COUNCILE OF SCIENTIFIC & INDUSTRIAL RESEARCH

Mathematical Science Code: 04

Unit – 3 :

SYLLABUS

Sub Unit – 3: Numerical Analysis

Sl. No	Topic
1.	3.1 Errors 3.1.1 Significant figures/digits 3.1.2. Exact Numbers (N_E) 3.1.3. Approximate Numbers (N_A) 3.1.4. Error (E) 3.1.5. Rounding-off Error 3.1.6. Types of Errors
2.	3.2 Interpolation with Equal and Unequal Intervals 3.2.1 Forward differences 3.2.2. Backward differences 3.2.3. Shift operator E 3.2.4. Factorial notation 3.2.5. Newton's Forward Interpolation Formula 3.2.6 Newton's Backward Interpolation Formula 3.2.7. Lagrange's Interpolation Formula 3.2.8. Divided Difference 3.2.8. (ii) Divided difference for equispaced arguments 3.2.8. (iii) Newton's general divided difference formula 3.2.9. Hermite Polynomial 3.2.10. Hermite's Interpolation Formula 3.2.11. Spline Interpolation 3.2.12. Cubic spline
3.	3.3 Solution of Algebraic and transcendental Equations 3.3.1 Method to find the location of roots 3.3.2 Bisection Method 3.3.3. Method of iteration or fixed point iteration 3.3.4. Order of Convergence 3.3.5. Geometric interpretation 3.3.6. Newton – Raphson Method 3.3.7. Regula –Falsi Method

4.	**3.4 Solution of system of linear equations** **3.4.1. Gauss-Elimination Method** **3.4.2. Gauss-Jacobi Iteration Method** **3.4.3. Gauss-Seidel Iteration Method**
5.	**3.5 Numerical Integration** **3.5.1. Trapezoidal Rule** **3.5.2 Simpson's One-third Rule** **3.5.3 Simpson's three-eight Rule** **3.5.4. Weddle's Rule**
6.	**3.6 Numerical solution of Differential equations** **3.6.1. Euler's method** **3.6.2. Euler's Modified method (Euler-Cauchy Method)** **3.6.3. Picard's Method** **3.6.4 Taylor's series method** **3.6.5 Runge – Kutta Method** **3.6.6 Mid – point Method** **3.6.7. Adams – Bash forth Method** **3.6.8. Adams – Moulton Method** **3.6.9 Two dimensional Newton – Raphson Method**
7.	**3.7 Determination of eigenvalues by power method**

Numerical Analysis

3.1. Errors

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

Examples (3.1):

- **(i)** 0, 1, 2,….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.

3.1.2. Exact Numbers (N_E): Exact numbers are those numbers which have no approximation.

Examples (3.2): 3, $\frac{1}{7}$, e, $\sqrt{5}$,π etc

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

Examples (3.3):

- **(i)** 1.732 is the approximation of $\sqrt{3}$.
- **(ii)** 3.142 is the approximation of π.

3.1.4. 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 (3.4): $\sqrt{3}$ -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).

3.1.5. Rounding-off Error: Rounding-off error is the error for discarding all but a pre-decided 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 (3.4):

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)

3.1.6. Types of Errors: Significant Error (S_a), Absolute $(\boldsymbol{E_a})$, Relative $(\boldsymbol{E_r})$ and Relative Percentage Errors $(\boldsymbol{E_p})$

(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. $E_a = |\, N_E - N_A|$

(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-(3.5):

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_p).

Solution: $\frac{1}{3}$ = 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 ≈ 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 (3.6)

$V_T = 345.26132, V_A = 345.261$

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

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

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

Example (3.7): $V_T = \frac{2}{3}, V_A = 0.6667$

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

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

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

$E_p = 0.000033 < 0.00005$

$E_r < \frac{1}{k \times 10^{n-1}} = \frac{1}{6 \times 10^3} = 0.00166 \simeq 0.001\ 7\ \ (k = 6, n = 4)$

3.2. Interpolation with Equal and Unequal Intervals:

Let $y = f(x)$ defined in $[a, b]$. Let us consider the consecutive value of x, differing by $\hbar$ as

$a = x_0,\ x_1 = x_0 + \hbar, \ldots\ldots\ \ldots, x_r = x_0 + r\hbar, \ldots\ldots\ldots, x_n = x_0 + \hbar$

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

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

3.2.1 Forward differences:

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

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

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

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

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

3.2.2. Backward differences: -

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

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

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

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.

3.2.3. Shift operator E:-

$E\, f(x) = f(x+\hbar) \Rightarrow E = \Delta + 1 \quad and \quad E\Delta = \Delta E$

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

By Taylor's Theorem:-

$f(x+\hbar) = f(x) + \hbar\, f'(x) + \frac{\hbar^2}{2!} f''(x) + \ldots\ldots\ ..$

$or, E\, f(x) = f(x) + \hbar\, D\, f(x) + \frac{\hbar^2}{2!} D^2 f(x) + \ldots\ldots\ ..$

$or, (\Delta+1) f(x) = \left(1 + \hbar D + \frac{\hbar^2}{2!} D^2 + \ldots\ \ldots\right) f(x)$

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

$or,\ \hbar D = \log(1+\Delta)$

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

(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 –

$f(x + x\hbar) = E\, f(x) = (1+\Delta) f(x)$

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

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

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

3.2.4. Factorial notation:-

$x^{(n)} = x(x-\hbar)(x-2\hbar)\ldots\ldots\ \ldots\ldots(x-\overline{x-1}\,\hbar)$

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

Example (3.8): 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			
		9		
2	13		12	
		21		6
3	34		18	
		39		6
4	73		24	
		63		
5	136			

(3rd degree polynomial as 3rd order difference is constant)

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

Here $x = 1, \hbar = 1,\ x + n\hbar = 1 + n = x \qquad \therefore x = n - 1$

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

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

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

$= x^3 + 2x + 1$

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

3.2.5. 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 $x_r = x_0 + r\,\hbar \quad (r = 0, 1, \ldots\ldots .n-1), \hbar = setp\ length.$

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

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

Which is known as Newton's Forward Interpolation Formula.

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

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

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

3.2.6. Newton's Backward Interpolation Formula: -

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

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

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

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

3.2.7. Lagrange's Interpolation Formula:

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

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

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

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

3.2.8. Divided Difference:-

Let $y = f(x)$ is known for $x_j (j = 0, 1, \ldots..\ \ldots n)$ 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 $x_0, x_1, x_2, \ldots\ldots\ldots x_n$

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

Some Remarks: -

(i) The nth order divided difference of a polynomial of degree n is constant.

(ii) Divided difference for equispaced arguments:-

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

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

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

Error:-

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

3.2.9. Hermite Polynomial:

Definition: Suppose $f \in C^1[a, b]$. Let $x_0, \dots, x_n$ be distinct numbers in $[a, b]$, the Hermite polynomial $P(x)$ approximating f is that:

1. $P(x_i) = f(x_i)$, for $i = 0, \dots, n$

2. $\frac{dP(x_i)}{dx} = \frac{df(x_i)}{dx}$, $for\ i = 0, \dots, n$

3.2.10. Hermite's Interpolation Formula:

The interpolation formulae considered so far make use of the function values at some number of points, say, $n + 1$ number of points and an nth degree polynomial is obtained. But, if the values of the function y = f(x) and its first derivatives are known at n + 1 points then it is possible to determine an interpolating polynomial $\phi(x)$ of degree (2n +1) which satisfies the (2n + 2) conditions

$$\begin{Bmatrix} \phi(x_i) = f(x_i) \\ \phi'(x_i) = f(x_i), i = 0, 1, 2, \dots\dots, n. \end{Bmatrix}$$

This formula is known as Hermite's Interpolation formula. Here, the number of conditions is (2n + 2), the number of coefficients to be determined is (2n + 2) and the degree of the polynomial is (2n -1).

