Semester 3:

Computational Methods → [UNIT - 1]

★ **Introduction** → There are two types of equations, i) Algebraic Equations and, ii) Transcedental Equations.

- We already know how to find roots of an algebraic equation for any polynomial degree of 'x' from quadratic to cubic and even bi-quadratic equations.
  For examples,
  (a) Quadratic Equation : $ax^2 + bx + c = 0$
  → can be solved by : ① Factorisation Method
  ② Discriminant Method
  ③ Completing the Squares.

  (b) Cubic Equation : $ax^3 + bx^2 + cx + d = 0$
  → can be solved by: remainder theorem.

→ **Transcedental Equations** : A transcedental equation is an equation into which transcedental functions (such as logarithm, exponentials, trigonometric and inverse trigonometric) of one of the variables have been solved for. For examples,

1) $xe^x + 2\log x = 0$, 2) $\sin(\log x) + 4\cos^{-1}x = 0$

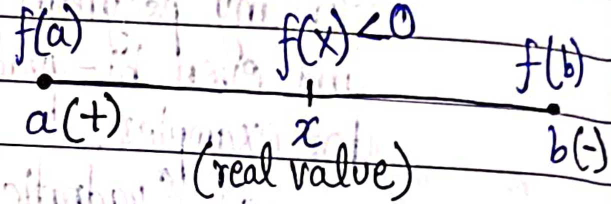
- To solve such equations and find its roots we have several methods which includes,
  1) Bisection Method
  2) Newton Raphson Method
  3) Secant Method
  → (In Syllabus)
  4) Regula-Falsi Method
  5) Iteration Method.

1) Methods to find roots of Transcedental Equations :-

1.1) BISECTION METHOD → Also called 'Bolzano Method'

→ Let $f(x)$ be a continous function in the closed interval $[a, b]$ and let,

$f(a)$ be positive.
$f(b)$ be negative.



Such that,

$$f(a) \cdot f(b) < 0$$

If it is true then there exists atleast one real root between a and b such that $f(x) = 0$.

Q.1) Solve the given equation by using the Bisection method to find its roots:

$$f(x) = x^3 - 4x - 9 = 0$$

Ans: Step 1: To find the range / interval $[a, b]$

By hit and trial for different values of x,

⇒ $f(0) = (0)^3 - 4(0) - 9 = -9$ (negative)
⇒ $f(1) = (1)^3 - 4(1) - 9 = -12$
⇒ $f(2) = (2)^3 - 4(2) - 9 = -9$
⇒ $f(3) = (3)^3 - 4(3) - 9 = +6$ (positive)

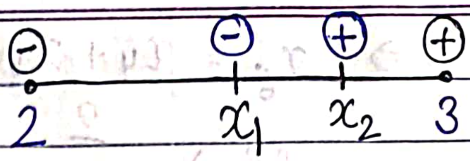
• The required interval for which $f(x)$ has two opposite sign values at a and b is, $[0, 3]$

⇒ The root of the given equation lies in between 2 and 3, i.e.,

$$f(2) \cdot f(3) < 0 ;$$

so closest and smallest interval is $[2, 3]$

Step 2:



- The root of the equation lies in between 2 and 3, so;

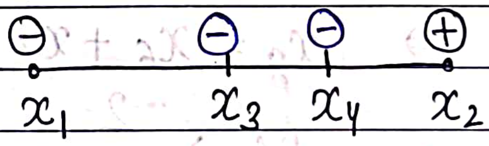
$$x_1 = \frac{2+3}{2} = 2.5$$

$\Rightarrow f(x_1) = f(2.5) = -3.375 < 0$

- The next shortest interval in which the root of the equation lies in is, $[x_1, 3]$.

$$x_2 = \frac{x_1+3}{2} = \frac{2.5+3}{2} = \frac{5.5}{2} = 2.75$$

$\Rightarrow f(x_2) = f(2.75) = 0.7969 > 0$



- The next shortest interval in which the root of the equation lies in is, $[x_1, x_2]$.

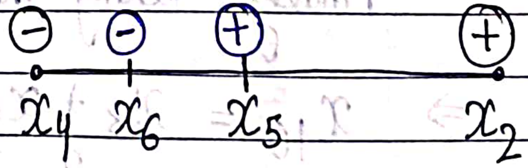
$$x_3 = \frac{x_1+x_2}{2} = \frac{2.5+2.75}{2} = 2.625$$

$\Rightarrow f(x_3) = -1.4121 < 0$

- Similarly, for interval $[x_3, x_2]$;

$$x_4 = \frac{x_2+x_3}{2} = \frac{2.75+2.625}{2} = 2.6875$$

$\Rightarrow f(x_4) = -0.33911 < 0$



- Similarly, for interval $[x_2, x_4]$

$$x_5 = \frac{x_2+x_4}{2} = \frac{2.75+2.687}{2} = 2.718$$

$\Rightarrow f(x_5) = 0.2072 > 0$

- Now, in interval $[x_4, x_5]$;

$\Rightarrow x_6 = \dfrac{x_4 + x_5}{2} = \dfrac{2.687 + 2.718}{2} = 2.7025$

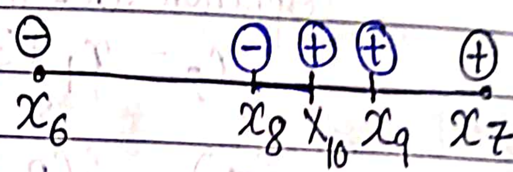
$\therefore f(x_6) = -0.0812 < 0$.

- The next root lies in range for $[x_5, x_6]$.

$\Rightarrow x_7 = \dfrac{x_5 + x_6}{2} = \dfrac{2.718 + 2.702}{2} = 2.710$

$\therefore f(x_7) = 0.0625 > 0$.

- Similarly, further in next interval $[x_6, x_7]$ i.e.,



$\Rightarrow x_8 = \dfrac{x_6 + x_7}{2} = \dfrac{2.702 + 2.710}{2} = 2.706$.

$\therefore f(x_8) = -0.00948 < 0$.

- Further in the next interval $[x_7, x_8]$;

$\Rightarrow x_9 = \dfrac{x_7 + x_8}{2} = \dfrac{2.71 + 2.706}{2} = 2.708$.

$\therefore f(x_9) = 0.0264 > 0$.

- Finally, taking the last iteration for interval $[x_8, x_9]$;

$\Rightarrow x_{10} = \dfrac{x_8 + x_9}{2} = \dfrac{2.706 + 2.708}{2} = 2.707$.

$\therefore f(x_{10}) = f(2.707) = 0.00848 > 0$.

→ Therefore, the closest root of this equation $f(x) = 0$ after 10 iterations is;

$$\boxed{X = 2.707}$$

Q.2) Solve the given below transcedental equation using the bisection method ?

$$f(x) = xe^{x} - 1$$ (Most Important)

Ans =

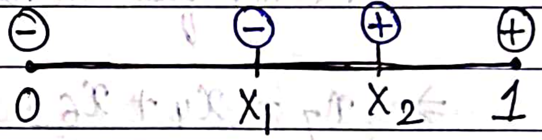
- First, we need to find the range in which $f(x)$ lies, i.e.,

$f(0) = 0 - 1 = -1$

$f(1) = e - 1 = 1.71$ ($\because$ Value of 'e' $= 2.718$)

- The required closed interval is $[0, 1]$ where at both end-points $f(x)$ has opposite signs.

Now, finding iteration 1,



$\Rightarrow x_1 = \frac{0+1}{2} = 0.5$

$\Rightarrow f(x_1) = f(0.5) = 0.5 \times e^{0.5} - 1 = -0.175 < 0$

Finding iteration 2 in interval $[x_1, 1]$;

$\Rightarrow x_2 = \frac{x_1 + 1}{2} = \frac{0.5+1}{2} = \frac{1.5}{2} = 0.75$

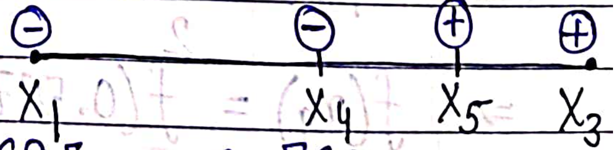
$\Rightarrow f(x_2) = f(0.75) = 0.587 > 0$

Finding iteration 3 in interval $[x_1, x_2]$,

$\Rightarrow x_3 = \frac{x_1 + x_2}{2} = \frac{0.5 + 0.75}{2} = 0.625$

$\Rightarrow f(x_3) = f(0.625) = 0.1676 > 0$

For iteration 4 in $[x_1, x_3]$,



$\Rightarrow x_4 = \frac{x_1 + x_3}{2} = \frac{0.5 + 0.625}{2} = 0.562$

$\Rightarrow f(x_4) = f(0.562) = -0.0127 < 0$

For iteration 5 in the interval $[x_3, x_4]$;

$\Rightarrow x_5 = \dfrac{x_3 + x_4}{2} = \dfrac{0.625 + 0.562}{2} = 0.593$

$\Rightarrow f(x_5) = 0.0729 > 0.$

Next, for iteration 6 in the interval $[x_4, x_5]$,

$\Rightarrow x_6 = \dfrac{x_4 + x_5}{2} = \dfrac{0.562 + 0.593}{2} = 0.577$

$\Rightarrow f(x_6) = 0.0274 > 0$

Next, for iteration 7 in the interval $[x_4, x_6]$,

$\Rightarrow x_7 = \dfrac{x_4 + x_6}{2} = 0.569$

$\Rightarrow f(x_7) = 0.005138 > 0$

Next, for iteration 8 in the interval $[x_4, x_7]$,

$\Rightarrow x_8 = \dfrac{x_4 + x_7}{2} = \dfrac{0.562 + 0.569}{2} = 0.565$

$\Rightarrow f(x_8) = f(0.565) = -0.00591 < 0$

Taking one last iteration 9 in the interval $[x_7, x_8]$,

$\Rightarrow x_9 = \dfrac{x_7 + x_8}{2} = \dfrac{0.569 + 0.565}{2} = 0.567.$

$\Rightarrow f(x_9) = f(0.567) = -0.0003958 < 0$

$\Rightarrow$ Hence, the closest root of this equation $f(x)$ after 9 iterations by bisection method is,

$$\boxed{x = 0.567}$$

1.2) Rate of Convergence of Bisection Method :-

(without PROOF)

→ If the bisection algorithm is applied to a continous function f on an interval [a, b] where,

$$f(a) \cdot f(b) < 0$$

then,

after n steps, an approximate root will be computed with error at most,

$$= \frac{(b-a)}{2^{n+1}} \qquad \text{[Linear Convergence]}$$

• If an error tolerance (ε) has been prescibed in advance then,

$$\frac{b-a}{2^{n+1}} < \varepsilon \qquad (\varepsilon\text{: very-very small number}).$$

⇒ Taking logarithms on both sides,

$$\Rightarrow \log(b-a) - \log(2^{n+1}) < \log \varepsilon$$

$$\Rightarrow \log\left(\frac{b-a}{\varepsilon}\right) < (n+1)\log 2$$

$$\Rightarrow \frac{\log(b-a) - \log \varepsilon}{\log 2} < n+1$$

or,

$$\Rightarrow n > \frac{\log(b-a) - \log(\varepsilon)}{\log 2}$$

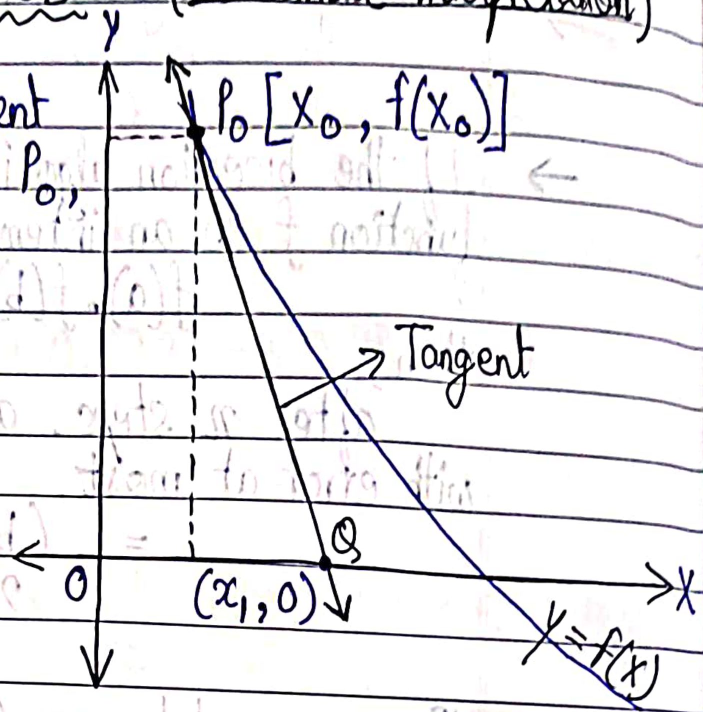
therefore,

$$\boxed{n > \frac{\log\left(\frac{b-a}{\varepsilon}\right)}{\log 2}}$$

→ 'n' is only dependent on the quantity ε.

(Asked in MT-2019, 3 MARKS).

1.3) NEWTON-RAPHSON METHOD → (Geometrical Interpretation)



- Applying the equation of tangent for the curve $f(x)$ at point P_0,

$\Rightarrow y - y_1 = m(x - x_1)$

$\Rightarrow y - y_1 = \frac{dy}{dx}(x - x_1)$

At point P_0,

$\Rightarrow y - f(x_0) = \frac{dy}{dx}(x - x_0)$

$\because y = f(x)$

$\Rightarrow \frac{dy}{dx} = f'(x)$

$\Rightarrow \left.\frac{dy}{dx}\right|_{(x_0)} = f'(x_0).$

Slope at point Q,

$\Rightarrow 0 - f(x_0) = f'(x_0)(x_1 - x_0)$

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

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

$\therefore$ General form can be written as,

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

where,

$f'(x_n) \neq 0.$

Note: It's rate of convergence is "Quadratic," and is a much faster way to find the roots.

Q.3) Find the root of the equation by Newton-Raphson's method :

$$f(x) = x^3 - 3x - 5$$

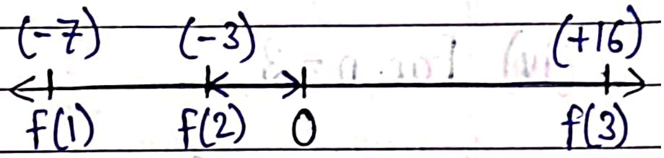
Ans: Step 1: To find the closest value of x to near '0', i.e.,

$\Rightarrow$ $f(1) = 1 - 3 - 5 = -7$

$\Rightarrow$ $f(-1) = -1 + 3 - 5 = -3$

$\Rightarrow$ $f(2) = 8 - 6 - 5 = -3$ $\rightarrow$ closest to 'zero'.

$\Rightarrow$ $f(3) = 27 - 9 - 5 = 16$



- Clearly, for $\boxed{x_0 = 2}$, $f(x)$ is closest for zero.

Step 2: Apply the formula.

Since,

$$f(n) = x_n^3 - 3x_n - 5$$

and,

$$f'(n) = 3x_n^2 - 3$$

- From Newton-Raphson's formula,

$$\Rightarrow x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^3 - 3x_n - 5}{3x_n^2 - 3}$$

or,

$$\Rightarrow x_{n+1} = \frac{2x_n^3 + 5}{3x_n^2 - 3}$$

(i) For $n = 0$,

$$\Rightarrow x_1 = \frac{2x_0^3 + 5}{3x_0^2 - 3} = \frac{2(2)^3 + 5}{3(2)^2 - 3} = \frac{21}{9} = 2.333$$

$(\because x_0 = 2)$.

(ii) For $n=1$,

$$\Rightarrow x_2 = \frac{2x_1^3+5}{3x_1^2-3} = \frac{2(2.333)^3+5}{3(2.333)^2-3} = \frac{30.396}{13.328} = 2.2806$$

(iii) For $n=2$,

$$\Rightarrow x_3 = \frac{2x_2^3+5}{3x_2^2-3} = \frac{2(2.280)^3+5}{3(2.280)^2-3} = 2.2790.$$

(iv) For $n=3$,

$$\Rightarrow x_4 = \frac{2x_3^3+5}{3x_3^2-3} = \frac{2(2.279)^3+5}{3(2.279)^2-3} = 2.2790.$$

→ Clearly, for the values of $n = 2$ and 3 both x_3 and x_4 are equal.

