\left|\frac{1}{\hbar} t(\hbar)\right| = 0(\hbar^2)$

8.6.5 Runge – Kutta Method:

$$y' = \frac{dy}{dx} = f(x, y) \text{ with } y(x_0) = y_0,$$

$$k_1 = h f(x_n, y_n)$$

$$k_2 = h f(x_n + h, y_n + k_1) \qquad Error = 0(h^3) i.e., order = 2$$

$$y_{n+1} = y_n + \frac{1}{2} (k_1 + k_2)$$

(b) Fourth order Runge – Kutta Method:

$$y_{1}' = \frac{dy}{dx} = f(x, y) \text{ with } y(x_{0}) = y_{0},$$

$$k_{1} = h f(x_{n}, y_{n})$$

$$k_{2} = h f\left(x_{n} + \frac{h}{2}, y_{n} + \frac{k_{1}}{2}\right), k_{3} = h f\left(x_{n} + \frac{h}{2}, y_{n} + \frac{k_{2}}{2}\right)$$

$$k_{4} = h f(x_{n} + h, y_{n} + k_{3})$$

$$y_{n+1} = y_{n} + \frac{1}{t} \left[k_{1} + 2(k_{2} + k_{3}) + k_{4}\right] \text{ with Technology}$$

(B) Multi – Step Method:

8.6.6 Mid – point Method:

$$\frac{dy}{dx} = f(x, y), \text{ with } y(x_0) = y_0
y_{n+1} = y_n + \hbar y_n' + \frac{\hbar^2}{2!} y_n'' + \frac{\hbar^3}{3!} + y''(\xi)
y_{n-1} = y_n - \hbar y_n' + \frac{\hbar^2}{2!} y_n'' - \frac{\hbar^3}{3!} + y''(\xi)
\Rightarrow y_{n+1} - y_{n-1} = 2\hbar y_n + t(\hbar) \qquad \left(\text{order} = \left| \frac{1}{h} t(w) \right| = 0(\hbar^2) \right)
\Rightarrow y_{n+1} = y_{n-1} + 2\hbar f(x_n, y_n), \quad n = 1, 2, 3, \dots \dots$$

8.6.7 Adams – Bash forth Method:

(i) Order – 1:

$$y_{n+1} = y_n + h f(x_n, y_n), t(h) = \frac{h}{2} y''(\xi)$$
 [Euler's method]

(ii) Order − 2:

$$y_{n+1} = y_n + \frac{\hbar}{2} \left[3y'_n - y'_{n-1} \right], t(\hbar) = \frac{5}{12} \hbar^3 y'''(\xi)$$

(iii) Order – 3:

$$y_{n+1} = y_n + \frac{\hbar}{12} \left[23y'_n - 16y'_{n-1} + y'_{n-2} \right], t(\hbar) = \frac{3}{8} \hbar^4 y^{(4)}(\xi)$$

8.6.8 Adams – Moulton Method:

(i) Order - 1:-

$$y_{n+1} = y_n + h f(x_{n+1}, y_{n+1}), \ t(h) = -\frac{1}{2} h y''(\xi)$$
 (Backward Euler's Method)

(ii) Order - 2:-

$$y_{n+1} = y_n + \frac{\hbar}{2} [y'_{n+1} + y'_n], \ t(\hbar) = \frac{\hbar^3}{12} y''(\xi)$$

(iii) Order - 3:-

$$y_{n+1} = y_n + \frac{\hbar}{12} \left[5 y'_{n+1} + 8 y'_n - y'_{n-1} \right] | t(\hbar) = -\frac{\hbar^4}{24} y^{(4)}(\xi)$$

8.6.9 Two dimensional Newton - Raphson Method:-

$$f(x,y) = 0, \ g(x,y) = 0$$

$$J = \begin{bmatrix} f_x & f_y \\ g_x & g_y \end{bmatrix}$$

$$\therefore {x_{k+1} \choose y_{k+1}} = {x_k \choose y_k} - J^{-1} (x_k, y_k) \cdot {f(x_k, y_k) \choose g(x_k, y_k)}.$$

Application:- Finding complex root of $f(z) = 0 \Rightarrow f(z) = u(x, y) + iv(x, y) = 0$

Then
$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ y_k \end{pmatrix} - J^{-1} (x_k, y_k) \cdot \begin{pmatrix} u(x_k, y_k) \\ v(x_k, y_k) \end{pmatrix}$$

8.7 Determination of eigenvalues by power method:

Let $A = (a_{ij})n \times n$ be a real symmetric matrix and $X_0 \neq 0$ be a real n component vector. Let $X_1 = AX_0$, $X_2 = AX_1$, $X_3 = AX_2$,...., $Y = AX_n = AX$ $(X_n = X)$

$$\boldsymbol{m}_0 = \boldsymbol{X}^T \boldsymbol{X}$$
 , $\boldsymbol{m}_1 = \boldsymbol{X}^T \boldsymbol{Y}$, $\boldsymbol{m}_2 = \boldsymbol{Y}^T \boldsymbol{Y}$.

Then $q = \frac{m_1}{m_0}$ is an approximate eigen values λ of A and if we set $q = \lambda + \varepsilon$ so that ε is the error of q, then $|\varepsilon| \le \sqrt{\frac{m_2}{m_0} - q^2}$

Example (8.8)

$$A = \begin{pmatrix} 8 & 1 & 1 \\ 1 & 5 & 2 \\ 1 & 2 & 5 \end{pmatrix}$$
, choose $X_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

Then
$$X_1 = \begin{pmatrix} 10 \\ 8 \\ 8 \end{pmatrix}$$
, $X_2 = \begin{pmatrix} 96 \\ 66 \\ 66 \end{pmatrix}$, $X_0 = \begin{pmatrix} 920 \\ 558 \\ 558 \end{pmatrix}$, $X_4 = \begin{pmatrix} 8 & 3 & 1 & 6 \\ 4 & 8 & 0 & 6 \\ 4 & 8 & 0 & 6 \end{pmatrix}$

Let $X = X_3$, $Y = X_4$ we have $m_0 = X^T X = 1432728$, $m_1 = X^T Y = 12847896$, $m_2 = Y^T Y = 115351128$

$$q = \frac{m_1}{m_0} = 8.967$$
 and $|\varepsilon| \le \sqrt{\frac{m_2}{m_0} - q^2} = 0.311$

$$\Rightarrow q - \varepsilon < \lambda < q + \varepsilon \Rightarrow 8.656 < \lambda < 9.278 \Rightarrow \lambda = 9$$