Let us assume the Hermite's interpolating polynomial in the form

$\phi(x) = \sum_{i=0}^{n} h_i(x) f(x_i) + \sum_{i=0}^{n} H_i(x) f'(x_i)$

Where $h_i(x)$ and $H_i(x)$, $i = 0, 1, 2, \ldots \ldots \ldots n,$ are polynomial in x of degree at most (2n +1).

Using conditions, we get

$h_i(x_j) = \begin{cases} 1, & if i = j \\ 0, & if i \neq j \end{cases}; \ H_i(x_j) = 0, \ for all \ i$

$h'_i(x_j) = 0, for all i; \quad H'_i(x_j) = \begin{cases} 1, & if i = j \\ 0, & if i \neq j \end{cases}$

Let us consider the Lagrangian function

$L_i(x) = \frac{(x-x_0)(x-x_1)\ldots(x-x_{i-1})(x-x_{i+1})\ldots(x-x_n)}{(x_i-x_0)(x_i-x_1)\ldots(x_i-x_{i-1})(x_i-x_{i+1})\ldots(x_i-x_n)}, i = 0,1,2, \ldots, n.$

Obviously, $L_i(x_j) = \begin{cases} 1, & if i = j \\ 0, & if i \neq j \end{cases}$

Since each $L_i(x)$ is a polynomial of degree, $[L_i(x)]^2$ is a polynomial of degree $2n$.

Since $h_i(x)$ and $H_i(x)$ are polynomials in x of degree $(2n + 1)$, their explicit form may be taken as

$h_i(x) = (a_i x + b_i)[L_i(x)]^2$

$H_i(x) = (c_i x + d_i)[L_i(x)]^2 \ldots$

Using the conditions, we obtain

$a_i x_i + b_i = 1$

$c_i x_i + d_i = 0$

$a_i + 2 L'_i(x_i) = 0$

$c_i = 1$

These relations give

$a_i = -2 L'_i(x_i), \ b_i = 1 + 2x_i a_i + 2x_i L'_i(x_i), \ c_i = 1 \ and d_i = x_i$

Hence,

$h_i(x) = \left(-2x L'_i(x_i) + 1 + 2x_i L'_i(x_i)\right)[L_i(x)]^2 = [1 - 2(x - x_i)L'_i(x_i)][L_i(x)]^2 and$

$H_i(x) = (x + x_i)[L_i(x)]^2$

Then finally becomes

$\phi(x) = \sum_{i=0}^{n} [1 - 2(x - x_i)L'_i(x_i)][L_i(x)]^2 f(x_i) + \sum_{i=0}^{n} (x + x_i)[L_i(x)]^2 f'(x_i)$

Which is the required Hermite's interpolation formula.

Problem - Determine the Hermite's polynomial of degree 5 which satisfies the following data and hence find an approximate value of $\sqrt[3]{2.8}$.

x	:	1.5	2.0	2.5
$y = \sqrt[3]{x}$	:	1.14471	1.25992	1.35721
$y' = \frac{1}{\left(3x^{\frac{2}{3}}\right)}$	:	0.25438	0.20999	0.18096

Solution:

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-2.0)(x-2.5)}{(1.5-2.0)(1.5-2.5)} = 2\,x^2 - 9x + 10,$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-1.5)(x-2.5)}{(2.0-1.5)(2.0-2.5)} = -4\,x^2 + 16\,x - 15,$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-1.5)(x-2.0)}{(2.5-1.5)(2.5-2.0)} = 2\,x^2 - 7x + 6,$$

Therefore,

$L'_0(x) = 4x - 9, L'_1(x) = -8x + 16, L'_2(x) = 4x - 7.$

Hence $L'_0(x_0) = -3, L'_1(x_1) = 0, L'_2(x_2) = 3.$

$h_0(x) = [1 - 2(x - x_0)L'_0(x_0)][L_0(x)]^2 = [1 - 2(x - 1.5)(-3)][L_0(x)]^2$

$= (6x - 8)(2x^2 - 9x + 10)^2$

$h_1(x) = [1 - 2(x - x_1)L'_1(x_1)][L_1(x)]^2 = (4x^2 - 16x + 15)^2,$

$h_2(x) = [1 - 2(x - x_2)L'_2(x_0)][L_2(x)]^2 = [1 - 2(x - 2.5)(3)](2x^2 - 7x + 6)^2$

$= (16 - 6x)(2x^2 - 9x + 6)^2$

$H_0(x) = (x - x_0)[L_0(x)]^2 = (x - 1.5)(2x^2 - 9x + 10)^2,$

$H_1(x) = (x - x_1)[L_1(x)]^2 = (x - 2.0)(4x^2 - 16x + 15)^2,$

$H_2(x) = (x - x_2)[L_2(x)]^2 = (x - 2.5)(2x^2 - 7x + 6)^2,$

The required Hermite polynomial is

$\phi(x) = (6x - 8)(2x^2 - 9x + 10)^2(1.14471) + (4x^2 - 16x + 15)^2(1.25992)$

$+(16 - 6x)(2x^2 - 7x + 6)^2(1.35721) + (x - 1.5)(2x^2 - 9x + 10)^2(0.25438)$

$+(x - 2.0)(4x^2 - 16x + 15)^2(0.20999) + (x - 2.5)(2x^2 - 7x + 6)^2(0.18096)$

To find the value of $\sqrt[3]{2.8}$, substituting $x = 2.8$ to the above relation.

Therefore,

$\sqrt[3]{2.8} = 10.07345 \times 0.23040 + 1.25992 \times 2.43360 - 1.08577 \times 4.32640$

$+0.33069 \times 0.23040 + 0.16799 \times 2.43360 + 0.05429 \times 4.32640 = 1.40948$

3.2.11. Spline Interpolation:

Spline interpolation is very powerful and widely used method and has many applications in numerical differentiation, integration, solution of boundary value problems, two and three – dimensional graph plotting etc. Spline interpolation method, interpolates a function between a given set of points by means of piecewise smooth polynomials. In this interpolation, the curve passes through the given set of points and also its slope and its curvature are continuous at each point. The splines with different degree are found in literature, among them cubic splines are widely used.

3.2.12. Cubic spline:

The name spline comes from the physical (instrument) spline draftsmen use to produce curves. A general cubic polynomial is represented by: $y = Ax^3 + Bx^2 + Cx + D$.

Mathematically, spline is a piecewise polynomial of degree k with continuity of derivatives of order $k-1$ at the common joints between the segments. Thus, the cubic spline has second order or $C2$ continuity.