Therefore, $\boxed{x = 2.2790}$

Q.4) Solve the given function using Newton-Raphson method?

$$x = (30)^{-1/5} \quad [\text{ET-2019, 4 MARKS}]$$

Ans: Given, $\Rightarrow x = (30)^{-1/5}$

$$\Rightarrow x^5 = \frac{1}{30} \Rightarrow 30x^5 = 1 \Rightarrow \boxed{30x^5 - 1 = 0}$$

therefore,

$$f(x) = 30x^5 - 1$$

Considering, $x_0 = 0.5$ to get $f(x)$ closest to zero.

$\Rightarrow f(x_n) = 30x_n^5 - 1 \quad \Rightarrow f'(x_n) = 150x_n^4$

★ From Newton's - Raphson formula,

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

$$\Rightarrow x_{n+1} = x_n - \frac{(30x_n^5 - 1)}{150x_n^4}$$

$$\therefore x_{n+1} = \frac{120x_n^5 + 1}{150x_n^4}$$

(i) For $n = 0$,

$$\Rightarrow x_1 = \frac{120x_0^5 + 1}{150x_0^4} = \frac{120(0.5)^5 + 1}{150(0.5)^4} = 0.5066$$

(ii) For $n = 1$,

$$\Rightarrow x_2 = \frac{120x_1^5 + 1}{150x_1^4} = \frac{120(0.506)^5 + 1}{150(0.506)^4} = \cancel{1.00098}\ 0.5064$$

(iii) For $n = 2$,

$$\Rightarrow x_3 = \frac{120x_2^5 + 1}{150x_2^4} = \frac{120(0.5064)^5 + 1}{150(0.5064)^4} = 0.50649$$

→ For the values of $n = 1$ and 2 both x_2 and x_3 are equal.

• Therefore, the root of this equation is,

$$\boxed{x = 0.5064} \qquad (x \in R)$$

Q.5) Solve the given equation by Newton's Method ?

$$f(x) = \cos x - xe^{x}$$ (Important)

Ans: For,

$x=0$: $f(0) = \cos 0 - 0 = 1 > 0$

$x=1$: $f(1) = \cos 1 - e = -1.718 < 0$.

- Required interval is : $[0, 1]$.

→ Considering $\boxed{x_0 = 0}$ as $f(x_0)$ is closest to zero,

i.e.,

$$f(x_n) = \cos x_n - x_n e^{x_n}$$

and,

$$\Rightarrow f'(x_n) = -\sin x_n - (e^{x_n} + x_n e^{x_n})$$

$$\Rightarrow f'(x_n) = -\sin x_n - x_n e^{x_n} - e^{x_n}$$

★ From Newton's - Raphson formula,

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

$$\Rightarrow x_{n+1} = x_n - \frac{\cos x_n - x_n e^{x_n}}{-(\sin x_n + x_n e^{x_n} + e^{x_n})}$$

further,

$$\Rightarrow x_{n+1} = \frac{x_n\left[-(\sin x_n + x_n e^{x_n} + e^{x_n})\right] - \cos x_n + x_n e^{x_n}}{-(\sin x_n + x_n e^{x_n} + e^{x_n})}$$

$$\Rightarrow x_{n+1} = \frac{\cancel{-}(x_n \sin x_n + x_n^2 e^{x_n} + \cos x_n)}{\cancel{-}(\sin x_n + x_n e^{x_n} + e^{x_n})}$$

now,

$$x_{n+1} = \frac{x_n(\sin x_n + x_n e^{x_n}) + \cos x_n}{e^{x_n}(x_n + 1) + \sin x_n}$$

(i) For $n=0$,

$$\Rightarrow x_1 = \frac{x_0\left(\sin x_0 + x_0 e^{x_0}\right) + \cos x_0}{e^{x_0}(x_0+1) + \sin x_0}$$

$$\Rightarrow x_1 = \frac{0 + \cos 0}{e^0(1) + 0} = \frac{1}{1} = \boxed{1}.$$

(ii) For $n=1$,

$$\Rightarrow x_2 = \frac{x_1\left(\sin x_1 + x_1 e^{x_1}\right) + \cos x_1}{e^{x_1}(x_1+1) + \sin x_1}$$

$$\Rightarrow x_2 = \frac{1\left(\sin 1^\circ + e\right) + \cos 1^\circ}{e(1+1) + \sin 1^\circ} = 0.684908.$$

(iii) For $n=2$,

$$\Rightarrow x_3 = \frac{x_2\left(\sin x_2 + x_2 e^{x_2}\right) + \cos x_2}{e^{x_2}(x_2+1) + \sin x_2}$$

$$\Rightarrow x_3 = \frac{0.6849\left[\sin(0.6849) + (0.6849)e^{0.6849}\right] + \cos x_2}{\exp(0.6849)\left[(0.6849+1)\right] + \sin(0.6849)}.$$

$$\therefore x_3 = 0.57797$$

(iv) For $n=3$,

$$\Rightarrow x_4 = 0.56725$$

(Substituting x_n values accordingly in the previous formula).

(v) For $n=4$,

$$x_5 = 0.56712$$

→ For the values of $n = 3$ and 4, x_4 and x_5 are almost equal or approximately equal.
Therefore, the real root of this equation is,

$$\boxed{x = 0.5671}$$

1.4) Rate of Convergence of Newton-Raphson's Method:-

- **Rate of Convergence:** It is a measure of how fast the difference between the solution point and its estimates goes to zero. By using iterative methods is approximate to close the exact root.

★ Show that the Rate of Convergence of Newton's method is always 'quadratic'? (IMPORTANT)

Ans: Let, x_k be the k^{th} iterate root and exact root be α, then error will be ϵ_k. So,

$$\Rightarrow x_k = \epsilon_k + \alpha.$$

or,

$$\Rightarrow x_n = \epsilon_n + \alpha \quad \text{—} (1) \Rightarrow x_{n+1} = \epsilon_{n+1} + \alpha \quad \text{—} (2)$$

- From Newton's formula,

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

$$\Rightarrow \epsilon_{n+1} + \cancel{\alpha} = \epsilon_n + \cancel{\alpha} - \frac{f(\epsilon_n + \alpha)}{f'(\epsilon_n + \alpha)}$$ [From equations (1) and (2)]

$$\Rightarrow \epsilon_{n+1} = \epsilon_n - \frac{f(\epsilon_n + \alpha)}{f'(\epsilon_n + \alpha)}$$

- From taylor series expansion,

$$\Rightarrow \epsilon_{n+1} = \epsilon_n - \frac{f(\alpha) + \epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2!} f''(\alpha) + \dots \infty}{f'(\alpha) + \epsilon_n f''(\alpha) + \frac{\epsilon_n^2}{2!} f'''(\alpha) + \dots \infty}$$

Since, 'α' is an exact root, So,

$$f(\alpha) = 0$$

$$\Rightarrow \epsilon_{n+1} = \epsilon_n - \frac{0 + \epsilon_n f'(\alpha)}{f'(\alpha) + \epsilon_n f''(\alpha)}$$ (further terms are neglected as, $\epsilon_n^2 \lll 0$).

$$\Rightarrow \epsilon_{n+1} = \frac{\cancel{\epsilon_n f'(\alpha)} + \epsilon_n^2 f''(\alpha) - \cancel{\epsilon_n f'(\alpha)}}{f'(\alpha) + \epsilon_n f''(\alpha)}$$

$$\Rightarrow \epsilon_{n+1} = \frac{\epsilon_n^2 f''(\alpha)}{f'(\alpha)} \times \frac{1}{\left(1 + \epsilon_n \frac{f''(\alpha)}{f'(\alpha)}\right)}$$

$$\Rightarrow \epsilon_{n+1} = \epsilon_n^2 \frac{f''(\alpha)}{f'(\alpha)} \times \left(1 + \epsilon_n \frac{f''(\alpha)}{f'(\alpha)}\right)^{-1}$$

$$\Rightarrow \epsilon_{n+1} = \epsilon_n^2 \frac{f''(\alpha)}{f'(\alpha)} \left(1 + \epsilon_n \frac{f''(\alpha)}{f'(\alpha)}\right).$$

$\because (1+x)^{-1} = 1 - x + x^2 - x^3 + x^4 \dots \infty$

but, $\epsilon_n^2 \lll 0 \Rightarrow$ so, the term is neglected.

$$\Rightarrow \epsilon_{n+1} = \epsilon_n^2 \frac{f''(\alpha)}{f'(\alpha)} + \epsilon_n^3 \left(\frac{f''(\alpha)}{f'(\alpha)}\right)^2$$

$\Rightarrow \epsilon_{n+1} = \epsilon_n^2 \left(\frac{f''(\alpha)}{f'(\alpha)} \right)$ ($\because \epsilon_n^3 <<< 0$, so second term is neglected)

- Taking modulus on both sides,

$\therefore$ $$\boxed{|\epsilon_{n+1}| = M |\epsilon_n|^2} \rightarrow \text{Quadratic.}$$

(Hence prooved)

where, $M = \frac{f''(\alpha)}{f'(\alpha)}$ (M is a function in terms of the term = 'α')

1.5) SECANT METHOD / CHORD METHOD →

- This method is quite similar to Regula-Falsi method except for the condition,

$$f(a) \cdot f(b) < 0$$

It is not necessary for this condition to be true always.

- It can be derived from Newton-Raphson's method.
- General formula that will be used is, (no proof needed)

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

where,

$n = 0, 1, 2, 3, 4, \ldots\ldots$ so on

and,

→ two points are always required to find the other iteration, i.e., if;

x_0 and x_1 are known then, x_2 can be calculated.

- Method fails if $f(x_n) = f(x_{n-1})$.

Q.6) Find the real root of the given function $f(x)$ in the interval [1, 2] by using Secant's method ?

$$f(x) = x^3 - 5x + 3$$

Ans : From the given interval,

$x_0 = 1$ and, $x_1 = 2$

So,

$f(x_0) = f(1) = 1 - 5 + 3 = -1$

and,

$f(x_1) = f(2) = 8 - 10 + 3 = +1.$

Now, $x_0 = 1$, $x_1 = 2$; $f(x_0) = -1$, $f(x_1) = +1$.

• Applying secant's formula,

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

(i) For $n = 1$,

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

$$\Rightarrow x_2 = \frac{1 \times 1 - 2 \times -1}{1 - (-1)} = \frac{1 + 2}{2} = 1.5$$

So,

$f(x_2) = f(1.5) = -1.125 < 0$.

(ii) For $n = 2$,

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

$$\Rightarrow x_3 = \frac{2 \times -1.125 - 1.5 \times 1}{-1.125 - 1} = 1.76470$$

So,

$$f(x_3) = f(1.7647) = -0.32793 < 0.$$

(iii) For $n = 3$,

$$\Rightarrow x_4 = \frac{x_2 f(x_3) - x_3 f(x_2)}{f(x_3) - f(x_2)}$$

$$\Rightarrow x_4 = \frac{1.5 \times -0.3279 - 1.7647 \times -1.125}{-0.3279 - (-1.125)}$$

$$\Rightarrow x_4 = 1.87358$$

So,

$$f(x_4) = f(1.8735) = 0.20848 > 0$$

(iv) For $n = 4$,

$$\Rightarrow x_5 = \frac{x_3 f(x_4) - x_4 f(x_3)}{f(x_4) - f(x_3)}$$

$$\Rightarrow x_5 = \frac{1.7647 \times 0.2084 - 1.8735 \times -0.3279}{0.2084 - (-0.3279)}.$$

$$\Rightarrow x_5 = 1.83122 \quad \text{and,} \quad f(x_5) = -0.01544 < 0$$

(v) For $n = 5$,

$$\Rightarrow x_6 = \frac{x_4 f(x_5) - x_5 f(x_4)}{f(x_5) - f(x_4)} = 1.83411$$

and, $f(x_6) = -0.000729 < 0$

(The first 'three' zeros indicate above in $f(x_6)$ after decimal that the iteration 6 is correct upto first three decimal places).

$\therefore$ The real root of $f(x)$ is : $\boxed{x = 1.834}$

Q.7) Find the real root of the given transcedental equation by using Secant method, correct upto first four decimal places ?

$$f(x) = xe^{x} - 1$$

Ans: • To find the interval at first, by hit and trial ;
For,
$x = 0$, $f(0) = 0 - 1 = -1 < 0$
$x = 1$, $f(1) = e - 1 = +1.718 > 0$

• Required interval is $[0, 1]$
now,
$x_0 = 0$, $x_1 = 1$; $f(x_0) = -1$, $f(x_1) = 1.718$.

→ From Secant's formula,

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

(i) For $n=1$,

$$\Rightarrow x_2 = \frac{x_0 f(x_1) - x_1 f(x_0)}{f(x_1) - f(x_0)} = \frac{0+1}{1.718+1} = 0.3679$$

$\Rightarrow f(x_2) = f(0.36791) = (0.3679)e^{(0.3679)} - 1$

$\rightarrow f(x_2) = -0.46849 < 0$

(ii) For $n=2$,

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

$$\Rightarrow x_3 = \frac{1 \times -0.4684 - 0.3679 \times 1.718}{-0.4684 - 1.718}$$

$\Rightarrow x_3 = 0.50331$

so, $f(x_3) = f(0.5033) = -0.16745 < 0$

(iii) For $n=3$,

$$\Rightarrow x_4 = \frac{x_2 f(x_3) - x_3 f(x_2)}{f(x_3) - f(x_2)} = 0.57860.$$

so, $f(x_4) = f(0.5786) = 0.03195 > 0$

(iv) For $n=4$,

$$\Rightarrow x_5 = \frac{x_3 f(x_4) - x_4 f(x_3)}{f(x_4) - f(x_3)} = 0.56654.$$

so, $f(x_5) = f(0.5665) = -0.001776 < 0$

(v) For $n=5$,

$\Rightarrow x_6 = \dfrac{x_4 f(x_5) - x_5 f(x_4)}{f(x_5) - f(x_4)} = 0.56711$

so,

$f(x_6) = f(0.5671) = -0.000196 < 0$.

(vi) For $n = 6$,

$\Rightarrow x_7 = \dfrac{x_5 f(x_6) - x_6 f(x_5)}{f(x_6) - f(x_5)} = 0.56717$

so,

$f(x_7) = f(0.56717) = 0.0000780 > 0$.

$\therefore$ The real root of this given equation (correct upto first four decimal places) is,

$$\boxed{x = 0.5671}$$

1.6) Order and Rate of Convergence of Secant Method :-

✯ i) Show that the rate of convergence of Secant method is Super-Linear?

(SKIP) ii) Further, proove that the order of convergence of Secant method is a golden ratio number, i.e., 1.62?

(IMPORTANT)

Ans = Let x_k be the k^{th} iterate root and the exact root be α. Then the error will be ϵ_k. So,

$\Rightarrow x_k = \epsilon_k + \alpha$

or,

$\Rightarrow x_n = \epsilon_n + \alpha$ ——— (1)

or,

$\Rightarrow x_{n-1} = \epsilon_{n-1} + \alpha$. ——— (2)

★ From Secant formula,

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

- It can be also written as,

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

→ From equations ① and ②,

$$\Rightarrow \epsilon_{n+1} + \cancel{\alpha} = \epsilon_n + \cancel{\alpha} - \frac{f(\epsilon_n+\alpha)[\epsilon_n + \cancel{\alpha} - \epsilon_{n-1} - \cancel{\alpha}]}{f(\epsilon_n+\alpha) - f(\epsilon_{n-1}+\alpha)}.$$

$$\Rightarrow \epsilon_{n+1} = \epsilon_n - \frac{f(\epsilon_n+\alpha)(\epsilon_n - \epsilon_{n-1})}{f(\epsilon_n+\alpha) - f((\epsilon_{n-1})+\alpha)}$$

- From taylor series expansion,

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

$$\Rightarrow \epsilon_{n+1} = \epsilon_n - \frac{(\epsilon_n - \epsilon_{n-1})\left(f(\alpha) + \epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2!} f''(\alpha) \dots\right)}{\left(f(\alpha) + \epsilon_n f'(\alpha) + \frac{\epsilon_n^2 f''(\alpha)}{2!}\right) - \left(f(\alpha) + \frac{\epsilon_{n-1}}{2!} f''(\alpha) + \epsilon_{n-1} f'(\alpha)\right)}$$

∵ 'α' is an exact root so, $f(\alpha) = 0$.

On RHS,

$$= \epsilon_n - \frac{(\epsilon_n - \epsilon_{n-1})\left(0 + \epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2} f''(\alpha) + \dots\right)}{\left(0 + \epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2} f''(\alpha) + \dots\right) - \left(0 + \epsilon_{n-1} f'(\alpha) + \frac{\epsilon_{n-1}^2}{2} f''(\alpha) + \frac{\epsilon_{n-1}^3}{6} f'''(\alpha) + \dots\right)}$$

$$= \epsilon_n - \frac{(\epsilon_n - \epsilon_{n-1})\left(\epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2} f''(\alpha) + \dots\right)}{(\epsilon_n - \epsilon_{n-1}) f'(\alpha) + (\epsilon_n^2 - \epsilon_{n-1}^2) \frac{f''(\alpha)}{2}}$$

(higher terms are ignored)

$$= \epsilon_n - \frac{\cancel{(\epsilon_n - \epsilon_{n-1})}\left(\epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2} f''(\alpha) + \dots\right)}{\cancel{(\epsilon_n - \epsilon_{n-1})}\left[f'(\alpha) + (\epsilon_n + \epsilon_{n-1}) \frac{f''(\alpha)}{2}\right]}$$

$$= \epsilon_n - \frac{\epsilon_n f'(\alpha) + \frac{\epsilon_n^2}{2} f''(\alpha)}{f'(\alpha) + (\epsilon_n + \epsilon_{n-1}) f''(\alpha)}$$

$$= \epsilon_n - \frac{\cancel{f'(\alpha)}\left[\epsilon_n + \frac{\epsilon_n^2}{2} \frac{f''(\alpha)}{f'(\alpha)}\right]}{\cancel{f'(\alpha)}\left[1 + \frac{(\epsilon_n + \epsilon_{n-1})}{2} \frac{f''(\alpha)}{f'(\alpha)}\right]}$$

$$= \epsilon_n - \left(\epsilon_n + \frac{\epsilon_n^2}{2} \frac{f''(\alpha)}{f'(\alpha)}\right)\left(1 + \frac{(\epsilon_n + \epsilon_{n-1})}{2} \frac{f''(\alpha)}{f'(\alpha)}\right)^{-1}$$

- Using expansion : $(1+x)^{-n} = 1 - nx + nx^2 \dots \infty$

$$= \epsilon_n - \left(\epsilon_n + \frac{\epsilon_n^2}{2}\frac{f''(\alpha)}{f'(\alpha)}\right)\left(1 - \frac{(\epsilon_n + \epsilon_{n+1})}{2}\frac{f''(\alpha)}{f'(\alpha)}\right)$$

(ignoring higher terms as, $(\epsilon_n + \epsilon_{n+1})^2 \lll 0$)

$$= \epsilon_n - \left(\epsilon_n + \epsilon_n^2 \frac{f''(\alpha)}{2f'(\alpha)}\right)\left(1 - \frac{\epsilon_n f''(\alpha)}{2f'(\alpha)} - \frac{\epsilon_{n-1} f''(\alpha)}{2f'(\alpha)}\right).$$

$$= \epsilon_n - \left[\epsilon_n - \cancel{\frac{\epsilon_n^2 f''(\alpha)}{2f'(\alpha)}} - \frac{\epsilon_n . \epsilon_{n+1} f''(\alpha)}{2f'(\alpha)} + \cancel{\frac{\epsilon_n^2 f''(\alpha)}{2f'(\alpha)}} \underbrace{- \epsilon_n^3 \left(\frac{f''(\alpha)}{2f'(\alpha)}\right)^2}_{\text{neglected}} \underbrace{- \epsilon_n^2 . \epsilon_{n-1}\left(\frac{f''(\alpha)}{2f'(\alpha)}\right)^2}_{\text{neglected}}\right]$$

$$= \cancel{\epsilon_n} - \cancel{\epsilon_n} + \frac{\epsilon_n . \epsilon_{n-1} f''(\alpha)}{2f'(\alpha)}$$

$$= \epsilon_n . \epsilon_{n-1} \frac{f''(\alpha)}{2f'(\alpha)}$$

We get,

$$\Rightarrow \epsilon_{n+1} = \epsilon_n . \epsilon_{n-1} . \frac{f''(\alpha)}{2f'(\alpha)}$$

→ Taking modulus on both sides and assuming,

$$C = \frac{f''(\alpha)}{2f'(\alpha)}.$$

$$\boxed{|\epsilon_{n+1}| = C\,|\epsilon_n|\,|\epsilon_{n-1}|} \quad \text{—— (3)}$$

→ Now, general equation of rate of convergence is,

$$|\epsilon_{n+1}| \leq C\,|\epsilon_n|^q \quad \text{—— (5)} \quad (q: \text{a constant}).$$

- Replacing 'n' by 'n-1' in above equation,

$$\Rightarrow \epsilon_{(n-1)+1} \leq C\,(\epsilon_{(n-1)})^q$$

$$\Rightarrow \epsilon_n \leq C.(\epsilon_{n-1})^q$$

$$\Rightarrow \frac{\epsilon_n}{C} \leq (\epsilon_{n-1})^q$$

- Taking q^{th} root on both sides,

$$\Rightarrow \sqrt[q]{\frac{\epsilon_n}{C}} \leq \epsilon_{n-1}$$

or,

$$\Rightarrow \epsilon_{n-1} \geq \epsilon_n^{1/q} \cdot C^{-1/q} \quad \text{—— (4)}$$

- Substituting the value of ϵ_{n-1} from eq-(4) in equation (3),

$$\Rightarrow \frac{\epsilon_{n+1}}{C.\epsilon_n} \geq \epsilon_n^{1/q} \cdot C^{-1/q}$$

$$\Rightarrow \epsilon_{n+1} \geq \epsilon_n^{1+1/q} \cdot C^{1-1/q}$$

- From equation-(5),

$$\Rightarrow C.\epsilon_n^q \geq \epsilon_n^{1+1/q} \cdot C^{1-1/q}$$

→ On comparing both sides we have,

$\Rightarrow 1 + \frac{1}{q} = q$ or, $\Rightarrow 1 + \left(-\frac{1}{q}\right) = 1$.

(this case is rejected as $q \neq 0$. If $q = 0$ then the inequality will not hold true).

So,

$\Rightarrow q + 1 = q^2$

or,

$\Rightarrow q^2 - q - 1 = 0$.

$\Rightarrow q = \frac{+1 \pm \sqrt{1 - 4(1)(-1)}}{2}$ (By Discriminant method)

$\Rightarrow q = \frac{1 \pm \sqrt{5}}{2}$

$\therefore q = \frac{1+\sqrt{5}}{2}$ $\left(q \neq \frac{1-\sqrt{5}}{2} \text{ as, } q > 0\right)$.

or, $\boxed{q = 1.62}$

Putting the value of 'q' in equation - 5,

$$\boxed{|\epsilon_{n+1}| \leq C\,|\epsilon_n|^{1.62}} \quad \left(C = \frac{f''(\alpha)}{2 f'(\alpha)}\right).$$

→ Golden ratio number

This shows that,

1) Order of Convergence is 1.62 for Secant method.

2) Rate of Convergence is "Super-Linear", i.e., it is not necessarily true that this method will always show convergence. It may fails at some times.

2) Review of Taylor's Series, Errors and Approximations :-

2.1) Review of Taylor Series :-

- Taylor series expansion for a function $f(x)$ at $x = x_0$ is,

$$\Rightarrow f(x) = f(x_0) + f'(x_0).(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \dots \infty.$$

- Taylor series expansion for a function $f(x+h)$ where, $h \approx 0$;

$$\Rightarrow f(x+h) = f(x) + h.f'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots \infty$$

★ **Special Expansions :-**

1) $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots + \frac{x^n}{n!}$

2) $(1+x)^{-1} = 1 - x + x^2 - x^3 + x^4 - x^5 + \dots \infty$

3) $(1-x)^{-1} = 1 + x + x^2 + x^3 + x^4 + x^5 + \dots \infty$

4) $\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} + \dots \infty$

5) $\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} + \dots \infty$

Note: Expansions 1, 2 and 3 are the MOST Important.

Examples: Compute the following values by using Taylor Series ?

1) $\ln(1.1) = ?$

Ans: Taylor series expansion for $\ln(1.1)$ is,

$$\Rightarrow \ln(x) = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \frac{(x-1)^4}{4} + \frac{(x-1)^5}{5}$$

For $x = 1.1$,

$$\Rightarrow \ln(1.1) = 0.1 - \frac{0.01}{2} + \frac{0.001}{3} - \frac{0.0001}{4} + \frac{0.00001}{5}$$

On solving, $\boxed{\ln(1.1) \approx 0.095310333....}$

2) $e^8 = ?$

Ans: Taylor series expansion for e^x is,

$$\Rightarrow e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + ...$$

For $x = 8$,

$$\Rightarrow e^8 = 1 + 8 + \frac{64}{2} + \frac{512}{6} + \frac{4096}{24} + \frac{32768}{120} + ...$$

On solving, $\boxed{e^8 = 570.066665}$

Q.8) What is the Taylor series of the function:

$$f(x) = 3x^5 - 2x^4 + 15x^3 + 13x^2 - 12x - 5$$

at the point $x_0 = 2$?

Ans: Taylor series expansion for a function $f(x)$ at $x = x_0$ is,

$$\Rightarrow f(x) = f(x_0) + (x-x_0) f'(x_0) + \frac{(x-x_0)^2}{2!} f''(x_0) + \frac{(x-x_0)^3}{3!} f'''(x_0) + \frac{(x-x_0)^4}{4!} f''''(x_0) + \ldots\ldots$$

Since,

$\Rightarrow$ given $x_0 = 2$. So,

$\Rightarrow f(x_0) = f(2) = 207$ (Substitute $x_0 = 2$ in function $f(x)$).

Now,

$\Rightarrow f'(x_0) = 15x^4 - 8x^3 + 45x^2 + 26x - 12$, $f'(2) = 396$

$\Rightarrow f''(x_0) = 60x^3 - 24x^2 + 90x + 26$, $f''(2) = 590$

$\Rightarrow f'''(x_0) = 180x^2 - 48x + 90$, $f'''(2) = 714$

$\Rightarrow f''''(x_0) = 360x - 48$, $f''''(2) = 672$

$\Rightarrow f'''''(x_0) = 360$, $f^5(2) = 360$.

$\Rightarrow f^6(x_0) = 0$, $f^6(2) = 0$.

$$\therefore f(x) = 207 + (x-2)(396) + \frac{(x-2)^2}{2} \times 590 + \frac{(x-3)^3}{6} \times 714 + \frac{(x-4)^4}{24} \times 672 + \frac{(x-5)^5}{120} \times 360$$

• Hence, approximate function is,

$$\therefore f(x) = 207 + 396(x-2) + 295(x-2)^2 + 119(x-2)^3 + 28(x-2)^4 + 3(x-2)^5.$$

2.2) Significant Digits and Rounding off :-

i) **Significant Digits :** The significant figures of a quantity are those starting from the first non-zero digit accurately on the left to the end of last digit specified on the right.

Examples	Number of Significant Figures
1) 58	2
2) 603	3
3) 1008	4
4) 95080	5
5) 7.0	2
6) 0.80	2
7) 18.00	4
8) 0.0003	1
9) 0.0090	2
10) 3.20	3
11) 0.6046	4
12) 2.134	4

Examples	(As whole)	(After Decimal)
13) 0.003	1	3
14) 3.40	3	1
15) 0.9999	4	4
16) 2.137	4	3
17) 2.0137	5	4
18) 2.1370	5	3
19) 2.13701	6	5
20) 1000.004	7	3

In total, the number of significant figures

Only after the decimal

ii) Rounding Off Rules :-

→ To round off a number to 'n' significant digits, discard all digits to right of the n^{th} digit, if the $(n+1)^{th}$ digit is :

Serial No.	RULES	Examples	Rounded off values to first three decimal places ($n = 3$)
1)	**Less than 5 :** Leave the n^{th} digit unchanged.		
		39.72431	39.724
		4.00342	4.003
2)	**Greater than 5 :** Increase the n^{th} digit by 1.	79.87293	79.873
		79.87893	79.879
		3.567	3.57
3)	**Exactly 5 :** Increase the n^{th} digit by 1 if it is odd, otherwise, leave it unchanged.	2.589951	2.5900
		59.4865	59.486
		47.6975	47.698
		50.0695	50.070
		6.3456	6.346
		9.864651	9.865

2.3) Errors and Approximations in Numerical Computations :-

Serial No.	Type of Error	Notation	Formula
1)	Absolute Error	E_a	$E_a = \lvert X - X' \rvert$.
2)	Relative Error	E_R	$E_R = \left\lvert \frac{X - X'}{X} \right\rvert = \frac{E_a}{\lvert X \rvert}$
3)	Percentage Error	E_P	$E_P = 100\, E_R = \frac{100\, E_a}{\lvert X \rvert}$
4)	Truncation Error	E_T	$E_T = X - X'$.

Here, $X \rightarrow$ True Value of a Quantity.
$X' \rightarrow$ Approximate Value of a Quantity.

Note : 1) Truncation Errors : Caused by using approximate results or on replacing an infinite process by a finite ones. For example,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots \infty = X \text{ (say)}$$

is replaced by,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} = X' \text{ (say)}.$$

So,

$$\text{Truncation Error} = \boxed{X - X'}.$$

2) If the first significant digit of a number is K, then the relative error is less than,

$$E_R < \frac{1}{K \times 10^{n-1}}$$

where, n : any number correct upto 'n' significant figures.

Example: For the given number (N),

$$N = 342.67392$$

then the relative error will be always less than for what value of N?

Ans: Total significant figures in 'N' ⇒ $n = 8$

First significant figure's value ⇒ $K = 3$.

So,

$$\Rightarrow E_R < \frac{1}{K \times 10^{n-1}} = \frac{1}{3 \times 10^{8-1}} = \frac{1}{3} \times 10^{-7} = 0.000005$$

therefore,

$$\boxed{E_R < 0.000005}$$

3) Error in a function $f(x)$:-

Let,

$$\Rightarrow y = f(x)$$

Suppose, 'x' be true value and Δx be absolute error in x

$$\Rightarrow E_A = \Delta x.$$

and,

$$\Rightarrow E_R = \Delta x / x$$

$$\Rightarrow E_P = \frac{\Delta x}{x} \times 100\%$$

and,

$$\boxed{\Delta y = \frac{dy}{dx} \cdot \Delta x}$$

here,
Δy = absolute error in 'y'.

Q.9) If $y(x) = 7x^7 + 3x^3$, find percentage error in y when $x = 1$ for absolute error in x given as, $\Delta x = 0.05$?

Ans: Given,

$\Rightarrow y = 7x^7 + 3x^3$. and, $y(1) = 7 + 3 = 10$.

$$\Rightarrow \frac{dy}{dx} = 49x^6 + 9x^2.$$

$$\Rightarrow \left.\frac{dy}{dx}\right|_{at\ x=1} = 49 + 9 = 58$$

Now,

$$\Rightarrow \Delta y = \frac{dy}{dx} \times \Delta x.$$

$$\Rightarrow \Delta y\Big|_{at\ x=1} = \left(\frac{dy}{dx}\right)_{at\ x=1} \times \Delta x.$$

$$= 58 \times 0.05$$

$$\therefore \Delta y = \boxed{2.9}$$

- Now, percentage error in $y = \frac{\Delta y}{y} \times 100\%$

$$\Rightarrow E_p = \frac{2.9}{\cancel{10}} \times 10\cancel{0}\,\%$$

$$\therefore \boxed{E_p = 29\,\%}.$$

Note: If $u = f(x_1, x_2, x_3, \ldots\ldots, x_n)$ be a function of several variables and Δx be the error in x, where $i = 1, 2, 3, 4, \ldots\ldots, n$. Then the error (Δu) in x is given by,

$$\Delta u = \frac{\partial f}{\partial x_1}\Delta x + \frac{\partial f}{\partial x_2}\Delta x + \frac{\partial f}{\partial x_3}\Delta x + \ldots\ldots$$

Date

Q.10) If, $u(x, y, z) = xyz^2 + x^2y^2z$ and error for each parameters x, y and z is 0.001 at $x = 2$, $y = 4$ and $z = 5$.