A function $y(x)$ is called cubic spline in $[x_0, x_n]$ if there exist cubic polynomials $p_0(x), p_1(x), \ldots\ldots \ldots p_{n-1}(x)$ such that

$y(x) = p_i(x)$ on $[x_i, x_{i+1}]$, $i = 1, 2, . \ldots\ldots n-1 \ldots\ldots\ldots\ldots\ldots\ldots (i)$

$p'_{i-1}(x_i) = p'_i(x_i), i = 1, 2, \ldots\ldots \ldots, n-1$ $(equal\ slope) \ldots\ldots\ldots\ldots\ldots\ldots (ii)$

$p''_{i-1}(x_i) = p''_i(x_i), i = 1, 2, \ldots\ldots \ldots, n-1$ $(equal\ curvature) \ldots\ldots\ldots\ldots\ldots\ldots (iii)$

And $p_i(x_i) = y_i, p_i(x_{i+1}) = y_{i+1}$ $i = 1, 2, \ldots\ldots \ldots, n-1$ $\ldots\ldots\ldots\ldots\ldots\ldots (iv)$

It may be noted that, at the end points x_0 and x_n , no continuity on slope and curvature are assigned. The conditions at these points are assigned, generally, depending on the applications.

Let the interval $[x_i, x_{i+1}]$, $i = 0, 1, \ldots\ldots\ldots, n-1$ be denoted by i-th interval.

Let $h_i = x_i - x_{i-1}, i = 1, 2, \ldots\ldots, n$ and $M_i = y''(x_i), i = 0, 1, 2, \ldots\ldots\ldots, n$

Let the cubic spline for the $i - th$ interval be

$y(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$ in $[x_i, x_{i+1}] \ldots\ldots\ldots\ldots\ldots\ldots\ldots (v)$

Since, it passes through the end points x_i and x_{i+1}, therefore,

$y_i = d_i \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (vi)$

And

$y_{i+1} = a_i(x_{i+1} - x_i)^3 + b_i(x_{i+1} - x_i)^2 + c_i(x_{i+1} - x_i) + d_i$

$= a_i {h_{i+1}}^3 + b_i {h_{i+1}}^2 + c_i h_{i+1} + d_i \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (vii)$

Equation (v) is differentiated twice and obtained the following equations.

$y'(x) = 3a_i(x-x_i)^2 + 2b_i(x-x_i) + c_i$ ……………….$(viii)$

And $y''(x) = 6a_i(x-x_i) + 2b_i$ ………………………(ix)

From (ix), $y_i'' = 2b_i$ and $y_{i+1}'' = 6a_ih_{i+1} + 2b_i, that\ is, M_i = 2b_i\ , M_{i+1} = 6a_ih_{i+1} + 2b_i$

Therefore $b_i = \frac{M_i}{2}$ ………………………..(x)

$a_i = \frac{M_{i+1}-M_i}{6\,h_{i+1}}$ ……………………..(xi)

Using (vi), (x) and (xi), equation (vii) becomes

$y_{i+1} = \frac{M_{i+1}-M_i}{6\,h_{i+1}}h_{i+1}{}^3 + \frac{M_i}{2}h_{i+1}{}^2 + c_ih_{i+1} + y_i$

$i.e., c_i = \frac{y_{i+1}-y_i}{h_{i+1}} - \frac{2h_{i+1}M_i+h_{i+1}M_{i+1}}{6}$

Thus, the coefficients $a_i, b_i. c_i$ and d_i of (v) are determined in terms of $n+1$ unknowns $M_0, M_1, \ldots\ldots, M_n$. These unknowns are determined in the following way.

The condition of equation (ii) state that the slopes of the two cubics p_{i+1} and p_i are same at x_i.

Now for the $i-th$ interval

$y'_i(x) = 3a_i(x-x_i)^2 + 2b_i(x-x_i) + c_i = c_i$ ………………………(xii)

And for the $(i-1)th$ interval

$y'_i(x) = 3a_{i-1}(x-x_{i-1})^2 + 2b_{i-1}(x-x_{i-1}) + c_{i-1}$ ………………$(xiii)$

Equation (xii) and $(xiii)$, we obtain $c_i = 3a_{i-1}h_i{}^2 + 2b_{i-1}h_i + c_{i-1}$

The values of $a_{i-1}, b_{i-1}\ , c_{i-1}$ and c_i are substituted to the above equation and obtained the following equation.

$$\frac{y_{i+1}-y_i}{h_{i+1}} - \frac{2h_{i+1}M_i + h_{i+1}M_{i+1}}{6} = 3\left(\frac{M_i - M_{i-1}}{6h_i}\right)h_i{}^2 + \frac{y_i - y_{i-1}}{h_i} - \frac{2h_iM_{i-1} + h_iM_i}{6}$$

After simplification the above equation reduces to

$h_iM_{i-1} + 2\,(h_i + h_{i+1})M_i + h_{i+1}M_{i+1} = 6\left(\frac{y_{i+1}-y_i}{h_{i+1}} - \frac{y_i-y_{i-1}}{h_i}\right)$

This relation is true for $i = 1, 2, \ldots\ldots\ldots, n-1$. Thus $n-1$ equations are available for the $n+1$ unknown quantities $M_0, M_1, \ldots\ldots, M_n$. Now, two more conditions are required to solve these equations uniquely. These conditions can be assumed to take one of the following forms:

(i) $M_0 = M_n = 0$. If this conditions are satisfied then the corresponding spline is called natural spline.

(ii) $M_0 = M_n,\ M_1 = M_{n+1}, y_0 = y_n,\ y_1 = y_{n+1},\ h_1 = h_{n+1}$. The corresponding spline satisfying these conditions is called periodic spline.

(iii) $y'(x_0) = y'_0, y'(x_n) = y'_n, i.e., 2M_0 + M_n = \frac{6}{h_1}\left(\frac{y_1 - y_0}{h_1} - y'_0\right)$ and

$M_{n-1} + 2M_n = \frac{6}{h_n}\left(y'_n - \frac{y_n - y_{n-1}}{h_n}\right)$

The corresponding spline satisfying the above conditions is called non – periodic spline or clamped cubic spline.

(iv) If $M_0 = M_n - \frac{h_1(M_2 - M_1)}{h_2}$ and $M_n = M_{n-1} + \frac{h_n(M_{n-1} - M_{n-2})}{h_{n-1}}$. The corresponding spline is called extrapolated spline.

(v) If $M_0 = y_0''\ and\ M_n = y_n''$ are specified. If a spline satisfy these conditions then it is called endpoint curvature – adjusted spline.

Problem: Fit a cubic spline curve that passes through $(0,0.0), (1, 0.5), (2, 2.0)\ and\ (3, 1.5)$ with the natural end boundary conditions, $y''(0) = y''(3) = 0$.

Solution: Here the invervals are (0,1), (1,2) and (2,3), i.e., three intervals of x, in each of which we can construct a cubic spline. These piecewise cubic spline polynomials together gives the cubic spline curve $y(x)$ in the entire interval (0,3).

Here $h_1 = h_2 = h_3 = 1$.

Then equation becomes

$M_{i-1} + 4M_i + M_{i+1} = 6(y_{i+1} - 2y_i + y_{i-1}),\ i = 1,2, (\mathbf{3})$.