Compute the maximum relative error (E_R) in u?

Ans: Given,

$\Rightarrow$ $u = xyz^2 + x^2y^2z$

also,

$$\Delta x = \Delta y = \Delta z = 0.001 \text{ for } \begin{cases} x = 2 \\ y = 4 \\ z = 5 \end{cases}$$

$\Rightarrow$ $u(2, 4, 5) = (2)(4)(5)^2 + (2)^2(4)^2(5)$

$\Rightarrow$ $u_T = 200 + 320$

$\therefore$ $u_T = 520$. —— (1)

Now,

$$\Rightarrow \Delta u = yz^2\Delta x + xz^2\Delta y + 2xyz\Delta z + 2xy^2z\Delta x + 2x^2yz\Delta y + x^2y^2\Delta z.$$

$$\Rightarrow \Delta u = (yz^2 + 2xy^2z)\Delta x + (xz^2 + 2x^2yz)\Delta y + (2xyz + x^2y^2)\Delta z.$$

$$\Rightarrow \Delta u = (4 \times 25 + 2 \times 4 \times 16 \times 5)\,0.001 + (2 \times 25 + 2 \times 4 \times 4 \times 5) \times 0.001 + (2 \times 2 \times 4 \times 5 + 4 \times 16) \times 0.001.$$

$\therefore$ $\Delta u = 0.774$ —— (2) (on solving).

Now, relative error;

$$\Rightarrow E_R = \frac{\Delta u}{u_T} \times 100\% = \frac{0.774}{520} \times 100 = \boxed{0.149\%}$$

Q.11) ① Find E_p in the numerical computation of $f(z)$,
$$f(z) = Z(x, y) = x - y$$
for $x = 12.05$ and $y = 8.02$ having absolute errors $\Delta x = 0.005$ and $\Delta y = 0.006$.

Ans: Let, $Z = x - y$. So,

$\Rightarrow Z_T = 12.05 - 8.02 = 4.03$

and,

$\Rightarrow \Delta Z = \Delta x - \Delta y$

$\Rightarrow \Delta Z = 0.005 - 0.006$

$\Rightarrow |\Delta Z| = 0.001$ ($\because$ Error can't be negative).

- So, percentage error (E_p) is,

$$\Rightarrow E_p = \frac{|\Delta Z|}{|Z_T|} \times 100\%$$

$$\Rightarrow E_p = \frac{0.001}{4.03} \times 100\%$$

On solving,
$$\boxed{E_p = 0.024813\,\%}$$

② Find the relative error if the number $X = 0.004997$ is truncated to three decimal digits?

Ans: Given, $X = 0.004997$

or, $X = 4.997 \times 10^{-3} = 0.4997 \times 10^{-2}$.

After truncating to three decimal digits,

$$X' = 0.499 \times 10^{-2}.$$

$$\therefore E_R = \left|\frac{X - X'}{X}\right| = \left|\frac{0.4997 \times 10^{-2} - 0.499 \times 10^{-2}}{0.4997 \times 10^{-2}}\right|$$

hence,
$$\boxed{E_R = 0.140 \times 10^{-2}}$$

3) Unconstrained One Variable Function Minimization :-

3.1) Fibonacci Search Method :- [IMPORTANT]

★ **Working Procedure →**

- Consider a function $f(x)$ defined in an interval $[a, b]$.

Step 1: Calculate L_0.
$\Rightarrow L_0 = b - a$ for a finite interval.

Step 2: Calculate x_1 (iteration 1) and x_2 (iteration 2) as:
$x_1 = a + L_2^* \rightarrow a + L_2^*$
$x_2 = b - L_2^*$

Step 3: Here, $L_k^* = \frac{F_{n-k}}{F_n} \times L_0$ (n : no. of iterations specified in the question)

So,
$L_2^* = \frac{F_{n-2}}{F_n} \times L_0$

and, ($K \rightarrow$ Iteration to be calculated : $K < n$).

Note: Fibonacci Series is defined as:
$$F_n = F_{n-1} + F_{n-2} \quad (n = 2, 3, 4, 5, \dots \infty)$$
and,
$F_0 = F_1 = 1$
i.e.,

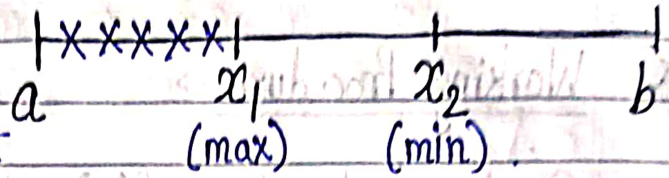
Series →	0,	1,	1,	2,	3,	5,	8,	13,	21,	34, ...
Term no. →		F_0	F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8

Step 4: Now, find $F(x_1)$ and $F(x_2)$ and compare both the values :

i) If $F(x_1) > F(x_2)$:

It means function is maximized at x_1 and is minimum at x_2.

- Discard the interval $[a, x_1]$, if you want to minimize the function.



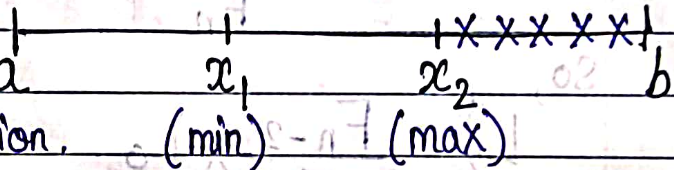
- And, discard the interval $[b, x_2]$, if you want to maximize the function.

ii) If $F(x_1) < F(x_2)$:

It means function is maximized at x_2 and is minimized at x_1.

→ Follow the above approach but opposite, i.e.,

- Discard the interval $[b, x_2]$, if you want to minimize the function.



- Discard the interval $[a, x_1]$, if you want to maximize the function.

Step 5: Calculate the next iteration, i.e., (x_3).

- First, find L_3^*, using the previously mentioned formula.

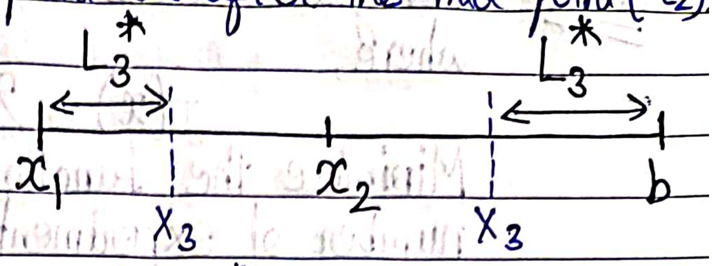
$$L_3^* = \frac{F_{n-3}}{F_n} \times L_0 \qquad \left(\begin{array}{l} L_0 = b - a \text{ (from Step 1)} \\ K = 3 \end{array} \right)$$

- Now, find x_3 [Considering Step 4: Case-1]

As,

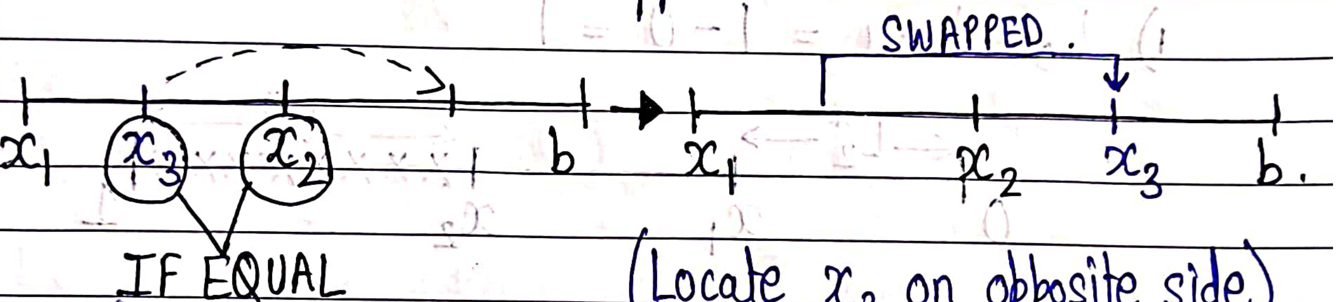
x_3 should lie in the interval $[x_1, b]$ and, could be before the mid-point or after the mid-point (x_2)

x_3 could be located only at one position either,



$x_3 = x_1 + L_3^*$ OR $x_3 = b - L_3^*$

i) If, $x_3 \approx x_2$ in the interval $[x_1, x_2]$, so x_3 should must be located on the opposite side.



(Locate x_3 on opposite side).

ii) Vice-Versa, would be followed if, $x_3 \approx x_2$ in the interval $[x_2, b]$, so swap x_3 on the opposite side.

Step 6: Similarly, as step 4, compare $F(x_3)$ and $F(x_2)$ and decide the next interval based on either condition of maximization or minimization.

Step 7: Calculate the next iteration, i.e., (x_4) and repeat steps 5 and step 4 till $\boxed{K = n}$ th iteration.
i.e.,

$$L_K^* = \frac{F_{n-K}}{F_n} \times L_0$$

→ At $K = n$,

$$L_n^* = \frac{F_0}{F_n} \times L_0$$

- this will be the last iteration to be calculated.

Q.12) For given unconstrained one variable function $y = f(x)$ where,

$$f(x) = 2x^2 - e^x$$

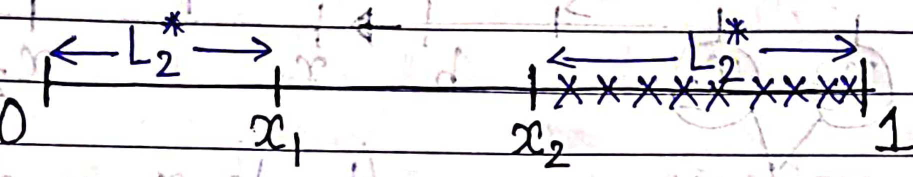
Minimize the function in the interval $[0, 1]$ for number of experiments / iterations $(n) = 10$?

(7.5 marks)

Ans: Given,

$f(x) = 2x^2 - e^x$, $n = 10$, $[0, 1]$

1) $L_0 = b - a = 1 - 0 = 1$



$\Rightarrow L_2^* = \frac{F_{n-2}}{F_n} \times L_0 = \frac{F_{10-2}}{F_{10}} \times 1 \qquad (n = 10)$

$\Rightarrow L_2^* = \frac{F_8}{F_{10}} = \frac{34}{89} = 0.382022$

So,

$\Rightarrow x_1 = a + L_2^* = 0 + 0.382022 = 0.382022$

$\Rightarrow x_2 = b - L_2^* = 1 - 0.382022 = 0.618$

$\Rightarrow F(x_1) = F(0.382022) = -1.17336$

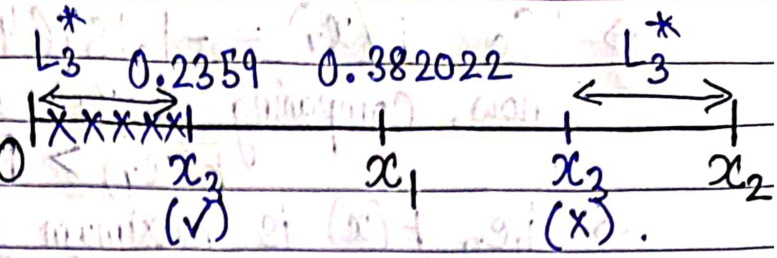
$\Rightarrow F(x_2) = F(0.618) = -1.09136$

(substitued values of x_1 and x_2 in function $f(x)$).

$\because$ $F(x_2) > F(x_1)$, for minimization discarding the max^n value and the interval $[x_2, 1]$.

$\rightarrow$ Rejecting the interval $[x_2, 1]$.

2) To find x_3.



$\Rightarrow L_3^* = \frac{F_{n-3}}{F_n} \times L_0$

$\Rightarrow L_3^* = \frac{F_7}{F_{10}} \times 1 = \frac{21}{89} = 0.2359$

So,

$\Rightarrow x_3 = 0 + L_3^* = 0 + 0.2359 = 0.2359$ (✓)

$\Rightarrow x_3 = x_2 - L_3^* = 0.618 - 0.2359 = 0.3821 \approx x_1$

- The value of x_3 will be the ones, that is not approximately equal to x_1. So,

$$x_3 = 0.2359.$$

Now,

$\Rightarrow F(x_3) = F(0.2359) = 2 \times (0.2359)^2 - e^{(0.2359)}$

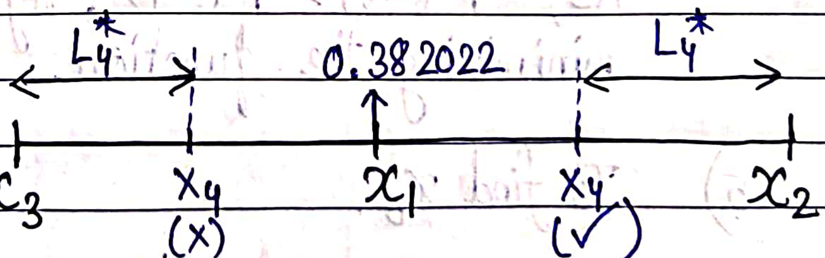
i.e.,

$$F(x_3) = -1.15475$$

and, $$F(x_1) = -1.17336.$$

$\because F(x_3) > F(x_1)$, rejecting the interval $[0, x_3]$.

3) To find x_4.



$\Rightarrow L_4^* = \frac{F_{n-4}}{F_n} \times L_0$

$\Rightarrow L_4^* = \frac{F_6}{F_{10}} \times 1 = \frac{13}{89} = 0.14606$

So,

$\Rightarrow x_4 = x_3 + L_4^* = 0.2359 + 0.14606 = 0.38196$

$\Rightarrow x_4 = x_2 - L_4^* = 0.618 - 0.14606 = 0.47194$ (✓)

$\rightarrow$ Value of $x_4 = 0.47194 \neq x_1$.

$\Rightarrow$ So, $F(x_4) = -1.157646$.

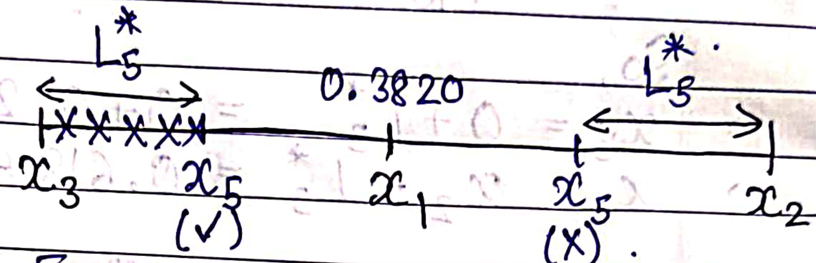
now, comparing $F(x_1)$ and $F(x_4)$,

$F(x_4) > F(x_1)$ $\quad (F(x_1) = -1.157646)$.

$\rightarrow$ i.e., $F(x)$ is maximum at x_4. So,

$\rightarrow$ rejecting the interval $[x_4, x_2]$.

4) To find x_5.



$\Rightarrow L_5^* = \frac{F_{n-5}}{F_n} \times L_0$

$\Rightarrow L_5^* = \frac{F_5}{F_{10}} \times 1 = \frac{F_5}{F_{10}} = \frac{8}{89} = 0.089887$

So,

$\Rightarrow x_5 = x_3 + L_5^* = 0.2359 + 0.089887 = 0.32578$ (✓)

$\Rightarrow x_5 = x_4 - L_5^* = 0.47194 - 0.089887 = 0.38206$.