That is ,

$M_0 + 4M_1 + M_2 = 6(y_2 - 2y_1 + y_0) = 6 \times (2.0 - 2 \times 0.5 + 0.0) = 6$

$M_1 + 4M_2 + M_3 = 6(y_3 - 2y_2 + y_1) = 6 \times (1.5 - 2 \times 2.0 + 0.5) = -12.$

Imposing the conditions $M_0 = y''(0) = 0\ \ and\ \ M_3 = y''(3) = 0$ to the above equations, and they simplify as

$4M_1 + M_2 = 6,\ M_1 + 4M_2 = -12$

These equations give $M_1 = \frac{12}{5}\ \ and\ \ M_2 = -\frac{18}{5}$

Let the natural cubic spline be given by

$p_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$

Where the coefficients $a_i, b_i. c_i\ and\ d_i$ are given by the relations

$a_i = \frac{M_{i+1} - M_i}{6\, h_{i+1}}\ ,\ b_i = \frac{M_i}{2},\ c_i = \frac{y_{i+1} - y_i}{h_{i+1}} - \frac{2h_{i+1}M_i + h_{i+1}M_{i+1}}{6}\ \ and\ d_i = y_i$ for $i = 0,1,2.$

Therefore,

$a_0 = \frac{M_1 - M_0}{6} = 0.4$ $\quad b_0 = \frac{M_0}{2} = 0$ $\quad c_0 = \frac{y_1 - y_0}{1} - \frac{2M_0 + M_1}{6} = 0.1$ $\quad d_0 = y_0 = 0$

$a_1 = \frac{M_2 - M_1}{6} = 1$ $\quad b_1 = \frac{M_1}{2} = \frac{6}{5}$ $\quad c_1 = \frac{y_2 - y_1}{1} - \frac{2M_1 + M_2}{6} = 1.3$ $\quad d_1 = y_1 =$ 0.5

$a_2 = \frac{M_3 - M_2}{6} = \frac{3}{5} b_2 = \frac{M_2}{2} = -\frac{9}{5}$ $\quad c_2 = \frac{y_3 - y_2}{1} - \frac{2M_2 + M_3}{6} = 0.7$ $\quad d_2 = y_2 = 2.0$

Hence the required piecewise cubic splines in each interval are given by

$p_0(x) = 0.4\, x^3 + \ 0.1\, x, \ \ 0 \le x \le 1$

$p_1(x) = -\,(x-1)^3 - \ 1.2\ \ (x-1)^2 + 1.3\,(x-1) + 0.5, \ \ 1 \le x \le 2$

$p_2(x) = 0.6\,(x-2)^3 - \ 1.8\ \ (x-2)^2 + 0.7\,(x-2) + 2.0, \ \ 12 \le x \le 3$

Problem: Fit a cubic spline curve for the following data with end conditions $y'(0) = 0.2\ and\ y'(3) = -1$.

x	:	0	1	2	3
y	:	0	0.5	3.5	5

Solution: Here, the three intervals $(0,1), (1,2)\ and\ (2,3)$ are given in each of which the cubic splines are to be constructed. These cubic spline functions are denoted by $y_0, y_1\ and\ \ y_2$. In this example, $h_0 = \ h_1 = h_2 = h_3 = 1$

For the boundary conditions, equation (3.99) is used. That is,

$M_0 + \ 4\,M_1 + M_2 = 6(y_2 - 2y_1 + \ y_0)$

$M_1 + \ 4\,M_2 + M_3 = 6(y_3 - 2y_2 + \ y_1)$

Also, from equations

$2M_0 + \ \ M_1 = 6(y_1 - 2y_0 + \ y_0{}')$ $\ \ and\ \ $ $M_2 + 2M_3 = 6(y_3{}' - 2y_3 + \ y_2)$

$M_0 + \ 4\,M_1 + M_2 = 15$

$M_1 + \ 4\,M_2 + M_3 = -9$

$2M_0 + \ \ M_1 = 1.8$

$M_2 + 2M_3 = 6(-1 - 5 + 3.5) = -15$

These equations give $M_0 = -1.36, M_1 = 4.52, M_2 = -1.72\ and\ M_3 = -6.64.$

Let the cubic spline in each interval be given by

$y'_i(x) = \ 3a_i(x - x_i)^3 + 2b_i(x - x_i)^2 + c_i(x - x_i) + d_i$

The coefficients are computed as

$a_i = \frac{M_{i+1} - M_i}{6\,h_{i+1}}$, $b_i = \frac{M_i}{2}$, $c_i = \frac{y_{i+1} - y_i}{h_{i+1}} - \frac{2h_{i+1}M_i + h_{i+1}M_{i+1}}{6}$ $\ and\ d_i = y_i$ for $i = 0,1,2.$

Therefore,

$a_0 = \frac{M_1 - M_0}{6} = 0.98$ $b_0 = -0.68$ $c_0 = 0.2$ $d_0 = 0$

$a_1 = \frac{M_2 - M_1}{6} = -1.04$ $b_1 = 2.26$ $c_1 = 1.78$ $d_1 = 0.5$

$a_2 = \frac{M_3 - M_2}{6} = -0.82$ $b_2 = \frac{M_2}{2} = -0.86$ $c_2 = 3.18$ $d_2 = 3.5$

Hence, the required piecewise cubic spline polynomials in each interval are given by

$y_0(x) = 0.98\,x^3 - \ 0.68\,x + 0.2\,x \quad 0 \le x \le 1$

$y_1(x) = -1.04\,(x-1)^3 + \ 2.26\ \ (x-1)^2 + 1.78\,(x-1) + 0.5,\ \ 1 \le x \le 2$

$y_2(x) = -0.82\,(x-2)^3 - \ 0.86\ \ (x-2)^2 + 3.18\,(x-2) + 3.5,\ \ 12 \le x \le 3$

Problem: Consider the function

$$f(x) = \begin{cases} -\frac{11}{2}x^3 + 26\,x^2 - \frac{75}{2}x + 18, & 1 \le x \le 2, \\ \frac{11}{2}x^3 - 40\,x^2 + \frac{189}{2}x - 70, & 2 \le x \le 3 \end{cases}$$

Show that $f(x)$ is cubic spline.

Solution: Let,

$p_0(x) = -\frac{11}{2}x^3 + 26\,x^2 - \frac{75}{2}x + 18,\ 1 \le x \le 2,$ and

$p_1(x) = \frac{11}{2}x^3 - 40\,x^2 + \frac{189}{2}x - 70,\ 2 \le x \le 3$

Here, $x_0 = 1, x_1 = 2 \ and\ x_2 = 3$. The function $f(x)$ will be a cubic spline if

(a) $p_i(x_i) = f(x_i)p_i(x_{i+1}) = f(x_{i+1}) \quad i = 0,1\ and$

(b) $p'_{i-1}(x_i) = p'_i(x_i)p''_{i-1}(x_i) = p''_i(x_i) \qquad i = 1$

The values of $f(x_0), f(x_1)$ and $f(x_2)$ are not supplied, so only the conditions

$p'_0(x) = -\frac{33}{2}x^2 + 52\,x - \frac{75}{2}$ $p'_1(x) = \frac{33}{2}x^2 - 80\,x + \frac{189}{2}$

$p''_0(x) = -33\,x + 52$ $p'_1(x) = \ 33\,x - 80$

$p'_0(x_1) = p'_0(2) = 0.5,\ p'_1(x_1) = p'_1(2) = 0.5, i.e.,\ p'_0(x_1) = p'_1(x_1)$

$p''_0(x_1) = p''_0(2) = -14,\ p''_1(x_1) = p''_1(2) = -14, Thus\ \ p''_0(x_1) = p''_1(x_1)$

Hence, $f(x)$ is a spline.