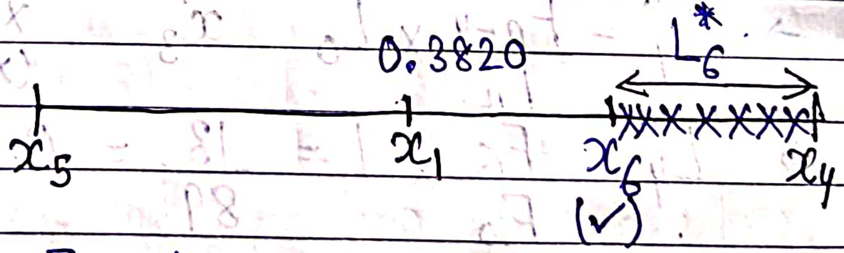
$\therefore F(x_5) = F(0.32578) = -1.17284$.

and,

$F(x_1) = -1.17336$.

As, $F(x_5) > F(x_1)$, reject interval $[x_3, x_5]$ for minimizing the function.

5) To find x_6.



$\Rightarrow L_6^* = \frac{F_{n-6}}{F_n} \times L_0$

$\Rightarrow L_6^* = \frac{F_4}{F_{10}} \times 1 = \frac{5}{89} \times 1 = 0.056179$

Value of x_6 will be

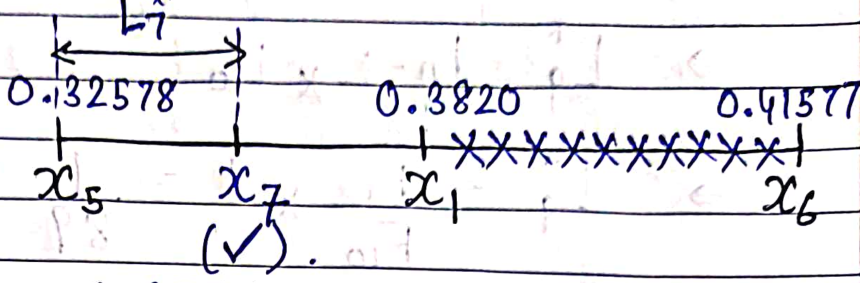
$\Rightarrow x_6 = x_4 - L_6^* = 0.47194 - 0.056179 = 0.41577 \neq x_1$

So,

$\Rightarrow F(x_6) = F(0.41577) = -1.169807$.

$\rightarrow$ As, $F(x_6) > F(x_1)$, so to minimize the function rejecting the maximized interval : $[x_6, x_4]$.

6) To find x_7.



$\Rightarrow L_7^* = \frac{F_{n-7}}{F_n} \times L_0$

$\Rightarrow L_7^* = \frac{F_3}{F_{10}} \times 1 = \frac{3}{89} = 0.033707$.

So,

$\Rightarrow x_7 = x_5 + L_7^* = 0.32578 + 0.033707 = 0.359487 \neq x_1$

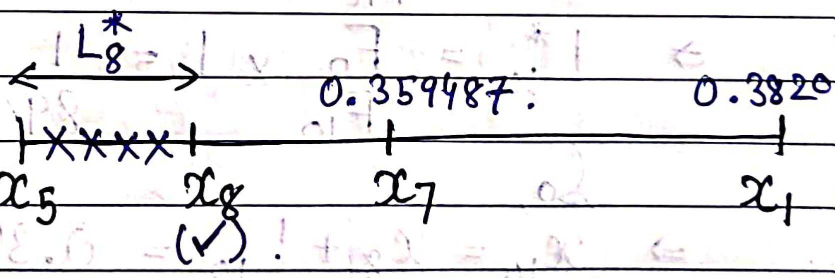
$\Rightarrow F(x_7) = F(0.359487) = -1.1741324$ <

and,

$\Rightarrow F(x_1) = -1.1733627$.

$\because F(x_7) < F(x_1)$, for minimizing the function rejecting the maxima at x_1, i.e., interval $[x_1, x_6]$.

7) To find x_8.



$\Rightarrow L_8^* = \frac{F_{n-8}}{F_n} \times L_0$

$\Rightarrow L_8^* = \frac{F_2}{F_{10}} \times L_0 = \frac{2}{89} = 0.022471$.

So,

$\Rightarrow x_8 = x_5 + L_8^* = 0.32578 + 0.022471 = 0.34825 \neq x_7$

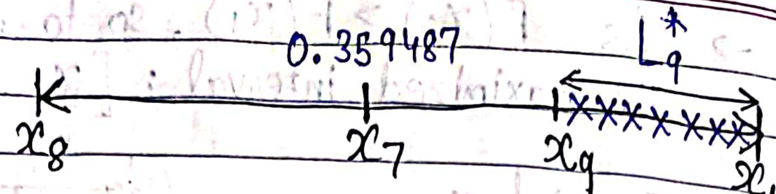
$\Rightarrow F(x_8) = F(0.34825) = -1.1740302$

and,

$\Rightarrow F(x_7) = -1.1741324$

• So, rejecting the interval $[x_5, x_8]$ as, $F(x_8) > F(x_7)$.

8) To find x_9.



$\Rightarrow L_9^* = \frac{F_{n-9}}{F_n} \times L_0$

$\Rightarrow L_9^* = \frac{F_1}{F_{10}} \times 1 = \frac{1}{89} = 0.011235$

So,

$\Rightarrow x_9 = x_1 - L_9^* = 0.382022 - 0.011235 = 0.37079$

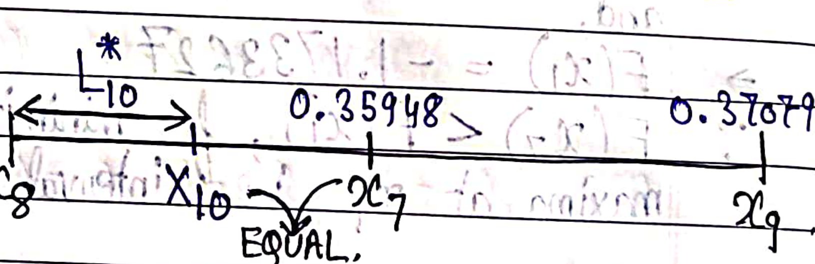
i.e.,

$\Rightarrow F(x_9) = F(0.37079) = -1.1739083$

$\because F(x_7) = -1.1741324.$

$\Rightarrow F(x_9) > F(x_7)$, so rejecting the interval $[x_9, x_1]$.

9) To find x_{10}.



$\Rightarrow L_{10}^* = \frac{F_{n-10}}{F_n} \times L_0$

$\Rightarrow L_{10}^* = \frac{F_0}{F_{10}} \times 1 = \frac{1}{89} = 0.011235$

So,

$\Rightarrow x_{10} = x_8 + L_{10}^* = 0.34825 + 0.011235 = 0.359485$

and,

$\Rightarrow F(x_{10}) = F(0.359485) = -1.17413251.$

$\Rightarrow F(x_7) = F(0.35948) = -1.1741324.$

$\rightarrow$ Here, values of x_{10} and x_7 show convergence, i.e., they are both equal.

Therefore, the value of x for which the function $F(x)$ is minimum is,

$$\boxed{x = 0.359485}$$

and,

$$\boxed{F(x_{min}) = F(0.359485) = -1.17413251}$$

Q.13) For the given unconstrained one variable function $y = f(x)$ where,

$$f(x) = x^2 + 4x + 5$$

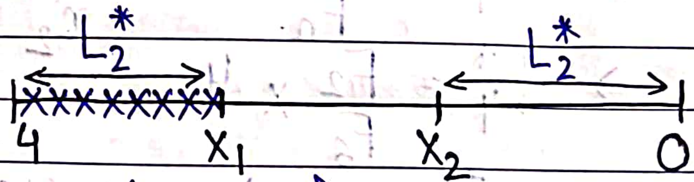
Maximize the function in the interval $[-4, 0]$ for number of iterations $(n) = 6$, using the Fibonacci Search Method ?

Ans: Given,

$$f(x) = x^2 + 4x + 5 \quad , \; n = 6 \quad , \; [-4, 0].$$

1) $L_0 = b - a = 0 - (-4) = 4.$

$\Rightarrow L_2^* = \dfrac{F_{n-2}}{F_n} \times L_0$



$\Rightarrow L_2^* = \dfrac{F_4}{F_6} \times 4 \qquad (\because n = 6).$

$\Rightarrow L_2^* = \dfrac{5}{13} \times 4 = 1.53846$

So,

$\Rightarrow x_1 = a + L_2^* = -4 + 1.53846 = -2.46154$

$\Rightarrow x_2 = b - L_2^* = 0 - 1.53846 = -1.53846$

and,

$\Rightarrow F(x_1) = 1.212521$

$\Rightarrow F(x_2) = 1.213444$

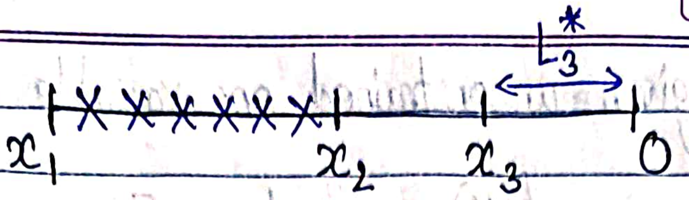
[Consider the values of x_1 and x_2 only upto first three decimal places.]

$\because F(x_2) > F(x_1)$, so for maximizing the function reject the minima, i.e., x_1, rejecting the interval $[-4, x_1]$.

2) $L_3^* = \dfrac{F_{n-3}}{F_n} \times L_0 = \dfrac{F_3}{F_6} \times 4 = \dfrac{3}{13} \times 4 = 0.92307$

Now,

$\Rightarrow x_3 = 0 - L_3^* = 0 - .92307 = -0.92307$



$\Rightarrow F(x_3) = F(-0.92307)$

$\Rightarrow F(x_3) = (-0.92307)^2 + 4 \times (-0.92307) + 5$

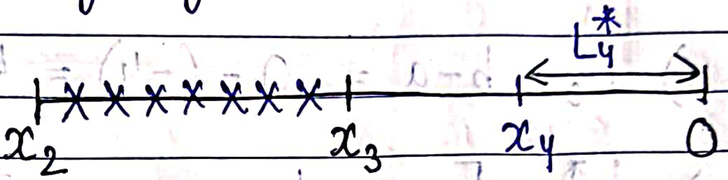
$\therefore F(x_3) = 2.1597782$

and,

$F(x_2) = 1.213444$

$\because F(x_3) > F(x_2)$, so rejecting the interval $[x_1, x_2]$.

3) $L_4^* = \frac{F_{n-4}}{F_n} \times L_0$



$\Rightarrow L_4^* = \frac{F_2}{F_6} \times 4$

$\Rightarrow L_4^* = \frac{2}{13} \times 4 = 0.61538$

$\Rightarrow x_4 = 0 - L_4^* = 0 - 0.61538 = -0.61538$.

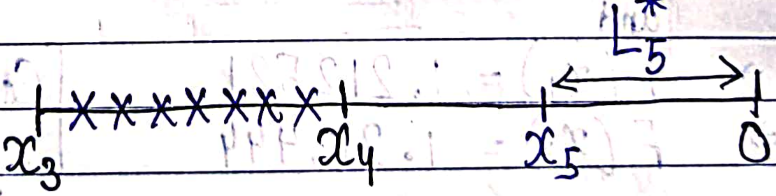
so,

$\Rightarrow F(x_4) = F(-0.61538) = 2.9171725$.

$\because F(x_4) > F(x_3)$, so rejecting the interval $[x_2, x_3]$.

4) To find x_5.

$\Rightarrow L_5^* = \frac{F_{n-5}}{F_n} \times L_0$



$\Rightarrow L_5^* = \frac{F_1}{F_6} \times 4$

$\Rightarrow L_5^* = \frac{1}{13} \times 4 = \cancel{0.6153}\ 0.30769$.

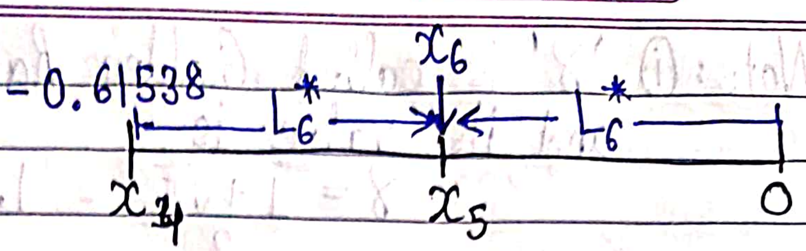
So,

$\Rightarrow x_5 = 0 - L_5^* = -0.30769$.

and,

$\Rightarrow F(x_5) = F(-0.30769) = 3.863913136$.

5) To find x_6



$\Rightarrow \; L_6^* = \dfrac{F_{n-6}}{F_n} \times L_0$

$\Rightarrow \; L_6^* = \dfrac{F_0}{F_6} \times L_0 = \dfrac{1}{13} \times 4 = 0.30769$.

So,

$\Rightarrow \; x_6 = x_4 + L_6^* = -0.61538 + 0.30769 = -0.30769$.

or,

$\Rightarrow \; x_6 = 0 - L_6^* = 0 - 0.30769 = -0.30769$.

and,

value of x_5 was $= -0.30769$.

i.e.,

'x_5' and 'x_6' show convergence and are clearly equal.

→ Therefore, the maxima of the function is,

$$\boxed{x_{max} = -0.30769}.$$

and,

→ The maximum value of the function is

$$F(x_{max}) = F(-0.30769) = \boxed{3.863913136}.$$

3.2) Golden Section Method :- [IMPORTANT]

✱ Working Procedure →

- Consider a function $f(x)$ defined in an interval $[a, b]$.

→ "Same procedure as Fibonacci Search Method, only change is in 'Step-3' → formula.."

Step-3: $L_n^* = \dfrac{1}{\gamma^n} \times L_0$; $L_0 = b - a$

$\gamma = 1.618$ (a constant).

Note: ① 'γ' is called Golden Ratio Number. It is a constant and its value is,

$$\gamma = \frac{1+\sqrt{5}}{2} = 1.618.$$

② If the value of 'n' is not given in the question, then calculate the value of x, till the number of iterations reach an error (ϵ) of 0.15 (approx.). That is,

$$\boxed{x \approx \epsilon = 0.15 \ldots\ldots \text{(approximately.)}}$$

Q.14) Using the Golden Section Method, minimize the following given function $f(x)$,

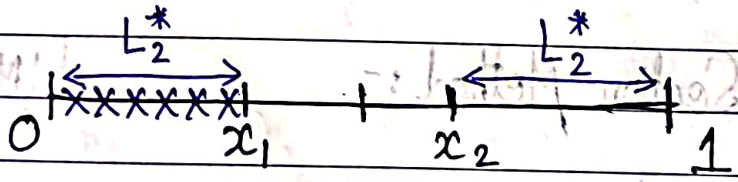
$$f(x) = 4x^3 + x^2 - 7x + 14$$

in the interval [0, 1] for $n = 6$?

Ans: Given,

$$f(x) = 4x^3 + x^2 - 7x + 14, \quad n = 6, \quad [0, 1].$$

1) $L_0 = b - a = 1 - 0 = 1$



$\Rightarrow L_2^* = \frac{1}{\gamma^2} \times L_0 = \frac{1}{(1.618)^2} \times 1 = 0.3819$

$\Rightarrow x_1 = a + L_2^* = 0 + 0.3819 = 0.3819$

$\Rightarrow x_2 = b - L_2^* = 1 - 0.3819 = 0.6181$

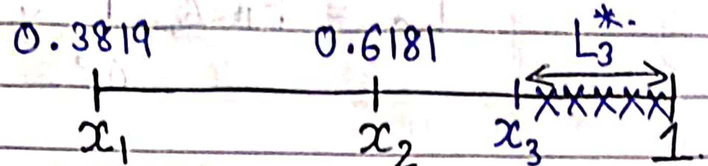
So,

$\Rightarrow F(x_1) = F(0.3819) = 11.6953$

$\Rightarrow F(x_2) = F(0.6181) = 10.9999$

As, $F(x_1) > F(x_2)$, so to minimize the function, rejecting the maxima (x_1) and interval $[0, x_1]$.

2) $L_3^* = \frac{1}{\gamma^3} \times L_0$



$\Rightarrow L_3^* = \frac{1}{(1.618)^3} \times 1 = 0.2361$.