3.3. 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 $f'(x)>0 \ or \ f'(x)<0$.

3.3.1. Method to find the location of roots:

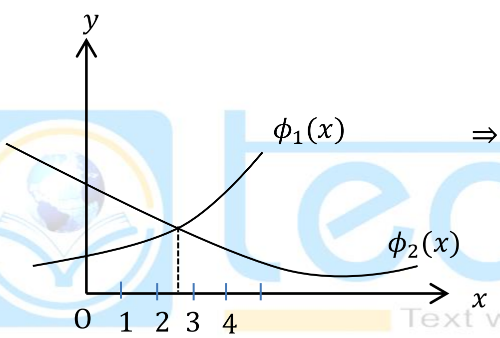
(a) Method of tabulation:

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

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

(b) Graphical method:

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



3.3.2. Bisection Method

We first find an interval $[\,a_0, \ b_0\,]$ such that the given function $f\colon [\,a_0, \ b_0\,] \to \boldsymbol{R}$ (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 $f(\,x_0\,)f(\,b_0) < 0$ 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

$$x_2 = \frac{a_2 + b_2}{2}.$$

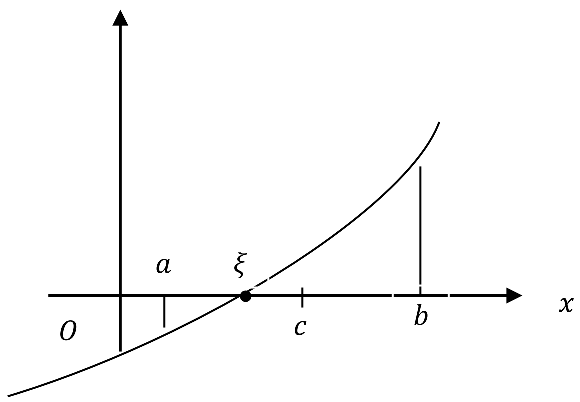
Continuing in this process we get a sequence $\{x_n\}$ of points in $[a_0, b_0]$. Now if $|x_n - x_{n-1}| < \varepsilon$ (a pre-assigned error) then the root of f will be x_n in $[a_0, b_0]$.

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	$a_2(= x_2)$	$b_2(= b_0)$	x_3	$f(x_3) > 0$ $(suppose)$
3	$a_3(= a_2)$	$b_3(= x_3)$	x_4	$f(x_3) > 0$ $(suppose)$



It may be noted that when the reduced interval be $[a_1, b_1]$ then the length of the interval is $\frac{b-a}{2}$, when the interval be $[a_2, b_2]$ then the length is $\frac{b-a}{2^2}$. At the n-the step the length of the interval being $\frac{b-a}{2^n}$. In the final step, when $\xi = \frac{a_n+b_n}{2}$ is chosen as a root then the length of the interval being $\frac{b-a}{2^{n+1}}$ and hence the error does not exceed $\frac{b-a}{2^{n+1}}$.

Thus, if ε be the error εt the $n-th$ step then the lower bound of n is obtained from the following relation

$$\frac{|b-a|}{2^n} \leq \varepsilon$$

The lower bound of n is obtained by rewriting this inequation as

$$n \geq \frac{\log(|b-a|)-\log \varepsilon}{\log 2}$$

Hence the minimum number of iterations required to achieve the accuracy ε is

$$\frac{\log_e\left(\frac{|b-a|}{e}\right)}{\log 2}$$

For example, if the length of the interval is $|b-a| = 1 \ \ and \ \ \varepsilon = 0.0001,$ then n is given by $n \geq 14.$

The minimum number of interations required to achieved the accuracy ε for $|b-a| = 1$ are shown in table.

Number of iterations for given ε						
ε	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
n	7	10	14	17	20	24

Property: Assume that $f(x)$ is a continuous function on $[a,b]$ and that there exists a number $\xi \in [a,b]$ such that $f(\xi) = 0$. If $f(a)$ and $f(b)$ have opposite signs, and $\{x_n\}$ represents the sequence of midpoints generated by the bisection method, then

$$|\xi - x_n| \leq \frac{b-a}{2^{n+1}} \ for \ n = 0,1,2 \ldots.$$

and therefore the sequence $\{x_n\}$ converges to the root ξ i.e., $\lim_{n\to\infty} x_n = \xi$

Note: If the function $f(x)$ is continuous on [a,b] then the bisection method is applicable. This is justified in Figure 3.3. For the function $f(x)$ of the graph, $f(a)\cdot f(b) < 0.$ but the equation $f(x) = 0$ has no root between $a \ and \ b$ as the function is not continuous at $x = c$.

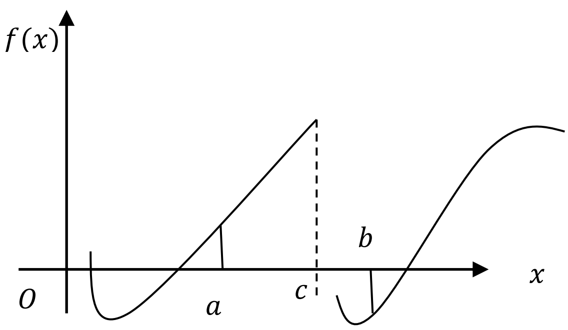


Figure-3.3: The function has no root between a and b, though $f(a)\cdot f(b) < 0.$

Note: This method is very slow, but it is very simple and will converge surely to the exact root. So the method is applicable for any function only if the function is continuous within the interval $[a, b]$, where the root lies.

In this method derivative of the function $f(x)$ and pre – manipulation of function are not required.

Note: This method is also called bracketing method since the method successively reduces the two endpoints (brackets) of the interval containing the real root.

Problem: Find a root of the equation $x^2 + x - 7 = 0$ by bisection method, correct up to two decimal places.

Solution: Let $f(x) = x^2 + x - 7$.

$f(2) = \; -1 < 0 \quad and \quad f(3) = \; 5 > 0$. So, a root lies between 2 and 3.

Left end point		Right end Point	Midpoint	
n	a_n	a_n	a_n	a_n
0	2	3	2.5	1.750
1	2	2.5	2.250	0.313
2	2	2.250	2.125	-0.359
3	2.125	2.250	2.188	-0.027
4	2.188	2.250	2.219	0.143
5	2.188	2.219	2.204	0.062
6	2.188	2.204	2.196	0.018
7	2.188	2.196	2.192	-0.003
8	2.192	2.196	2.194	0.008
9	2.192	2.194	2.193	0.002
10	2.192	2.193	2.193	0.002

Therefore, the root is 2.19 correct up to two decimal places.

3.3.3. 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 $x_{n+1} = \phi(x_n),\ x = 0, 1, \ldots\ldots (iteration\ formula.)$

Convergence of the method of iteration:

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

By MVT,

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

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

.

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.

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

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

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

$\therefore \log_{n\to\infty}|\alpha - x_{n+1}| \le |\alpha - x_0| \log_{n\to\infty} \rho^{n+1}$ $\quad \to 0\ if\ \rho < 1\ \ i.e., |\phi'(x)| < 1$

$\to 0\ if\ \rho > 1\ \ i.e., |\phi'(x)| > 1$

Estimation of error:

$Order = 1$

$|\varepsilon_{n+1}| \le \frac{\rho}{1-\rho}|\hbar_n|$ $\quad \downarrow$

$[|\varepsilon_{n+1}| \le \rho\,|\alpha - x_n|]$

3.3.4. Order of Convergence:

The convergence of an interation method depends on the suitable choice of the interation function $\phi(x)$ and x_0, the initial guess.

Let x_n converges to the exact root ξ, so that $\xi = \phi(\xi)$.

Thus $x_{n+1} - \xi = \phi(x_n) - \phi(\xi)$.

Let $\varepsilon_{n+1} = x_{n+1} - \xi$. Note that $\phi'(x) \neq 0$. Then the above relation becomes

$$\varepsilon_{n+1} = \phi(\varepsilon_n + \xi) - \phi(\xi)$$

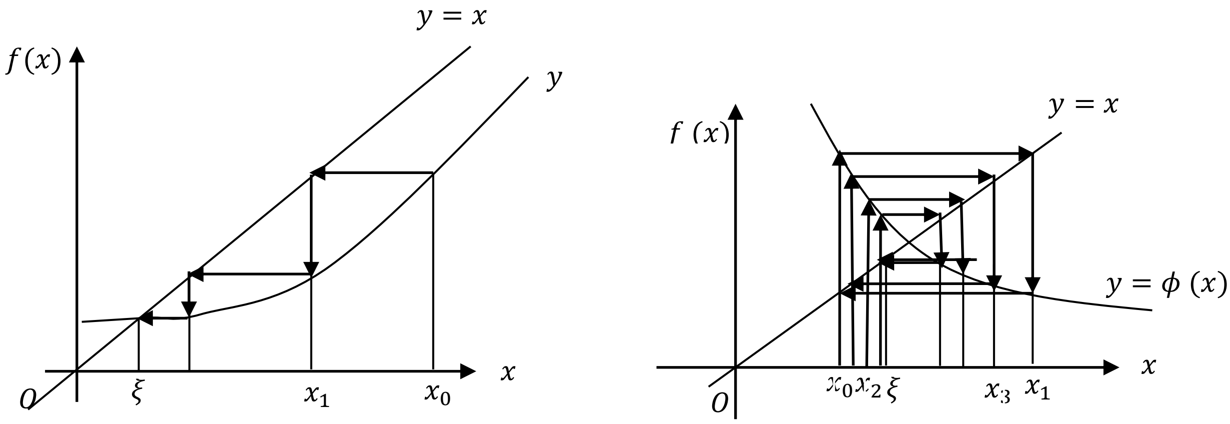
$$= \varepsilon_n\phi'(\xi) + \frac{1}{2}{\varepsilon_n}^2\phi'(\xi) + \ \ldots\ldots\ldots\ldots\ldots$$

$$= \varepsilon_n\phi'(\xi) + O({\varepsilon_n}^2)$$

i.e., $\varepsilon_{n+1} \simeq \varepsilon_n\phi'(\xi)$

Hence the order of convergence of iteration method is linear.

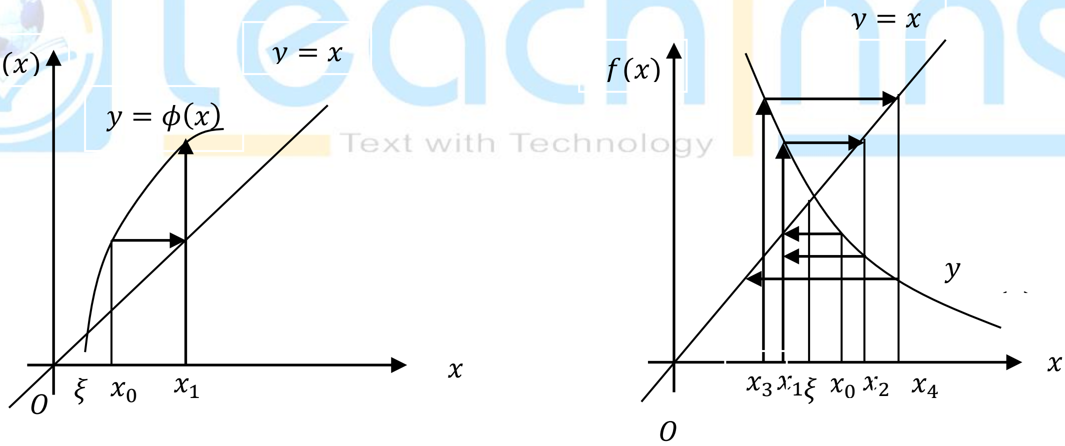
3.3.5. Geometric interpretation: Geometrically, the point of intersection of the line $y = x$ and the curve $y = \phi(x)$ is a root of the equation $f(x) = 0$. Depending on the value of $\phi'(\xi)$ the convergence and divergence cases are illustrated in figures.



(a)*Stair case solution* $0 < \phi'(\xi) < 1$

(b)*Sprial case solution* $-1 < \phi'(\xi) < 0$

Figure: Convergent for $|\phi'(\xi)| < 1$.



(a)*Divergent for* $\phi'(\xi) > 1$

(b)*Divergent for* $\phi'(\xi) < -1$

Figure: Divergent for $\phi'(\xi) > 1$.

Merit and Demerits:

The disadvantage of iteration method is that a pre – calculation is required to rewrite $f(x) = 0\ into\ x = \phi(x)$ in such a way that $|\phi'(x)| < 1$. But the main advantage of this method is that the operation carried out at each stage are of the same kind, and this makes easier to develop computer program.

This method is sometimes called a linear iteration due to its linear order of convergence.

Problem: Consider the equation $5x^3 - 20x + 3 = 0$. Find the root laying on the interval $[0,1]$ with an accuracy of 10^{-4}.

Solution: The given equation is written as $x = \frac{5x^3+3}{20} = \phi(x)(say)$.

Now, $\phi'(x) = \frac{15x^2}{20} = \frac{3x^2}{4} < 1$ on $[0,1]$.

Let $x_0 = 0.5$. The calculations are shown in the following table.

n	x_n	$\phi(x_n) = x_{n+1}$
0	0.5	0.18125
1	0.18125	0.15149
2	0.15149	0.15087
3	0.15087	0.15086
4	0.15086	0.15086

Problem: Find a root of the equation $\cos x - xe^x = 0$ correct up to three decimal places.

Solution: It is easy to see that one root of the given equation lies between 0 and 1.Let $x_0 = 0$.

The equation can be written as $x = e^{-x}\cos x = \phi(x)(say)$.

The calculations are shown in the following table.

n	0	1	2	3	4	5	6
x_n	0.50000	0.53228	0.50602	0.52734	0.51000	0.52408	0.51263
x_{n+1}	0.53228	0.50602	0.52734	0.51000	0.52408	0.51263	0.52193

n	7	8	9	10	11	12	13
x_n	0.52193	0.51437	0.52051	0.51552	0.51958	0.51628	0.51896
x_{n+1}	0.51437	0.52051	0.51552	0.51958	0.51628	0.51896	0.51678

n	14	15	16	17	18	19	20
x_n	0.51678	0.51855	0.51711	0.51828	0.51733	0.51810	0.51748
x_{n+1}	0.51855	0.51711	0.51828	0.51733	0.51810	0.51748	0.51798

Therefore, the required root is 0.518 correct up to three decimal places.

3.3.6. 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: [$a_0,\ b_0$]→**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 [$a_0,\ b_0$].

Let x be an approximation of α. Then $x_1 = x_0 + h$ is correct root

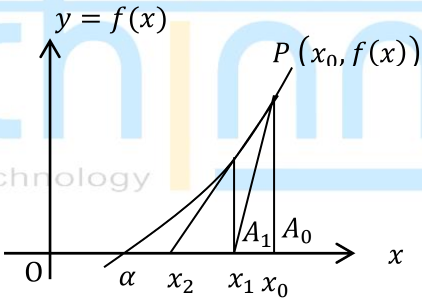
$$\Rightarrow f(x_0 + h) = f(x_1) = 0$$
$$\Rightarrow f(x_0) + h f'(x_0) + \frac{h}{2} f''(x_0) + \ldots\ldots = 0$$
$$\Rightarrow h = -\frac{f(x_n)}{f'(x_n)} \quad (\because h \to 0, h^n = 0, n \geq 2)$$
$$\therefore x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} x_2$$

Convergence of this method:

Comparing with the iteration method

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

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



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 ∃ a finite number C such that $|x_{n+1} - \alpha| \leq C|x_n - \alpha|^p$ i.e.,

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

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

Problem: Use Newton – Raphson method to find a root or the equation $x^3 + x - 1 = 0$.

Solution: Let $f(x) = x^3 + x - 1$. Then $f(0) = -1 < 0$ and $f(1) = 1 > 0$.

So one root lies between 0 and 1. Let $x_0 = 0$ be the initial root.

The iteration scheme is $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n{}^3 + x_n - 1}{3x_n{}^2 + 1} = \frac{2x_n{}^3 + 1}{3x_n{}^2 + 1}$

The sequence $\{x_n\}$ for different values of n is shown below.

n	x_n	x_{n+1}
0	0	1
1	1	0.7500
2	0.7500	0.6861
3	0.6861	0.6823
4	0.6823	0.6823

Therefore, a root of the equation is 0.682 correct up to three decimal places.

3.3.5. Regula –Falsi Method:

We first find an interval $[x_0, x_1]$ such that the given function f: $[x_0, x_1] \to$ **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 $f(x_1)f(x_2) < 0$ 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.

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

Graphically,

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

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

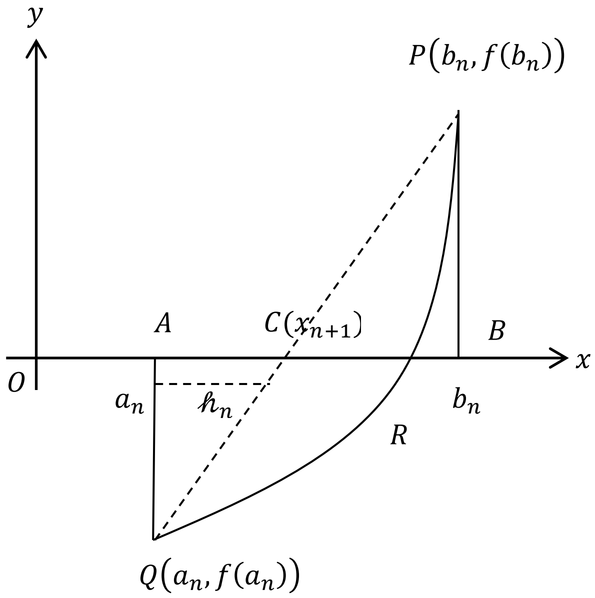
$$\Rightarrow x_{n+1} - a_n = \frac{|f(a_n)|}{|f(b_n)|}\,(b_n - a_n - (x_{n+1} - a_n)$$

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

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

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

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



3.4. Solution of system of linear equations: -

3.4.1. Gauss-Elimination Method:

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

$$\begin{aligned}
a_{11}\ x_1\ + a_{12}\ x_2\ + \cdots + a_{1n}\ x_n\ &= b_1 \\
a_{21}\ x_1\ + a_{22}\ x_2\ + \cdots + a_{2n}\ x_n\ &= b_2 \\
a_{31}\ x_1\ + a_{32}\ x_2\ + \cdots + a_{3n}\ x_n\ &= b_3 \\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
a_{n1}\ x_1\ + a_{n2}\ x_2\ + \cdots + a_{nn}\ x_n\ &= b_n
\end{aligned}$$

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

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

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

$$(A|\,b) \approx \begin{pmatrix} a'_{11} & a'_{12} & & \cdots\cdots & a'_{1n} & b'_1 \\ 0 & a'_{22} & & \cdots\cdots & a'_{2n} & b'_2 \\ 0 & 0 & a'_{3n} & \cdots\cdots & a'_{3n} & b'_3 \\ & & \vdots & & & \vdots \\ 0 & 0 & 0 & \cdots\cdots & a'_{nn} & b'_n \end{pmatrix}$$

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

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

3.4.2. Gauss-Jacobi Iteration Method

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

$$a_{11}\ x_1 + a_{12}\ x_2 + \cdots + a_{1n}\ x_n = b_1$$

$$a_{21}\ x_1 + a_{22}\ x_2 + \cdots + a_{2n}\ x_n = b_2$$

$$a_{31}\ x_1 + a_{32}\ x_2 + \cdots + a_{3n}\ x_n = b_3$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.$$

$$a_{n1}\ x_1 + a_{n2}\ x_2 + \cdots + a_{nn}\ x_n = b_n$$

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

$$x_1 = \frac{1}{a_{11}}[b_1 - (a_{12}\ x_2 + a_{13}\ x_3 + \cdots + a_{1n}\ x_n)]$$

$$x_2 = \frac{1}{a_{22}}[b_2 - (a_{21}\ x_1 + a_{23}\ x_3 + \cdots + a_{2n}\ x_n)]$$

$$x_3 = \frac{1}{a_{33}}[b_3 - (a_{31}\ x_1 + a_{32}\ x_2 + \cdots + a_{3n}\ x_n)]$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.$$

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

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

$$x_1^{(k+1)} = \frac{1}{a_{11}}[b_1 - \left(a_{12}\ x_2^{(k)} + a_{13}\ x_3^{(k)} + \cdots + a_{1n}\ x_n^{(k)}\right)]$$

$$x_2^{(k+1)} = \frac{1}{a_{22}}[b_2 - (a_{21}\ x_1^{(k)} + a_{23}\ x_3^{(k)} + \cdots + a_{2n}\ x_n^{(k)})]$$

$$x_3^{(k+1)} = \frac{1}{a_{33}}[b_3 - (a_{31}\ x_1^{(k)} + a_{32}\ x_2^{(k)} + \cdots + a_{3n}\ x_n^{(k)})]$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.$$

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

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

3.4.3. Gauss-Seidel Iteration Method

Consider a system of linear algebraic equation in n unknown.

$$a_{11}\ x_1\ +\ a_{12}\ x_2\ +\ \cdots + a_{1n}\ x_n\ = b_1$$

$$a_{21}\ x_1\ +\ a_{22}\ x_2\ +\ \cdots + a_{2n}\ x_n\ = b_2$$

$$a_{31}\ x_1\ +\ a_{32}\ x_2\ +\ \cdots + a_{3n}\ x_n\ = b_3$$

… … … … … … … … … … … … … … … … … … ….

$$a_{n1}\ x_1\ +\ a_{n2}\ x_2\ +\ \cdots + a_{nn}\ x_n\ = b_n$$

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

$$x_1\ = \frac{1}{a_{11}}[b_1\ -(\ a_{12}\ x_2\ +\ a_{13}\ x_3\ +\ \cdots + a_{1n}\ x_n\ )]$$

$$x_2\ = \frac{1}{a_{22}}[\ b_2\ -(a_{21}\ x_1\ +\ a_{23}\ x_3\ +\ \cdots + a_{2n}\ x_n\ )]$$

$$x_3\ = \frac{1}{a_{33}}[b_3\ -(a_{31}\ x_1\ +\ a_{32}\ x_2\ +\ \cdots + a_{3n}\ x_n\ )]$$

… … … … … … … … … … … … … … … … … … ….