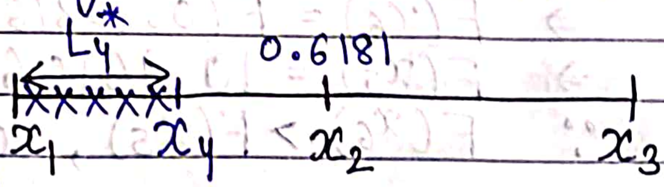
$\Rightarrow x_3 = 1 - L_3^* = 1 - 0.2361 = 0.7639$

so,

$\Rightarrow F(x_3) = 11.019317$ and, $F(x_2) = 10.9999$

$\because F(x_3) > F(x_2)$, so rejecting the interval $[x_3, 1]$.

3) $L_4^* = \frac{1}{\gamma^4} \times L_0$



$\Rightarrow L_4^* = \frac{1}{(1.618)^4} = 0.1459102$

so,

$\Rightarrow x_4 = x_1 + L_4^* = 0.52781$ (✓).

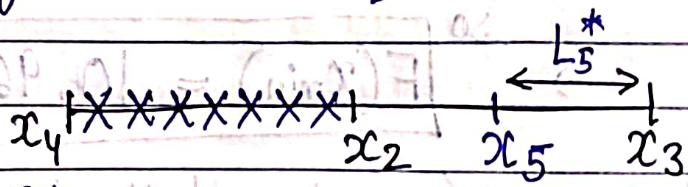
$\Rightarrow x_4 = x_3 - L_4^* = 0.61799$

so,

$\Rightarrow F(x_4) = 11.1720698$ and, $F(x_2) = 10.9999$.

$\because F(x_4) > F(x_2)$, so rejecting the interval $[x_1, x_4]$.

4) $L_5^* = \frac{1}{\gamma^5} \times L_0$



$\Rightarrow L_5^* = \frac{1}{(1.618)^5} = 0.0901794$

so,

$\Rightarrow x_5 = x_3 - L_5^* = 0.7639 - 0.090179 = 0.673721$

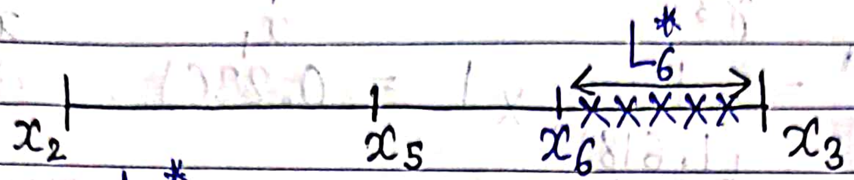
i.e.,

$\Rightarrow F(x_5) = 10.9610608$, and, $F(x_2) = 10.9999$

$\because F(x_2) > F(x_5)$, so rejecting the interval $[x_4, x_2]$.

5) For $n=6$,

$$L_6^* = \cancel{F_{n-6}}\ \frac{1}{\gamma_1^6} \times L_0 = \frac{1}{(1.618)^6} \times 1 = 0.055735$$



$\Rightarrow x_6 = x_3 - L_6^*$

$\Rightarrow x_6 = 0.7639 - 0.055735$

$\Rightarrow x_6 = 0.708165 \neq x_5$.

So,

$\Rightarrow F(x_6) = F(0.708165) = 10.964915$

$\Rightarrow F(x_5) = 10.9610608$.

$\because F(x_6) > F(x_5)$, so rejecting the interval $[x_6, x_3]$.

→ Hence, the interval remains $[x_2, x_6]$. So, optimised value of x_{min} will be;

$\Rightarrow x_{min} = \dfrac{x_2 + x_6}{2} \quad \left(\because x_{opt} = \dfrac{a+b}{2} \text{ for } [a, b]\right)$

$\Rightarrow x_{min} = \dfrac{0.6181 + 0.708165}{2} = \boxed{0.6631325}$

So,

$\Rightarrow \boxed{F(x_{min}) = 10.964253 \sim F(x_5)}$

Note: (Important) If, number of iterations (n) and interval (L_0) is not given for either Fibonaci Search and Golden Section method, but error (ϵ) is given then, assume,
$L_0 = [0, 1]$ for both the methods and 'n' shall be calculated as;

1). Fibonaci Search Method: Assume, $L_0 = [0, 1]$
$\because$ 'ϵ' is given, but 'n' is not, so

★ Using the formula,

$$\boxed{\epsilon = \frac{L_n}{L_0}}$$

where,
① 'ϵ' is called as measure of efficiency.
② L_n = Length of interval of uncertainity after 'n' iterations
L_0 = Length of initial interval of uncertainity.
③ Ratio $\left(\frac{L_n}{L_0}\right)$ is called as "Reduction Ratio."

So, assume value of $L_n = \frac{1}{F_n} L_0$.

$\therefore \epsilon = \left(\frac{\cancel{L_0}}{F_n}\right) \times \frac{1}{\cancel{L_0}} \Rightarrow \boxed{F_n \geq \frac{1}{\epsilon}}$ { 'ϵ' will be given, For fibonacci method }

$\geq$ → Greater than or equal to.

→ When calculated 'F_n', compare this value to the fibonacci series to find the nearest value of 'n'. For example, if F_n comes out to be 377 then, $\boxed{n = 14}$.

Sequence (F_n)	1	1	2	3	5	8	13	21	34	55	89	144	233	377 ✓
No. of term (n)	1	2	3	4	5	6	7	8	9	10	11	12	13	$\boxed{14}$ ↑

2) Golden Section Method: Assume $L_0 = [0, 1]$.
Applying above formula,

$$\epsilon = \frac{L_n}{L_0}$$

So, in this case, assume $L_n = \frac{1}{\gamma^{n-1}} L_0$.

$\therefore \epsilon = \left(\frac{\cancel{L_0}}{\gamma^{n-1}}\right) \times \frac{1}{\cancel{L_0}} \Rightarrow \boxed{\epsilon = (0.618)^{n-1} = (1.618)^{1-n}}$

→ Use this formula, to solve and find 'n'.

4) Multivariate Two Variables Function Minimization :-

4.1) Steepest Descent Method :-

★ **Working Procedure :-**

Step 1 : Start with an arbitary initial point X_1, considering it as iteration 1 where,

$$X_1 = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \text{(for two variables)}$$

Step 2 : Find the Search Direction (S_n), where n: number of iteration;

$$S_n = -\nabla f_n = -\begin{bmatrix} \partial f / \partial x_1 \\ \partial f / \partial x_2 \end{bmatrix}_{X_n}$$

- Example : If $n=1$,

$$S_1 = -\underset{\substack{\downarrow \\ \text{(Gradient Symbol)}}}{\nabla} f_1 = -\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_1} \text{ or } -\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} \text{ at } \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

Step 3 : Determine the optimal step Length (L_1^*). For minimizing the function,

① Find $f(X_1 + L_1^* S_1) = ?$ (for $n=1$)

② Now, differentiate this value w.r.t L_1^*, i.e., find

$$\Rightarrow \frac{d}{dL_1^*}\left[f(X_1 + L_1^* S_1)\right]$$

③ Put the above value equal to zero and find L_1^*.

$$\Rightarrow \frac{d}{dL_1^*}\left[f(X_1 + L_1^* S_1)\right] = 0 \quad \Rightarrow \boxed{L_1^* = ?}$$

Step 4: Now, determine the next arbitary point X_2 using the formula,

$$\boxed{X_2 = X_1 + L_1^* S_1}$$

Step 5: Find the next Search Direction (S_2) at point X_2.

$$S_2 = -\nabla f_2 = -\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_2} \text{ or } -\begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} \text{ at } \begin{bmatrix} x_K \\ x_{K+1} \end{bmatrix}$$

Step 6: Check whether, $|\nabla f_2| \cong X_1$. [$\cong$: Approximately Equal].
If NOT,
then perform the next iteration, i.e., find X_3 then S_3 and compare it to X_1. If not approximately equal then repeat the procedure till it shows convergence.

Note: Break the iteration, if it does not show convergence or gets maximized instead of minimizing.

Q.15) Minimize the given function $f(x_1, x_2)$ where,

$$f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2$$

Starting from the point $X_1 = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ where, $x_1 = x_2 = 0$ using the Steepest Descent Method? (HARD)

Ans: Given, initial arbitary point $(X_1) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

Now,

Iteration 1:

$$\Rightarrow \nabla f_1 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_1} = \begin{bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{bmatrix} \text{ at } \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\Rightarrow \nabla f_1 = \begin{bmatrix} 1 + 4(0) + 2(0) \\ -1 + 2(0) + 2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

hence,

$$\Rightarrow S_1 = -\nabla f_1 = -\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix},$$

$\Rightarrow$ To find λ_1^* or L_1^*, minimizing the function,

$$\Rightarrow f(X_1 + L_1^* S_1) = f\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + L_1^* \begin{bmatrix} -1 \\ 1 \end{bmatrix}\right]$$

$$\Rightarrow f\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} -L_1^* \\ L_1^* \end{bmatrix}\right] = f\begin{bmatrix} -L_1^* \\ +L_1^* \end{bmatrix} = f(\underbrace{-L_1^*}_{x_1}, \underbrace{L_1^*}_{x_2})$$

$$\Rightarrow -L_1^* - L_1^* + 2(L_1^*)^2 + 2L_1^*(-L_1^*) + (L_1^*)^2$$

$$\Rightarrow -2L_1^* + \cancel{2L_1^{*2}} - \cancel{2L_1^{*2}} + L_1^{*2}$$

$$\Rightarrow L_1^{*2} - 2L_1^*$$

$\rightarrow$ Differentiating this value w.r.t L_1^* and equating to zero,

$$\Rightarrow \frac{d}{dL_1^*}\left[f(-L_1^*, L_1^*)\right] = \frac{d}{dL_1^*}(L_1^{*2} - 2L_1^*)$$

$\Rightarrow 2L_1^* - 2 = 0 \qquad \Rightarrow 2L_1^* = 2$

$\Rightarrow \boxed{L_1^* = 1}$.

So,

$\Rightarrow X_2 = X_1 + L_1^* S_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$.

Iteration 2: Now,

$$\Rightarrow \nabla f_2 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_2} = \begin{bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{bmatrix} \text{ at } \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

$$\Rightarrow \nabla f_2 = \begin{bmatrix} 1 + 4(-1) + 2(1) \\ -1 + 2(-1) + 2(1) \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \end{bmatrix} \neq X_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$\because \nabla f_2 \neq X_1$, we have to continue with next iteration.

hence,

$S_2 = -\nabla f_2 = -\begin{bmatrix} -1 \\ -1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

→ To find L_2^*, finding the function : $f(X_2 + L_2^* S_2)$.

$$= f\left(\begin{bmatrix} -1 \\ 1 \end{bmatrix} + L_2^* \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) = f\left(\begin{bmatrix} -1 + L_2^* \\ 1 + L_2^* \end{bmatrix} \begin{matrix} \rightarrow x_1 \\ \rightarrow x_2 \end{matrix} \right)$$

$\Rightarrow f\left([-1 + L_2^*], [1 + L_2^*] \right)$

$\Rightarrow (-1+L_2^*) - (1+L_2^*) + 2(-1+L_2^*)^2 + 2(-1+L_2^*)(1+L_2^*)$

$+ (1+L_2^*)^2$

$\Rightarrow -1+\cancel{L_2^*}-1-\cancel{L_2^*}+2\left(L_2^{*2}+1-2L_2^*\right)+2\left(L_2^{*2}-1\right)$

$+\left(1+L_2^{*2}+2L_2^*\right)$

$\Rightarrow -2+5L_2^{*2}-2L_2^*+1$

$\Rightarrow 5L_2^{*2}-2L_2^*-1$

$\rightarrow$ On differentiating w.r.t L_2^*;

$$\Rightarrow \frac{d}{dL_2^*}\left(5L_2^{*2}-2L_2^*-1\right)=10L_2^*-2$$

$\Rightarrow 10L_2^*-2=0$ (for minimization)

$\Rightarrow L_2^*=\frac{2}{10}$

$\therefore \boxed{L_2^*=\frac{1}{5}}$

So,

$$\rightarrow X_3=X_2+L_2^*S_2=\begin{bmatrix}-1\\1\end{bmatrix}+\frac{1}{5}\begin{bmatrix}1\\1\end{bmatrix}=\begin{bmatrix}-1+0.2\\1+0.2\end{bmatrix}$$

$$\Rightarrow X_3=\begin{bmatrix}-0.8\\1.2\end{bmatrix}$$

Now,

$$\Rightarrow \nabla f_3=\begin{bmatrix}\frac{\partial f}{\partial x_1}\\\frac{\partial f}{\partial x_2}\end{bmatrix}_{\text{at } X_3}=\begin{bmatrix}1+4x_1+2x_2\\-1+2x_1+2x_2\end{bmatrix}\text{at}\begin{bmatrix}-0.8\\+1.2\end{bmatrix}.$$

$$\Rightarrow \nabla f_3=\begin{bmatrix}1+4(-0.8)+2(1.2)\\-1+2(-0.8)+2(1.2)\end{bmatrix}$$

$\Rightarrow \nabla f_3 = \begin{bmatrix} 0.2 \\ -0.2 \end{bmatrix} \neq X_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

$\because$ $\nabla f_3 \neq X_1$, we have to continue with the next iteration.

Iteration 3: So,

$S_3 = -\nabla f_3 = \begin{bmatrix} -0.2 \\ +0.2 \end{bmatrix}$

→ Now, L_3^* shall be calculated as : $f(X_3 + L_3^* S_3) =$

$\Rightarrow f\left(\begin{bmatrix} -0.8 \\ 1.2 \end{bmatrix} + L_3^* \begin{bmatrix} -0.2 \\ 0.2 \end{bmatrix}\right)$

$\Rightarrow f\left(\left[-0.8 + (-0.2) L_3^*\right], \left[1.2 + (0.2) L_3^*\right]\right)$.

$\Rightarrow (-0.8 - 0.2 L_3^*) - (1.2 + 0.2 L_3^*) + 2(-0.8 - 0.2 L_3^*)^2$

$+ 2(-0.8 - 0.2 L_3^*)(1.2 + 0.2 L_3^*) + (1.2 + 0.2 L_3^*)^2$

$\Rightarrow -2 - 0.4 L_3^* + 2(0.64 + 0.04 L_3^{*2} + 0.32 L_3^*)$.

$+ 2(-0.96 - 0.16 L_3^* - 0.24 L_3^* - 0.04 L_3^{*2}) +$

$(1.44 + 0.04 L_3^{*2} + 0.48 L_3^*)$.

$\Rightarrow 0.04 L_3^{*2} - 0.08 L_3^* - 1.2$ (on solving..)

→ Now, differentiating this value, and equating it to zero.

$\Rightarrow \frac{d}{dL_3^*}(0.04 L_3^{*2} - 0.08 L_3^* - 1.2) = 0$.

$\Rightarrow 0.08L_3^* - 0.08 = 0$

so, $\boxed{L_3^* = 1}$

$\Rightarrow X_4 = X_3 + L_3^* S_3$

$\Rightarrow X_4 = \begin{bmatrix} -0.8 \\ 1.2 \end{bmatrix} + 1 \begin{bmatrix} -0.2 \\ 0.2 \end{bmatrix}$

$\Rightarrow X_4 = \begin{bmatrix} -0.8 - 0.2 \\ 1.2 + 0.2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1.4 \end{bmatrix}$

Now,

$\Rightarrow \nabla f_4 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_4} = \begin{bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{bmatrix} \text{ at } \begin{bmatrix} -1 \\ 1.4 \end{bmatrix}$

$\Rightarrow \nabla f_4 = \begin{bmatrix} 1 + 4(-1) + 2(1.4) \\ -1 + 2(-1) + 2(1.4) \end{bmatrix} = \begin{bmatrix} -0.2 \\ -0.2 \end{bmatrix} \neq X_1$

$\because \nabla f_4 \neq X_1$, we have to continue with the next iteration.

<u>Iteration 4</u>: So,

$S_4 = -\nabla f_4 = -\begin{bmatrix} -0.2 \\ -0.2 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix}$

Now,

$\Rightarrow X_5 = X_4 + L_4^* S_4 = \begin{bmatrix} -1 \\ 1.4 \end{bmatrix} + L_4^* \begin{bmatrix} 0.2 \\ 0.2 \end{bmatrix}$

$\Rightarrow X_5 = \begin{bmatrix} -1 + 0.2 L_4^* \\ 1.4 + 0.2 L_4^* \end{bmatrix}$

→ Now, to find the value of L_4^*, first finding $f:(X_4+L_4^* S_4)$

⇒ $f\left(\left[\underbrace{-1+0.2L_4^*}_{x_1},\ \underbrace{1.4+0.2L_4^*}_{x_2}\right]\right)$.

⇒ $(-1+\cancel{0.2L_4^*}) - (1.4+\cancel{0.2L_4^*}) + 2(-1+0.2L_4^*)^2$
$+ 2(-1+0.2L_4^*)(1.4+0.2L_4^*) + (1.4+0.2L_4^*)^2$.

⇒ $-2.4 + 2(0.04L_4^{*2}+1-0.4L_4^*) + 2(-1.4-0.2L_4^*$
$+0.28L_4^*+0.04L_4^{*2}) + (1.96+0.04L_4^{*2}+0.56L_4^*)$

⇒ $-2.4+0.08L_4^{*2}+2-0.8L_4^*-2.8-0.4L_4^*+0.56L_4^*$
$+0.08L_4^{*2}) + (1.96+0.04L_4^{*2}+0.56L_4^*)$.

⇒ $0.2L_4^{*2} - 0.08L_4^* - 1.24$.

→ On differentiating, w.r.t. L_4^*,

⇒ $\frac{d}{dL_4^*}(0.2L_4^{*2} - 0.08L_4^* - 1.24) = 0$.

⇒ $0.4L_4^* - 0.08 = 0$

hence,

$$\boxed{L_4^* = 0.2}$$

so,

$$X_5 = \begin{bmatrix}-1+0.2L_4^* \\ 1.4+0.2L_4^*\end{bmatrix} = \begin{bmatrix}-1+0.04 \\ 1.4+0.04\end{bmatrix} = \begin{bmatrix}-0.96 \\ 1.44\end{bmatrix}$$

→ Now, evaluating ∇f_5:

$$\Rightarrow \nabla f_5 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_5} = \begin{bmatrix} 1+4x_1+2x_2 \\ -1+2x_1+2x_2 \end{bmatrix} \text{ at } \begin{bmatrix} -0.96 \\ 1.44 \end{bmatrix}$$

$$\Rightarrow \nabla f_5 = \begin{bmatrix} 1+4(-0.96)+2(1.44) \\ -1+2(-0.96)+2(1.44) \end{bmatrix}$$

$$\therefore \nabla f_5 = \begin{bmatrix} 0.04 \\ -0.04 \end{bmatrix} \approx X_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Here,

∇f_5 is approximately close to X_1 (initial point).

So,

stopping the iteration here, we have;

$x_1 = 0.04$ and $x_2 = -0.04$.

i.e.,

the minimised value of the function $f(x_1, x_2)$ at ∇f_5 is,

$$f(\nabla f_5) = f(0.04, -0.04)$$

$$\boxed{f_{min} = 0.0816}$$

4.2) Newton's Method :-

Q.16) Minimize the given function $f(x_1, x_2)$, starting from the point $X_1 = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, given $x_1 = x_2 = 0$ using Newton's method if :

$$f(x_1, x_2) = x_1 - x_2 + 2x_1^2 + 2x_1 x_2 + x_2^2.$$

Ans : i) Step 1: Find the Hessian's matrix $[H_1]$.

Here,

$$[H_1] = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial^2 x_1 x_2} \\ \frac{\partial^2 f}{\partial^2 x_2 x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

where,

$\Rightarrow \frac{\partial f}{\partial x_1} = 1 + 4x_1 + 2x_2$ $\qquad \Rightarrow \frac{\partial^2 f}{\partial x_1^2} = 4.$

$\Rightarrow \frac{\partial f}{\partial x_2} = -1 + 2x_1 + 2x_2$ $\qquad \Rightarrow \frac{\partial^2 f}{\partial x_2^2} = 2.$

$$\Rightarrow \frac{\partial^2 f}{\partial^2 x_1 x_2} = \frac{\partial}{\partial x_1}\left(\frac{\partial f}{\partial x_2}\right) = 2$$

$$\Rightarrow \frac{\partial^2 f}{\partial^2 x_2 x_1} = \frac{\partial}{\partial x_2}\left(\frac{\partial f}{\partial x_1}\right) = 2$$

$\therefore$ Value of matrix $[H_1]$ is,

$$H_1 = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}.$$

ii) Step 2: Find inverse of the matrix H.

$$\Rightarrow [H_1]^{-1} = \frac{1}{4\times 2 - 2\times 2}\begin{bmatrix} 2 & -2 \\ -2 & 4 \end{bmatrix}$$

$$\Rightarrow [H_1]^{-1} = \frac{1}{4}\begin{bmatrix} 2 & -2 \\ -2 & 4 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1 \end{bmatrix}.$$

Note: (INVERSE OF A MATRIX): For a given matrix A, if,

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \quad \text{where, } ad - bc \neq 0.$$

Then, $[A^{-1}]$ is,

$$\Rightarrow [A^{-1}] = \frac{1}{(ad-bc)} \times \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

iii) Step 3: Find ∇f_1 at the given initial point X_1 using the formula,

$$\Rightarrow \nabla f_1 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_1} = \begin{bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{bmatrix} \text{at} \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

iv) Step 4: Find the next iteration X_2 using the formula,

$$\Rightarrow X_2 = X_1 - ([H_1]^{-1}).\nabla f_1$$

$$\Rightarrow X_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

$$\Rightarrow X_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ -3/2 \end{bmatrix} = \begin{bmatrix} -1 \\ 3/2 \end{bmatrix}$$

v) Step 5: Find ∇f_2 at the point X_2.

$$\Rightarrow \nabla f_2 = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}_{X_2} = \begin{bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{bmatrix} \text{ at } \begin{bmatrix} -1 \\ 3/2 \end{bmatrix}$$

on solving,

$$\Rightarrow \nabla f_2 = \begin{bmatrix} 1 - 4 + 3 \\ -1 - 2 + 3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = X_1.$$

vi) Step 6: (If $\nabla f_2 \neq X_1$ or $\nabla f_2 \not\approx X_1$ then..)

Find the next iteration X_3, i.e., also ~~ca~~ find matrix $[H_2]$

$$X_3 = X_2 - [H_2]^{-1} \cdot \nabla f_2$$

* (General Formula): To find $(n+1)^{th}$ iteration we have,

$$X_{n+1} = X_n - [H_n]^{-1} \cdot \nabla f_n$$

vii) Step 7: (Continuation of Step-6;)

→ Find ∇f_3 at the point X_3. Then compare ∇f_3 with X_1, if approximately equal then stop at this iteration, and if not equal then repeat steps - 6 and 7 again...

∵ In this question, at step-5; $\nabla f_2 = X_1$, i.e., the minimum value of the function is X_2: $(-1, 1.5)$ and $\boxed{F_{min} = \cancel{1.75}}$ $\boxed{-1.25}$

4.3) Nelder-Mead Downhill Simplex Method :- (HARD).

(Nelder-Mead's Algorithm for Two Dimensions and Three Sides → A Triangle...)

- Nelder-Mead Method is a simplex method for finding a local minimum of a function of several variables.

→ Simplex : Elementary Geometrical figure formed in N Dimensions and has (N+1) sides.

For example,

1) A 2-simplex is a triangle (2 dimensions and 3 sides).
2) A 3-simplex is a tetrahedron (3 dimensions and 4 sides).

⊙ We will study this method only for a 2-simplex figure.

Goal: To find the local minima (minimum point) by,

1) Moving the Simplex towards the (local) minimum. (R/E).
2) Surrounding the minimum, then,
3) Contracting the Simplex around the minimum. (C/S)

- This procedure shall be repeated till an acceptable error (ϵ) has been reached.

- Four Searching Movements are involved, i.e.,

1) Reflection (R)
2) Expansion (E)
3) Contraction (C)
4) Shrinking (S).

★ Notations to be involved :-

1)	B	Best Vertex
2)	G	Good Vertex
3)	W	Worst Vertex
4)	R	Reflection Point
5)	E	Expanding Point
6)	C	Contraction Point
7)	S	Shrinking Point
8)	M	Mid-Point of $\overline{BG}$.
9)	C_1	Mid-Point of Contracting Point (C) of $\overline{WM}$.
10)	C_2	Mid-Point of Contracting Point (C) of $\overline{MR}$.

B, G, W → Vertices of the Triangle.

R, E, C, S → Searching Movements.

★ Working Procedure :-

Step 1: Consider initial triangle BGW and choose the three vertices : (x_K, y_K) where, K = 1, 2 and 3.

① $B = (x_1, y_1)$ (the best vertex)
② $G = (x_2, y_2)$ (the good vertex)
③ $W = (x_3, y_3)$ (the worst vertex).

⇒ To select which will be B or G or W vertex, use the relation,

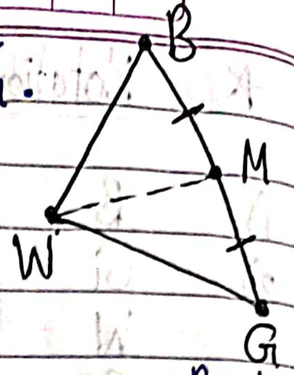
$$\boxed{f(B) \leq f(G) \leq f(W)} \quad \text{——— ①}$$

Example: Given, $f(x,y) = x + y$. And vertices of the triangle are $(0,0)$, $(2,3)$ and $(4,-1)$. Determine B, G & W?

Ans:
$$\left.\begin{aligned} f(0,0) &= 0+0 = 0 \longrightarrow B \\ f(2,3) &= 2+3 = 5 \longrightarrow W \\ f(4,-1) &= 4-1 = 3 \longrightarrow G \end{aligned}\right\} \text{Selected on the basis of relation - ①.}$$

$\therefore$ $B = (0,0)$, $G = (4,-1)$, $W = (2,3)$.

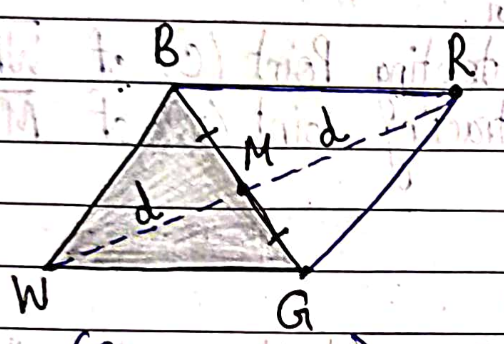
Step 2: Find the Mid-Point of the Good Side $\overline{BG}$.



$$\Rightarrow \boxed{M = \frac{B+G}{2}} = \left(\frac{x_1+x_2}{2}, \frac{y_1+y_2}{2}\right)$$

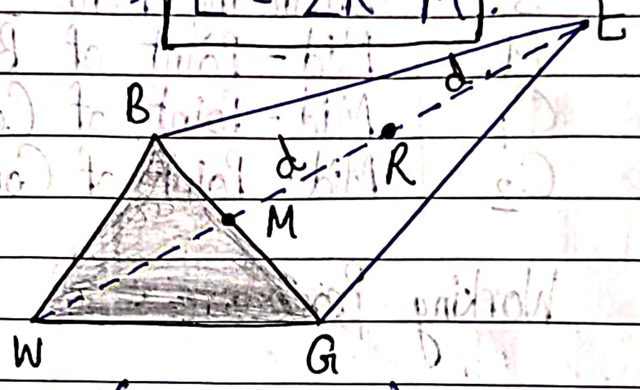
Step 3: Determine the Reflection Point (R) or Expansion Point (E) based on the conditions.. (discussed later)

$$\Rightarrow \boxed{R = 2M - W}$$



(REFLECTION)

$$\Rightarrow \boxed{E = 2R - M}$$



(EXPANSION)

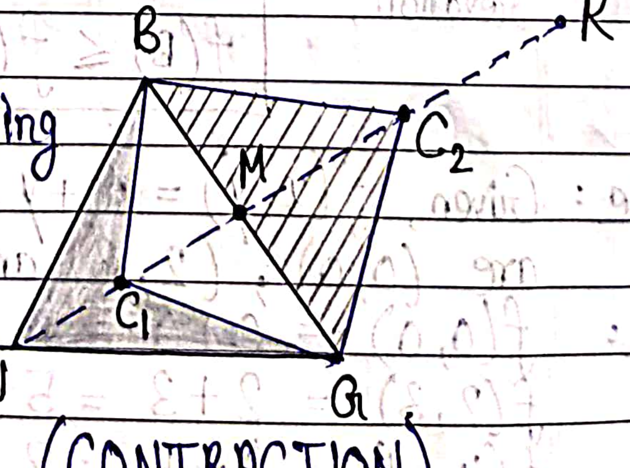
Step 4: Determine the Contraction Point (C).
There will be two contracting points, i.e.,

1). Contraction Point (C_1) lying between $\overline{WM}$.

$$\boxed{C_1 = \frac{W+M}{2}}$$

2) Contraction Point (C_2) lying between $\overline{MR}$.

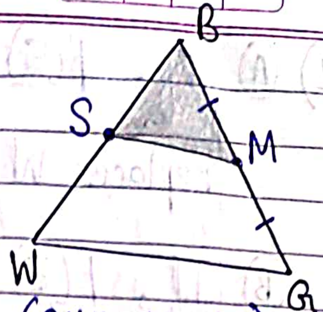
$$\boxed{C_2 = \frac{M+R}{2}}$$



(CONTRACTION)

Step 5: Determine the Shrinking Point (S).

⇒ $\boxed{S = \frac{B+W}{2}}$ (shrink towards B)



(SHRINKING).

★ BUT,
on what conditions will steps - 2, 3, 4 and 5 be applied and which point will we determined among R, E, C or S?

→ **Order of Procedure :-**

1) If, $f(R) < f(G)$, then the searching movement will be either Reflection (R) or Expansion / Extension (E), and CASE-1 shall be performed.

2) If, $f(R) \nless f(G)$, then the searching movement will be either Contraction (C) or Shrinking (S), and CASE-2 shall be performed.

Step Number	CASE-1	CASE-2
(1) Ⓐ	If, $f(B) < f(R)$ then, Replace W with R.*	If, $f(R) < f(W)$, then Replace W with R. AND, Compute C and $f(C)$, i.e., $C_1 = \frac{W+M}{2}$, $C_2 = \frac{M+R}{2}$ and, $f(C_1) = f(C_2) = f(C)$. Note: Use the new point W to find C_1 and further on..
Ⓑ	If, $f(B) \nless f(R)$ then, Compute $E = 2R-M$ and, evaluate $f(E)$.	
		If $f(R) \geq f(W)$ then Compute C and $f(C)$ directly. $C = C_1 = \frac{W+M}{2} = C_2 = \frac{M+R}{2}$

(2) (A)	If, $f(E) < f(B)$ then, Replace W with E.*	If, $f(C) < f(W)$ then, Replace W with C.*
(B)	If, $f(E) \nless f(B)$ then, Replace W with R.*	CONTINUED...
	– CASE (1) ENDS –	
(3)		If, $f(C) \nless f(W)$ then, find S, i.e., $S = \frac{B+W}{2}$ and $f(S)$. Replace W with S.* Replace G with M.*
		– CASE (2) ENDS –

Q.17) Using Nelder-Mead Downhill Simplex method, find the minimum value of the function : (upto 6 iterations).

$$f(x,y) = x^2 - 4x + y^2 - y - xy$$

Given vertices for the 2-D simplex as :

$V_1 = (0,0)$, $V_2 = (1.2, 0)$, $V_3 = (0, 0.8)$.

Ans : ① Iteration 1 : First find BGW triangle,

$\Rightarrow f(V_1) = f(0,0) = 0 \longrightarrow W$

$\Rightarrow f(V_2) = f(1.2, 0) = -3.36 \longrightarrow B$

$\Rightarrow f(V_3) = f(0, 0.8) = -0.16 \longrightarrow G$.