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

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

$$x_1^{(k+1)} = \frac{1}{a_{11}}[b_1\ -\left(\ a_{12}\ x_2^{(k)} +\ a_{13}\ x_3^{(k)}\ +\ \cdots + a_{1n}\ x_n^{(k)}\right)]$$

$$x_2^{(k+1)} = \frac{1}{a_{22}}[\ b_2\ -(a_{21}\ x_1^{(k+1)} +\ a_{23}\ x_3^{(k)}\ +\ \cdots + a_{2n}\ x_n^{(k)})]$$

$$x_3^{(k+1)} = \frac{1}{a_{33}}[b_3\ -(a_{31}\ x_1^{(k+1)} +\ a_{32}\ x_2^{(k+1)} +\ a_{34}\ x_4^{(k)}\ \ \cdots + a_{3n}\ x_n^{(k)})]$$

… … … … … … … … … … … … … … … … … … . … … … … … … … … … … … … … … ….

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

Here the iteration depends on given error (ε >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

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

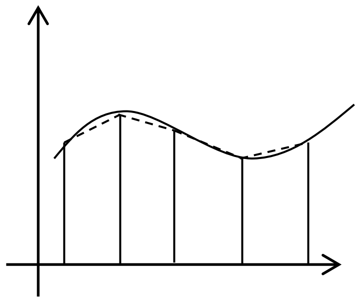
3.5. Numerical Integration

3.5.1. Trapezoidal Rule:

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

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

Then



$\int_a^b f(x)dx \simeq \frac{h}{2}[(y_0 + y_n) + 2(y_1 + y_2 + \ldots\ldots + y_{n-1})],\ h = \frac{b-a}{n}$

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

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

3.5.2. 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 $a = x_0$, $x_0 + h,\ x_0 + 2h,\ x_0 + 3h, \ldots\ldots\ x_0 + (n-1)h,\ x_0 + nh = x_n = b$ where h is the step length.

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

Then

$$\int_a^b f(x)dx \simeq \frac{h}{3}[y_0 + y_n + 4(y_1 + y_3 + \ldots\ldots + y_{n-1}) + 2(y_2 + y_4 + \ldots\ldots + y_{n-2})]$$

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

3.5.3. 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 $a = x_0$, $x_0 + h,\ x_0 + 2h,\ x_0 + 3h, \ldots\ldots\ x_0 + (n-1)h,\ x_0 + nh = x_n = b$ where h is the step length.

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

Then

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

3.5.4. 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 $a = x_0$, $x_0 + h,\ x_0 + 2h,\ x_0 + 3h, \ldots\ldots x_0 + (n - 1)h,\ x_0 + nh = x_n = b$where h is the step length.

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

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

3.6. Numerical solution of Differential equations

(A) Single step Method:

3.6.1. Euler's method:

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

$y_{n+1} = y_n + \hbar f(x_n, y_n),\ n = 0, 1, 2, \ldots\ldots .p$ where $x_r = x_r + r\hbar, r = 1, 2, \ldots\ldots .p$

3.6.2. Euler's Modified method (Euler-Cauchy Method):

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

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

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

3.6.3. Picard's Method:

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

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 $y^n(x) = y_0$

3.6.4 Taylor's series method:

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

$y(x) = y(x + \hbar) = y_0 + \hbar\, y_0' + \frac{\hbar^2}{2!} y_0'' + \frac{\hbar^3}{3!} y_0''' + \ldots\ldots$

$y' = f(x, y)$

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

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 $= \left|\frac{1}{\hbar}\ t(\hbar)\right| = 0(\hbar^2)$

3.6.5 Runge – Kutta Method:

(a) Second order Runge – Kutta Method:

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

$k_1 = \hbar\, f(x_n, y_n)$

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

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

(b) Fourth order Runge – Kutta Method:

$y_1{}' = \frac{dy}{dx} = f(x, y)$ with $y(x_0) = y_0,$

$k_1 = \hbar\, f(x_n, y_n)$

$k_2 = \hbar\, f\left(x_n + \frac{\hbar}{2}, y_n + \frac{k_1}{2}\right), k_3 = \hbar\, f\left(x_n + \frac{\hbar}{2}, y_n + \frac{k_2}{2}\right)$

$k_4 = \hbar\, f(x_n + \hbar, y_n + k_3)$

$y_{n+1} = y_n + \frac{1}{t}[k_1 + 2(k_2 + k_3) + k_4]$

(B) Multi – Step Method:

3.6.6 Mid – point Method:

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

$y_{n+1} = y_n + \hbar\, y_n{}' + \frac{\hbar^2}{2!} y_n{}'' + \frac{\hbar^3}{3!} + y''(\xi)$

$y_{n-1} = y_n - \hbar\, y_n{}' + \frac{\hbar^2}{2!} y_n{}'' - \frac{\hbar^3}{3!} + y''(\xi)$

$\Rightarrow y_{n+1} - y_{n-1} = 2\hbar\, y_n + t(\hbar)$ $\qquad \left(order = \left|\frac{1}{h} t(w)\right| = 0(\hbar^2)\right)$

$\Rightarrow y_{n+1} = y_{n-1} + 2\hbar\, f(x_n, y_n)\quad , n = 1, 2, 3, \ldots\ldots\ \ldots$

3.6.7. Adams – Bash forth Method:

(i) Order – 1:

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

(ii) Order – 2:

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

(iii) Order – 3:

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

3.6.8. Adams – Moulton Method:

(i) Order – 1:-

$y_{n+1} = y_n + \hbar\, f(x_{n+1}, y_{n+1}),\ t(\hbar) = -\frac{1}{2}\,\hbar\, y''(\xi)$ (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:-

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

3.6.9 Two dimensional Newton – Raphson Method:-

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

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

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

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

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

3.7. 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 $X_1 = AX_0,\ X_2 = AX_1,\ X_3 = AX_2, \ldots\ldots\ ..,Y = AX_n = AX \quad (X_n = X)$

$m_0 = X^T X\ , m_1 = X^T Y, m_2 = Y^T Y$.

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 $|\varepsilon| \leq \sqrt{\frac{m_2}{m_0} - q^2}$

Example (3.8) $A = \begin{pmatrix} 8 & 1 & 1 \\ 1 & 5 & 2 \\ 1 & 2 & 5 \end{pmatrix}$, 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 $m_0 = X^T X = 1432728,\ m_1 = X^T Y = 12847896,$

$m_2 = Y^T Y = 115351128$

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

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