$\because$ The relation $f(B) < f(G) < f(W)$ should be satisfied.
So,
$$B = (1.2, 0), \; G = (0, 0.8), \; W = (0, 0).$$

$\rightarrow$ Now, finding mid-point (M) of $\overline{BG}$.

$$\Rightarrow M = \frac{B+G}{2} = \left(\cancel{\frac{1+2}{}}\frac{1.2+0}{2}, \frac{0+0.8}{2}\right) = (0.6, 0.4).$$

$\rightarrow$ Now, $R = 2M - W = 2(0.6, 0.4) - (0, 0)$.
$\Rightarrow R = (1.2, 0.8) - (0, 0)$.
So,
$$R = (1.2, 0.8)$$
$\Rightarrow f(R) = (1.2)^2 - 4(1.2) + (0.8)^2 - (0.8) - (1.2)(0.8)$
$\Rightarrow f(R) = -4.48$.

$\rightarrow$ Since, $f(R) = -4.48$ and, $f(G) = -0.16$
As, $\boxed{f(R) < f(G)}$, so CASE-1 will be followed.

$\rightarrow$ Now, $f(B) = -3.36 \nless f(R) = -4.48$. So, computing value of E,
$\Rightarrow E = 2R - M = 2(1.2, 0.8) - (0.6, 0.4)$
$\Rightarrow E = (2.4, 1.6) - (0.6, 0.4)$
$\Rightarrow E = (1.8, 1.2)$.
and
$f(E) = (1.8)^2 - 4(1.8) + (1.2)^2 - (1.2) - (1.8)(1.2)$
$f(E) = -4.68 - 1.2 = -5.88$.

$\rightarrow$ Now, $f(E) = \overset{-5.88}{\cancel{-4.68}} < f(B) = -3.36$, so replacing W with E, i.e.,
$$W = (1.8, 1.2).$$

② Iteration 2: Find BGW triangle again,

$\Rightarrow f(1.2, 0) = -3.36 \longrightarrow G$
$\Rightarrow f(0, 0.8) = -0.16 \longrightarrow W$
$\Rightarrow f(1.8, 1.2) = -5.88 \longrightarrow B$

$\because$ The relation $f(B) \le f(G) \le f(W)$ should be satisfied, so
$B = (1.8, 1.2) \quad G = (1.2, 0) \quad W = (0, 0.8)$

→ Now, mid-point (M) of line segment $\overline{BG}$.

$$\Rightarrow M = \frac{B+G}{2} = \left(\frac{1.8+1.2}{2}, \frac{1.2+0}{2}\right) = (1.5, 0.6)$$

→ Value of Reflextion Point (R),
$\Rightarrow R = 2M - W = 2(1.5, 0.6) - (0, 0.8) = (3, 0.4)$
and,
$\Rightarrow f(R) = (3)^2 - 4(3) + (0.4)^2 - (0.4) - (3)(0.4)$
$\therefore f(R) = -4.44$

$\because$ $\boxed{f(R) < f(G)}$, so CASE-1 will be followed.

i) Now, because $f(B) < f(R)$, so replacing W with R, i.e.,
$W = (3, 0.4)$.

ii) Since, $f(B) < f(R)$, so there was no expansion point (E) so, case-1 will end here and we move to the next iteration. (No Step-2 will be performed).

③ Iteration 3: Find BGW triangle again,

$\Rightarrow f(1.2, 0) = -3.36 \longrightarrow W$.

$\Rightarrow$ $f(3, 0.4) = -4.44 \longrightarrow G$
$\Rightarrow$ $f(1.8, 1.2) = -5.88 \longrightarrow B$

$\because$ The relation $f(B) \leq f(G) \leq f(W)$ should be satisfied, so
$B = (1.8, 1.2)$, $G = (3, 0.4)$, $W = (1.2, 0)$.

$\rightarrow$ Now, mid-point (M) of line segment $\overline{BG}$.

$\Rightarrow$ $M = \dfrac{B+G}{2} = \left(\dfrac{1.8+3}{2}, \dfrac{1.2+0.4}{2}\right) = (2.4, 0.8)$

$\rightarrow$ Value of Reflextion Point (R),
$\Rightarrow$ $R = 2M - W = 2(2.4, 0.8) - \cancel{(0, 0.8}\ (1.2, 0)$
$\Rightarrow$ $R = (4.8, 1.6) - (1.2, 0)$
$\therefore$ $R = (3.6, 1.6)$
and,
$\Rightarrow$ $f(R) = (3.6)^2 - 4(3.6) + (1.6)^2 - (1.6) - (3.6)(1.6)$
$\therefore$ $f(R) = -6.24$.

$\because$ $\boxed{f(R) < f(G)}$, so CASE-1 begins.

i) Now, because $f(B) \nless f(R)$ then, finding the expanding point (E) and $f(E)$.
$\Rightarrow$ $E = 2R - M = 2(3.6, 1.6) - (2.4, 0.8)$
$\Rightarrow$ $E = (4.8, 2.4)$
and,
$\Rightarrow$ $f(E) = -4.32$

ii) Now, because $f(E) \nless f(B)$ so, replacing W with R.
That is,
$$W = (3.6, 1.6)$$

④ Iteration 4: Find BGW triangle again.

⇒ $f(3.6, 1.6) = -6.24 \rightarrow B$
⇒ $f(3, 0.4) = -4.44 \rightarrow W$
⇒ $f(1.8, 1.2) = -5.88 \rightarrow G$

∵ The relation $f(B) \leq f(G) \leq f(W)$ should be satisfied so,
$B = (3.6, 1.6)$, $G = (1.8, 1.2)$, $W = (3, 0.4)$.

→ Mid-Point of line segment of $\overline{BG}$.
⇒ $M = \frac{B+G}{2} = \left(\frac{3.6+1.8}{2}, \frac{1.6+1.2}{2}\right) = (2.7, 1.4)$

→ Value of Reflextion Point (R),
⇒ $R = 2M - W = 2(2.7, 1.4) - (3, 0.4) = (2.4, 2.4)$
and,
⇒ $f(R) = (2.4)^2 - 4(2.4) + (2.4)^2 - (2.4) - (2.4)(2.4)$
∴ $f(R) = -6.24$.

∵ $\boxed{f(R) < f(G)}$, so CASE-1 begins.

i) ∵ Here, $f(B) = f(R) = -6.24$, but the condition was strictly for $f(B) < f(R)$ so, we can say;
$f(B) \nless f(R)$
We will find E and f(E).
⇒ $E = 2R - M = 2(2.4, 2.4) - (2.7, 1.4)$
∴ $E = (2.1, 3.4)$
and,
→ $f(E) = -2.97$

ii) ∵ $f(E) \nless f(B)$ $[-2.97 \nless -6.24]$, so replacing W with R.

$$W = (2.4, 2.4).$$

(5) Iteration 5: Find BGW triangle again with new vertices,

$\Rightarrow$ $f(3.6, 1.6) = -6.24 \longrightarrow B$
$\Rightarrow$ $f(2.4, 2.4) = -6.24 \longrightarrow G$
$\Rightarrow$ $f(1.8, 1.2) = -5.88 \longrightarrow W$

$\because$ The relation $f(B) \le f(G) \le f(W)$ should be satisfied,
$B = (3.6, 1.6)$ $G = (2.4, 2.4)$ $W = (1.8, 1.2)$.

$\rightarrow$ Mid-Point (M) of $\overline{BG}$.

$\Rightarrow$ $M = \frac{B+G}{2} = \left(\frac{3.6+2.4}{2}, \frac{1.6+2.4}{2}\right) = (3, 2)$

$\rightarrow$ Values of (R) and f(R).

$\Rightarrow$ $R = 2M - W = 2(3, 2) - (1.8, 1.2) = (4.2, 2.8)$

and,

$\Rightarrow$ $f(R) = -5.88$

$\because$ $\boxed{f(R) \not< f(G)}$, so CASE-2 begins.

i) Since, $f(R) \le f(W)$, i.e., $-5.88 = -5.88 = f(R) = f(W)$
Now, computing the Contraction Point (C), i.e.,

$\Rightarrow$ $C_1 = \frac{W+M}{2} = \left(\frac{1.8+3}{2}, \frac{1.2+2}{2}\right) = (2.4, 1.6)$

and,

$\Rightarrow$ $C_2 = \frac{M+R}{2} = \left(\frac{3+4.2}{2}, \frac{2+2.8}{2}\right) = (3.6, 2.4)$

and,

$\rightarrow$ $f(C_1) = f(C_2) = -6.72$ (On solving..)

Both have the same value. So,

$$C = (2.4, 1.6)$$
$$f(C) = -6.72$$

ii) Now, because $f(C) < f(W)$, so replace W with C.

$$W = (2.4, 1.6).$$

⑥ Iteration 6: Find BGW triangle again,

$f(3.6, 1.6) = -6.24 \longrightarrow G$
$f(2.4, 2.4) = -6.24 \longrightarrow W$
$f(2.4, 1.6) = -6.72 \longrightarrow B$

$\because$ The relation $f(B) \leq f(G) \leq f(W)$ should be satisfied so,
$B = (2.4, 1.6)$, $G = (3.6, 1.6)$, $W = (2.4, 2.4)$

→ Mid-point (M) of $\overline{BG}$,

$\Rightarrow M = \dfrac{B+G}{2} = \left(\dfrac{2.4+3.6}{2}, \dfrac{1.6+1.6}{2}\right) = (3, 1.6)$

→ Value of Reflection Point (R) and f(R),

$\Rightarrow R = 2M - W = 2(3, 1.6) - (2.4, 2.4) = (3.6, 0.8)$

and,

$\Rightarrow f(R) = -4.48$

$\because f(R) \nless f(G)$, so CASE-2 begins.

i) Since, $f(R) \nless f(W)$, i.e., $-4.48 \nless -6.24$.
so, computing value of $f(C)$, i.e.,

$\Rightarrow C_2 = C = \dfrac{M+R}{2} = \left(\dfrac{3+3.6}{2}, \dfrac{1.6+0.8}{2}\right)$

$\therefore C = (3.3, 1.2)$

Note :
- In the question it will be specified as which value of C we have to assume either C_1 or C_2 throughout the whole process (procedure).
- If NOT mentioned, then assume C to be either C_1 or C_2 and solve the question throughout based on this assumption and then apply the further conditions.

⇒ Now, $f(C) = f(C_2) = -6.03$

and,

$f(W) = -6.24$.

ii) Since, $f(C) \nless f(W)$. So, we have to find the Shrinking Point (S) and f(S).

$$\Rightarrow S = \frac{B+W}{2} = \left(\frac{2.4+2.4}{2}, \frac{1.6+2.4}{2}\right) = (2.4, 2)$$

and,

$$\Rightarrow f(S) = (2.4)^2 - 4(2.4) + (2)^2 - (2) - (2.4)(2)$$

$$\Rightarrow f(S) = -6.64.$$

→ Further, Replacing W with S and G with M, i.e.,

updated Values → $B = (2.4, 1.6)$, $G = (3, 1.6)$, $\cancel{M}\ W = (2.4, 2)$.

Now, $f(2.4, 1.6) = -6.72 \longrightarrow G$

$f(3, 1.6) = -6.84 \longrightarrow B$

$f(2.4, 2) = -6.64 \longrightarrow W$.

ANSWER:

∴ Stopping the iteration here, so new vertices are:

$B = (3, 1.6)$, $G = (2.4, 1.6)$, $W = (2.4, 2)$.

→ The value of F_{min} upto 6 iterations is : $\boxed{-6.84}$ at B.

5) Rolle's Theorem and Mean Value Theorem :-

5.1) Rolle's Theorem :-

→ Let $f(x)$ be a function defined on $[a, b]$ such that,

① $f(x)$ is a continous function on $[a, b]$
② $f(x)$ is a differentiable function on (a, b).
③ $f(a) = f(b)$.

Then for a real number, $c \in (a, b)$ we have,

$$\boxed{f'(c) = 0}$$

5.2) Mean Value Theorem :-

Let $f(x)$ be a function defined on $[a, b]$ such that,

① $f(x)$ is a continous function on $[a, b]$.
② $f(x)$ is a differentiable function on (a, b).

Then, there exists some $c \in (a, b)$ such that,

$$\boxed{f'(c) = \frac{f(b) - f(a)}{b - a}}$$

Example: Verify Rolle's Theorem in $[-1, 1]$ for the function :
$f(x) = x^2$.

Ans: ⇒ $f(a) = f(b)$ $\quad (\exists\ a = -1\ \forall\ b = 1)$
⇒ $f(-1) = f(1)$
⇒ $(-1)^2 = (1)^2$
⇒ $1 = 1$ ⇒ LHS = RHS

also, given $f(x)$ is both continous and differentiable on $[-1, 1]$

→ For a real number, $c \in (-1, 1)$ we have,

⇒ $f'(c) = 0$

⇒ $\frac{d}{dc}[f(c)] = 0$ ⇒ $\frac{d}{dc}[c^2] = 0$

⇒ $2c = 0$

∴ $\boxed{c = 0}$ ⇒ $\boxed{c \in (-1, 1)}$

∴ Rolle's Theorem is verified for the given function.

Q.18) Verify Rolle's Theorem and Mean Value Theorem for the given function in the interval $[-3, 0]$.

$$f(x) = x(x+3)e^{\frac{-x}{2}} \quad \text{~~(IF POSSIBLE)~~}.$$

Ans: ① **Rolle's Theorem:**

i) We have, $a = -3$ and $b = 0$ for interval $[-3, 0]$. So,

⇒ $f(a) = f(b)$

⇒ $f(-3) = f(0)$

⇒ $(-3)(-3+3) \times \exp\left(\frac{+3}{2}\right) = (0)(0+3) \times \exp\left(\frac{-0}{2}\right)$.

⇒ $\boxed{0 = 0}$ ∴ LHS = RHS

Now,

ii) For a real number, $c \in (a, b)$ we have,

⇒ $f'(c) = 0$ or, $\frac{d}{dc}[f(c)] = 0$

⇒ $\frac{d}{dc}\left(c(c+3)\exp\left(\frac{-c}{2}\right)\right) = 0$.

⇒ $\frac{d}{dc}\left[(c^2+3c) \cdot e^{\frac{-c}{2}}\right] = 0$

$$\Rightarrow (2c+3)e^{\frac{-c}{2}} + (c^2+3c)\left(\frac{-1}{2}\right)e^{\frac{-c}{2}} = 0$$

$$\Rightarrow e^{\frac{-c}{2}}(4c+6-c^2-3c) = 0$$

$$\Rightarrow e^{\frac{-c}{2}}(c^2-c-6) = 0$$

$\because$ e^x is never equal to zero and graphically also, it always tend to zero. So,

$$e^{\frac{-c}{2}} \neq 0 \qquad \text{(Case Rejected)}$$

But,

$$\Rightarrow c^2-c-6 = 0$$

$$\Rightarrow \boxed{c = -2}$$

($c = 3$ rejected since it lies outside the interval $[-3, 0]$).

$\therefore$ For a real number, $\boxed{c = -2}$, $c \in (-3, 0)$ we have

$$\boxed{f'(-2) = 0}$$

hence,

Rolle's Theorem is verified.

② Mean Value Theorem :

$\rightarrow$ Since, $f(x)$ is already continous and differentiable for the interval $(-3, 0)$. So, there exists some $c \in (a, b)$ such that,

$$f'(c) = \frac{f(b) - f(a)}{b - a}$$

So,

$a = -3$, $f(a) = 0$.

$b = 0$, $f(b) = 0$

i.e.,

$$\Rightarrow \quad f'(c) = \frac{0-0}{0-(-3)} = 0.$$

$$\therefore \boxed{f'(c) = 0}$$

→ Same Condition as Rolle's theorem.

Hence, the value of c will be same again, i.e.,

$$\boxed{c = -2}$$

$\therefore$ Mean Value Theorem is also verified.

Note: Logically, if Rolle's Theorem is verified then MVT is automatically also verified or vice-versa.

—x—

Question) Using Newton-Raphson Method, find the root of the equation $f(x) = x\sin x + \cos x = 0$ which is near $x = \pi$ correct to three decimal places?
(DIY) (ET 2018, 6.5 marks)

Answer: