Root Finding of Non-Linear Equations:

→ For powers of x which are low, we can easily find the root using approaches like:

eg $f(x) = x^2 - 2x = 0$

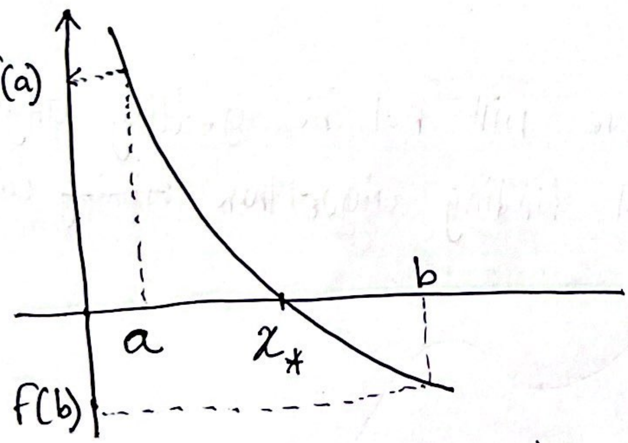
$\Rightarrow x(x-2) = 0$

$x = 2, \ x = 0$

→ But what if we are dealing with non-linear equations with high powers/ series/ polynomials/ rational functions? How can we find their root?

↳ We can apply some iterative algorithms to find the roots.

Bisection Root Finding Algorithm:



→ If root exists, the ~~graph~~ value of the function changes sign.

Here, $f(a) = +ve$, $f(b) = -ve$ } Roots lies within $[a, b]$ ~~changes~~ Therefore it changes sign

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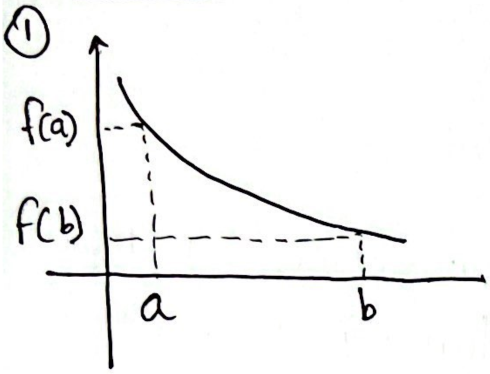
So, if $\boxed{f(a) * f(b) < 0}$ root exists between a and b.

Examples:

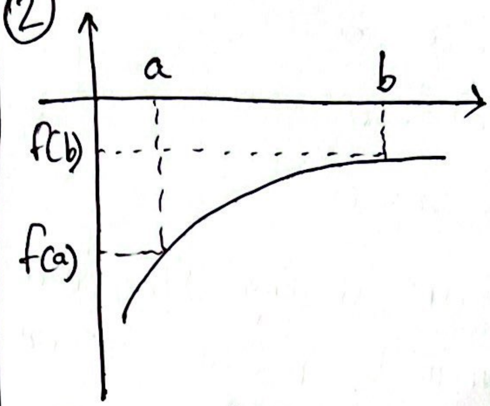
①



$f(a) * f(b)$
$= (+ve) * (+ve)$
$= (+ve)$
> 0

Root does not exist

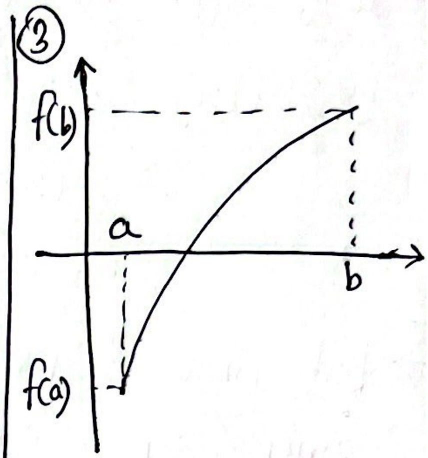
②



$f(a) * f(b)$
$= (-ve) * (-ve)$
$= (+ve)$
> 0

Root does not exit

③



$f(a) * f(b)$
$= (-ve) * (+ve)$
$= (-ve)$
< 0

Root exists

For example ① and ②, we will not be getting any roots if we apply ~~the~~ any root finding algorithm ~~withing~~ within the interval [a, b].

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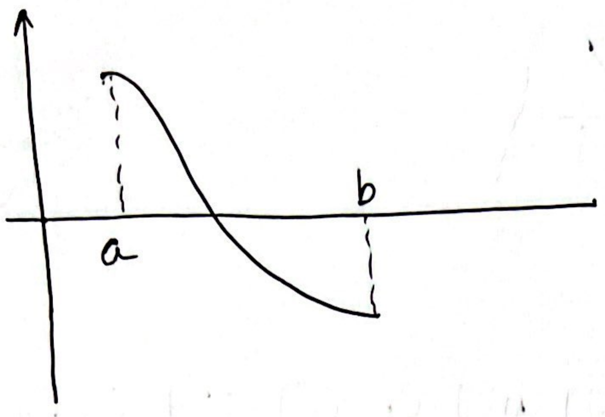
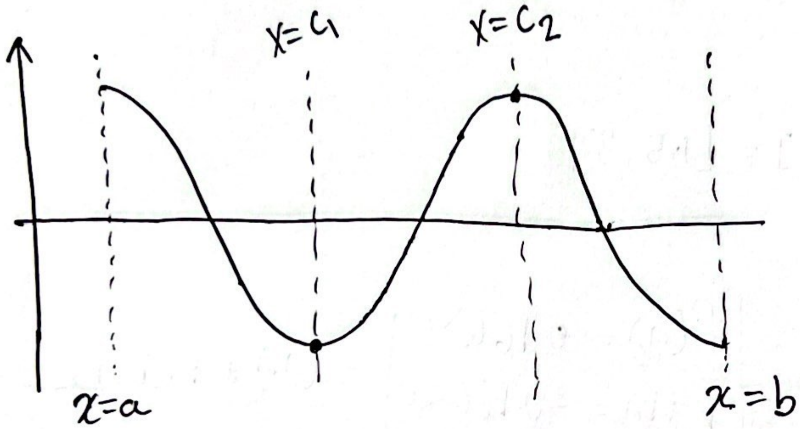
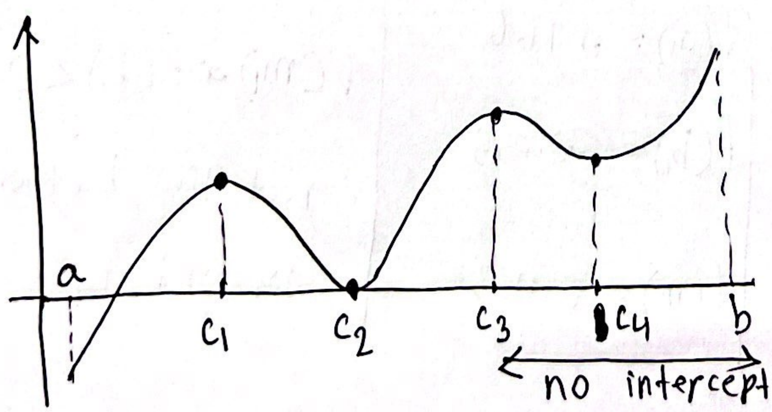
How to choose the right intervals :



$[a, b] \rightarrow$



$[a, b] = [a, c_1] \cup [c_1, c_2] \cup [c_2, b]$



no intercept here, therefore can avoid.

$[a, b] = [a, c_1] \cup [c_1, c_2] \cup [c_2, c_3]$

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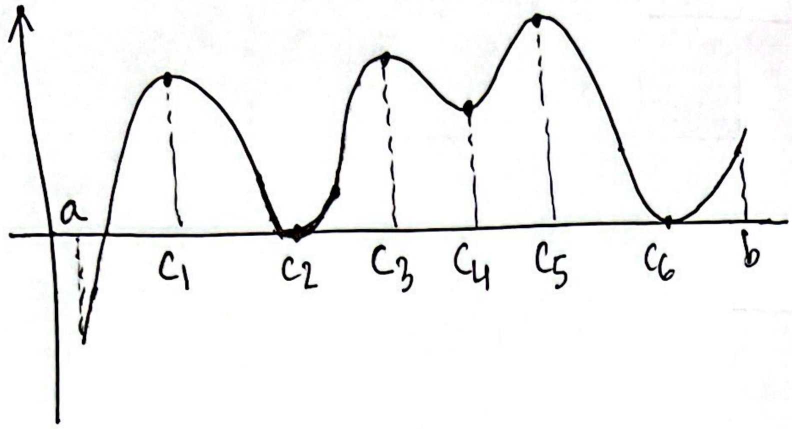

$[a,b] = [a,c_1] \cup [c_1,c_2] \cup [c_2,c_3] \cup [c_5,c_6] \cup [c_6,b]$

Bisection Method:

$f(x) = \frac{1}{x} - 0.5 \qquad I = [1.5, 3]$

$a_0 = 1.5$

$b_0 = 3$

$m_0 = \frac{a_0+b_0}{2} = \frac{1.5+3}{2} = 2.25$

$f(a_0) = 0.166 > 0$

$f(b_0) = -0.166 < 0$

$f(m_0) = -0.055 < 0$

$f(a_0) * f(m_0) < 0$

$\therefore$ root lies ~~beet~~ between a_0 and m_0

$a_1 = a_0 = 1.5$

$b_1 = m_0 = 2.25$

$m_1 = \frac{a_1+b_1}{2} = \frac{1.5+2.25}{2} = 1.875$

$f(a_1) = 0.166$

$f(b_1) = -0.055$

$f(m_1) = 0.033$

$f(m_1) * f(b_1) < 0$

$\therefore$ root lies beetween m_1 and b_1

$\vdots$

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Example

Use Bisection method to find solutions accurate within 10^{-3} for $f(x) = x^3 - 7x^2 + 14x - 6 = 0$ on interval $[1, 3.2]$

k	a_k	m_k	b_k	$f(a_k)$	$f(m_k)$	$f(b_k)$	$x_* \in [\ ,\ ]$
0	1	2.1	3.2	2	1.79	-0.11	[2.1, 3.2]
1	2.1	2.65	3.2	1.79	0.55	-0.11	[2.65, 3.2]
2	2.65	2.925	3.2	0.55	0.086	-0.11	[2.925, 3.2]
3	2.925	3.0625	3.2	0.86	-0.054	-0.11	[2.925, 3.0625]
⋮							
9	2.998	3.000195	3.002	1.96×10^{-3}	$\boxed{-1.95 \times 10^{-4}}$ $< 10^{-3}$	-2.3×10^{-3}	

$X_* = 3.\underbrace{000}$

Take upto 3 d.p. since error bound is 10^{-3}.

Finding number of iterations to find root :

Things that will be provided in the question:

1. interval, eg: [1.5, 3]
2. Machine epsilon / error/ accuracy, eg: 1.1×10^{-16}
   bound

Formula:

$$n \geq \frac{\log(|b-a|) - \log(\epsilon)}{\log(2)} - 1$$

put −1 if question specifies Machine epsilon or error. If question specifies accuracy, then do not put −1.

Example

interval = [1.5, 3]

$\epsilon_M = 1.1 \times 10^{-6}$

Find minimum amount of iteration required to find the root with the error bound of the machine epsilon.

Solution

$$n \geq \frac{\log|3-1.5| - \log(1.1 \times 10^{-16})}{\log(2)} - 1$$

≥ 52.59

≥ 53

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Fixed Point Iteration:

→ We want to solve $f(x)=0$

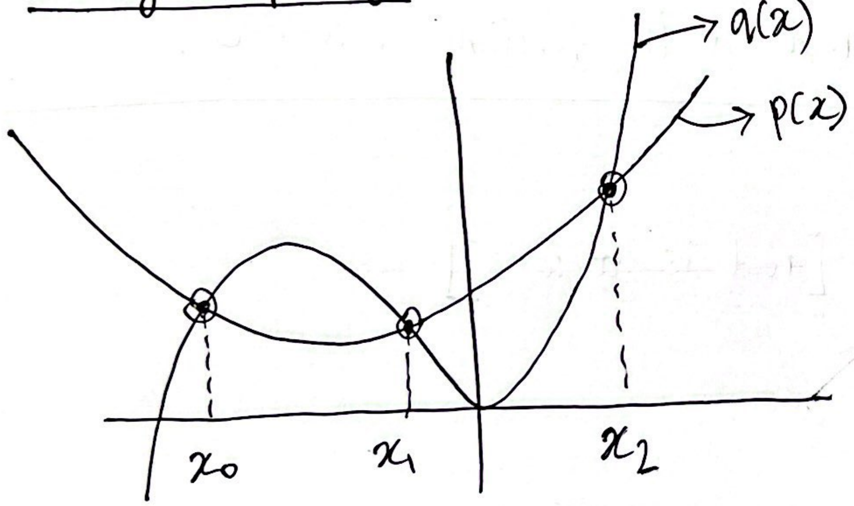
→ Need to transform $f(x)=0$ into a new form

→ convert $f(x)=0$ into $\boxed{g(x)=x}$

Algebra Recap:

$$\underbrace{x^2+5x+7}_{p(x)} = \underbrace{x^3+3x^2}_{q(x)} \longrightarrow \underbrace{x^3+2x^2-5x-7}_{f(x)}$$

Solving Graphically:



x_0, x_1, x_2 are the roots of the function $f(x)$

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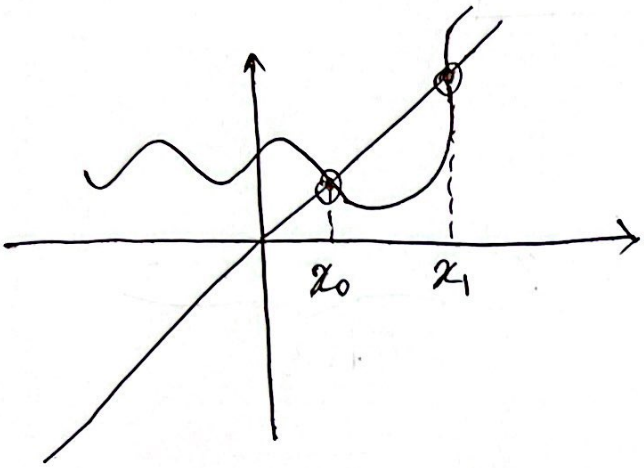
→ Now imagine we have a function $f(x)=0$

→ Convert the function $f(x)=0$ into $g(x)=x$

→ The intersection of $g(x)=x$ should give the root of the function $f(x)=0$.



x_0, x_1 should be the root of the function $f(x)=0$.

Example:

$f(x) = -\frac{1}{2}x + 1 = 0$ [root is at $x=2$]

$$\underbrace{\frac{x+2}{2}}_{g(x)} = \underbrace{x}_{x}$$

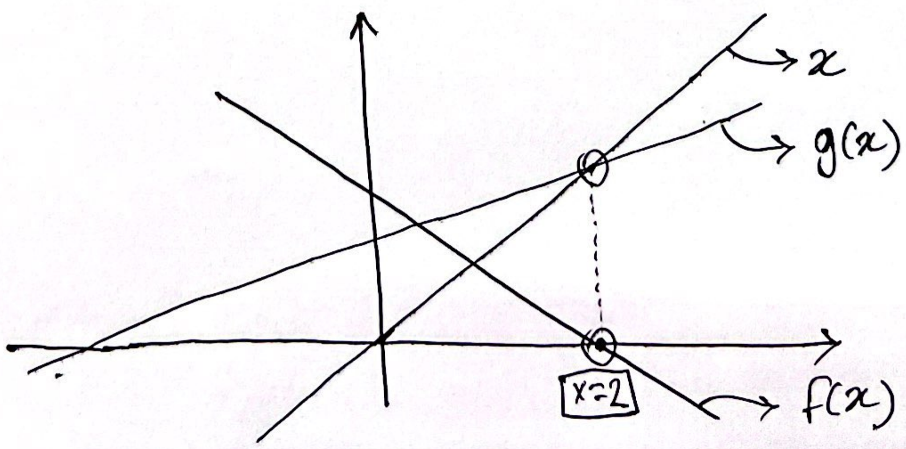
Solving numerically:

$\frac{x+2}{2} = x$

$x+2 = 2x$

$\boxed{x=2}$

Solving Graphically:



Converting $f(x)=0$ into $g(x)=x$:

$f(x) = x^2 - 2x - 3 = 0$

[Roots are at $x = -1, 3$]
[Found using middle term, or quadratic root finding formula]

$\boxed{\text{make } x \text{ the subject}}$

① $x^2 - 2x - 3 = 0$

$x^2 = 2x + 3$

$\underbrace{x}_{x} = \underbrace{\sqrt{2x+3}}_{g(x)}$

② $x^2 - 2x - 3 = 0$

$\Rightarrow x(x-2) - 3 = 0$

$\Rightarrow \underbrace{x}_{x} = \underbrace{\dfrac{3}{x-2}}_{g(x)}$

③ $x^2 - 2x - 3 = 0$

$\Rightarrow x^2 - x - x - 3 = 0$

$\Rightarrow \underbrace{x}_{x} = \underbrace{x^2 - x - 3}_{g(x)}$

④ $x^2 - 2x - 3 = 0$

$\Rightarrow 2x^2 - 2x = x^2 + 3$

$\Rightarrow x(2x-2) = x^2 + 3$

$\Rightarrow \underbrace{x}_{x} = \underbrace{\dfrac{x^2+3}{2x-2}}_{g(x)}$

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Root Finding Formula:

$$\boxed{g(x_k) = x_{k+1}}$$

① $g(x) = \sqrt{2x+3}$, $x_0 = 0$

$g(0) = 1.73$
$g(1.73) = 2.54$
$g(2.54) = 2.84$
$g(2.84) = 2.95$
$g(2.95) = 2.98$
$g(2.98) = 2.99$
$g(2.99) = 3$
$g(3) = 3 \longrightarrow$ Fixed point reached.

② $g(x) = x^2 - x - 3$, $x_0 = 0$

$g(0) = -3$
$g(-3) = 9$
$g(9) = 69$ } Diverges
⋮

③ $g(x) = \dfrac{x^2+3}{2x-2}$, $x_0 = 0$

$g(0) = -1.5$
$g(-1.5) = -1.05$
$g(-1.05) = -1$
$g(-1) = -1 \longrightarrow$ Fixed point reached.

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2 Questions to answer:

① At which root will it converge to?

→ It will depend on the initial choice of x_0

→ It will also depend on the value of the converging rate, λ.

② Which form of $g(x)$ is convergent?

→ It will depend on the value of the converging rate, λ.

Elaborating the first Q/A:

① $g(x) = \sqrt{2x+3}$, $x_0 = 0$

$g(0) = 1.73$
$g(1.73) = 2.54$
$g(2.54) = 2.84$
$g(2.84) = 2.95$
$g(2.95) = 2.98$
$g(2.98) = 2.99$
$g(2.99) = 3.00$
$g(3) = 3$

$g(x) = \sqrt{2x+3}$, $x_0 = 42$

$g(42) = 9.33$
$g(9.33) = 4.65$
$g(4.65) = 3.51$
$g(3.51) = 3.17$
$g(3.17) = 3.06$
$g(3.06) = 3.02$
$g(3.02) = 3.01$
$g(3.01) = 3$
$g(3) = 3$

→ Both $x_0 = 0$ & $x_0 = 42$ converges to the root, $x_* = 3$.
→ Even though $x_0 = 0$ is closer to $x_* = -1$, it converges to $x_* = 3$.

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② $g(x) = x^2 - x - 3, \quad x_0 = 0$

$g(0) = -3$

$g(-3) = 9$

$g(9) = 69$

$g(69) = 4.69 \times 10^3$

$\left.\begin{matrix} \vdots \\ \vdots \end{matrix}\right\}$ diverges

$g(x) = x^2 - x - 3, \quad x_0 = 42$

$g(42) = 1.72 \times 10^3$

$g(1.72 \times 10^3) = 2.95 \times 10^6$

$g(2.95 \times 10^6) = 8.72 \times 10^{12}$

$\left.\begin{matrix} \vdots \\ \vdots \end{matrix}\right\}$ Diverges

→ Both $x_0 = 0$ and $x_0 = 42$ diverges rapidly.

③ $g(x) = \dfrac{x^2+3}{2x-2}, \quad x_0 = 0$

$g(0) = -1.5$

$g(-1.5) = -1.05$

$g(-1.05) = -1$

$g(-1) = -1$

$g(x) = \dfrac{x^2+3}{2x-2}, \quad x_0 = 42$

$g(42) = 21.6$

$g(21.6) = 11.4$

$g(11.4) = 6.39$

$g(6.39) = 4.07$

$g(4.07) = 3.19$

$g(3.19) = 3.01$

$g(3.01) = 3$

$g(3) = 3$

→ $x_0 = 0$ and $x_0 = 42$ converges to 2 different roots.

→ $x_0 = 0$ converges to the nearest root, which is -1, and $x_0 = 42$ converges to the nearest root, which is 3. (42 is closer to 3 than -1).

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Contraction Mapping Theory:

Find $g'(x)$

Find $g'(\text{root}-1)$

Find $g'(\text{root}-2)$

if $|g'(\text{root})| < 1$, $g(x)$ will be convergent.

$\lambda = |g'(\text{root})|$

$\uparrow$ converging rate

---

① $g(x) = \sqrt{2x+3} = (2x+3)^{\frac{1}{2}}$

$g'(x) = \frac{1}{\cancel{2}}(2x+3)^{-\frac{1}{2}}\cancel{(2)}$

$= (2x+3)^{-\frac{1}{2}}$

$= \frac{1}{\sqrt{2x+3}}$

$\lambda = |g'(-1)| = 1$ (not <1)

$\lambda = |g'(3)| = \frac{1}{3}$ (<1)

$\therefore$ both $x_0 = 0$, $x_0 = 42$ converges to the root $x_* = 3$.

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② $g(x) = x^2 - x - 3$

$g'(x) = 2x - 1$

$\lambda = |g'(-1)| = |-3| = 3$ (not <1)

$\lambda = |g'(3)| = 5$ (not <1)

$\therefore$ no choices of x_0 will converge to any root. It will all diverge.

③ $g(x) = \dfrac{x^2+3}{2x-2}$

$\lambda = |g'(-1)| = 0$ (<1)

$\lambda = |g'(3)| = 0$ (<1)

$\therefore$ will converge to both $x_* = -1$ & 3.

Since $x_0 = 0$ is closer to -1, it will converge to -1.

$x_0 = 42$ is closer to 3, it will converge to 3.

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Example:

$$f(x) = x^3 - 2x^2 - x + 2$$

(a) State the roots of the function $f(x)$

(b) Construct 3 different fixed point function $g(x)$ such that $f(x)=0$

(c) Find the converging rate of $g(x)$ and which root it will converge to.

Solution:

(a) $f(x) = x^3 - 2x^2 - x + 2 = 0$

$\Rightarrow x^2(x-2) - 1(x-2) = 0$

$\Rightarrow (x^2-1)(x-2) = 0$

$x_* = +1$

-1

$+2$

(b) (i) $x^3 - 2x^2 - x + 2 = 0$

$$x = \underbrace{x^3 - 2x^2 + 2}_{g(x)}$$

(ii) $x^3 - 2x^2 - x + 2 = 0$

$\Rightarrow x(x^2 - 2x - 1) = -2$

$\Rightarrow x = \dfrac{-2}{x^2 - 2x - 1}$

(iii) $x^3 - 2x^2 - x + 2 = 0$

$\Rightarrow 2x^2 = x^3 - x + 2$

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

$$\Rightarrow \underbrace{x}_{x} = \underbrace{\frac{1}{\sqrt{2}}\sqrt{x^3 - x + 2}}_{g(x)}$$

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(C) (i) $g(x) = x^3 - 2x^2 + 2$

$g'(x) = 3x^2 - 4x$

$$\lambda = |g'(x_*)| = \left\{\begin{array}{ll} 7 & \text{at } x_* = -1 \\ 1 & \text{at } x_* = 1 \\ 4 & \text{at } x_* = 2 \end{array}\right\} \text{Divergent}$$

(ii) $g(x) = \dfrac{-2}{x^2 - 2x - 1}$

$g'(x) = \dfrac{4(x-1)}{(x^2 - 2x - 1)^2}$

$$\lambda = |g'(x_*)| = \begin{cases} 2 & \text{at } x_* = -1 \\ 0 & \text{at } x_* = 1 \\ 4 & \text{at } x_* = 2 \end{cases}$$

$\therefore$ $g(x)$ will converge to $x_* = 1$

(iii) $g(x) = \frac{1}{\sqrt{2}} (x^3 - x + 2)^{\frac{1}{2}}$

$g'(x) = \dfrac{3x^2 - 1}{2\sqrt{2}\,(x^3 - x + 2)^{1/2}}$

$$\lambda = |g'(x_*)| = \begin{cases} 0.5 & \text{when } x_* = -1 \\ 0.5 & \text{when } x_* = 1 \\ 1.375 & \text{when } x_* = 2 \end{cases}$$

$\therefore$ $g(x)$ will converge to $x_* = -1$ & 1.

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Order of convergence:

① $\lambda = 0 \rightarrow$ Super linear convergence
- → fastest convergence
- → less iterations required to converge.

② $0 < \lambda < 1 \rightarrow$ linear convergence
- → will converge
- → But not as fast as $\lambda = 0$.

③ $\lambda = 1 \rightarrow$ ignore

④ $\lambda > 1 \rightarrow$ Diverge.

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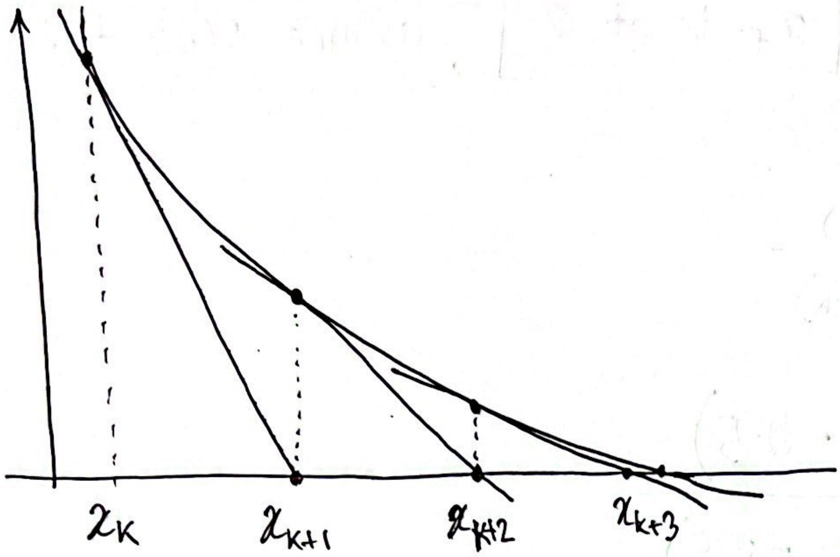
Newton's Method:



Slope of the tangent line:

$$\text{slope} = \frac{f(x_{k+1}) - f(x_k)}{x_{k+1} - x_k} = \frac{-f(x_k)}{x_{k+1} - x_k} \quad \text{—— (I)}$$

$$\text{slope} = f'(x_k) \quad \text{—— (II)}$$

Equating the two equations

$$f'(x) = \frac{-f(x_k)}{x_{k+1} - x_k}$$

$$\boxed{x_{k+1} = \underbrace{x_k - \frac{f(x_k)}{f'(x_k)}}_{g(x)}}$$

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Example:

$f(x) = \frac{1}{x} - 0.5$ $[x_* \text{ is at } 2]$, assume $x_0 = 1$.

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

$$= x_k - \frac{\left(\frac{1}{x_k} - 0.5\right)}{\frac{d}{dx}\left(\frac{1}{x_k} - 0.5\right)}$$

$$x_{k+1} = 2x_k - 0.5x_k^2$$

k	x_k
0	1
1	1.5
2	1.875
3	1.9921875
4	1.999969482
5	2
6	2

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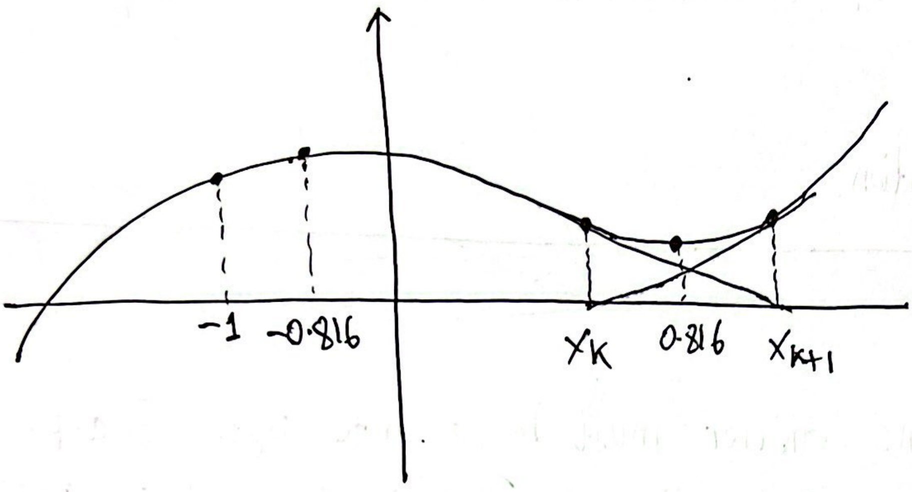
Newton's Method will not work if there is a turning point between x_k and x_{k+1}.

Example:



Lets say the above function is $f(x) = x^3 - 2x + 2$

Finding the turning points:

$$f'(x) = 3x^2 - 2 = 0$$

$$\Rightarrow x = \pm\sqrt{\frac{2}{3}}$$

$$= \pm 0.816$$

Make sure $x_0 < -0.816$

Example, $x_0 = -1$.

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Example:

$$f(x) = x^2 - 2xe^{-x} + e^{-2x}, \quad x_0 = 1$$

Find the solution of this function within 10^{-5} using

a) Newton's Method

b) Aitken Acceleration.

Note:

0.00001

→ Within 10^{-5} means answer must be accurate upto 5 d.p.
[Calculate answers upto 6 dp, then round upto 5 dp at the last]

→ In the above question, what should we compare our answers to? Should we compare our answers to $f(x)=0$ or compare our answer to the actual root, x_*?

→ If we compare to $f(x)=0$, we will reach our answer when $f(x_k) < 0.00001$, where k is the iteration number.

→ If we compare to the actual root, x_*, we will reach our answer when $|x_* - x_k| < 0.00001$.

→ This means that we compare to $f(x)=0$ when x_* is not given, or x_* cannot be found numerically.

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Solution:

$$f(x) = x^2 - 2xe^{-x} + e^{-2x}$$

$$f'(x) = 2x - 2e^{-x} - 2x(-e^{-x}) - 2e^{-2x}$$

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

$$= x_k - \frac{x_k^2 - 2x_k e^{-x_k} + e^{-2x_k}}{2x_k - 2e^{-x_k} + 2x_k e^{-x_k} - 2e^{-2x_k}}$$

K	x_k	$f(x_k)$	if $\lvert f(x_k) \rvert < 0.0001$?
0	1 $\xrightarrow{\text{put } f(1)}$ ↓ put (1) in iteration formula	0.399576	NO
1	0.768941	0.093292	NO
2	0.664590	0.022532	NO
3	0.615033	0.005537	NO
4	0.590884	0.00137	NO
5	0.578963	0.000342	NO
6	0.573041	0.000085	NO
7	0.570089	2×10^{-5}	NO
8	0.568615	0.5×10^{-5}	Yes

Answer: $x_* = 0.56862$ (upto 5 d.p)

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Aitken Acceleration:

→ Used to accelerate convergence

Formula:

$$\boxed{\hat{x}_{k+2} = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k}}$$

→ starting from x_0, every 2 iteration acceleration occurs.
eg: $x_2, x_4, x_6 \ldots$

$$x_0 \to x_1 \to x_2 \to \hat{x}_2 \to x_3 \to x_4 \to \hat{x}_4 \to x_5 \to x_6 \to \hat{x}_6$$

Example:

$f(x) = \frac{1}{x} - 0.5$ [x_* is at 2]

→ construct a $g(x)$ so that $x=2$ is a fixed point of $g(x)$.

$$g(x) = x + \frac{1}{16}\left(\frac{1}{x} - 0.5\right)$$

$$g(2) = 2$$

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$$g'(x) = 1 + \frac{1}{16}\left(-\frac{1}{x^2}\right)$$

$$\lambda = \left|g'(2)\right| = 1 + \frac{1}{16}\left(-\frac{1}{2^2}\right) = 0.984375 \quad (<1)$$

→ λ is close to 1. It will converge, but it will be very slow.

→ lets start using $x_0 = 1.5$, keeping the calculations upto 7 s.f.

$$g(x) = x + \frac{1}{16}\left(\frac{1}{x} - 0.5\right), \quad x_0 = 1.5$$

$x_0 = 1.5$

$x_1 = g(x_0) = 1.510417$

$x_2 = g(x_1) = 1.520546$

$x_3 = g(x_2) = 1.530400$

$x_4 = g(x_3) =$

$\vdots$

$x_{818} = g(x_{817}) = 1.999999$

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Now, Applying Aitken Acceleration:

$$\hat{x}_{k+2} = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k}$$

$$x_0 \rightarrow x_1 \rightarrow x_2 \xrightarrow{\text{Accelerate}} \hat{x}_2 \rightarrow x_3 \rightarrow x_4 \xrightarrow{\text{Accelerate}} \hat{x}_4 \rightarrow x_5 \rightarrow x_6$$

$$x_6 \xrightarrow{\text{Accelerate}} \hat{x}_6$$

$$\hat{x}_8 \xleftarrow{\text{Accelerate}} x_8 \leftarrow x_7 \leftarrow \hat{x}_6$$

$x_0 = 1.5$

$x_1 = g(x_0) = 1.510417$

$x_2 = g(x_1) = 1.520546$

$$\hat{x}_2 = x_0 - \frac{(x_1 - x_0)^2}{x_2 - 2x_1 + x_0} = 1.877604$$

$x_3 = g(\hat{x}_2) = 1.879641$

$x_4 = g(x_3) = 1.881642$

$$\hat{x}_4 = \hat{x}_2 - \frac{(x_3 - \hat{x}_2)^2}{x_4 - 2x_3 + \hat{x}_2} = 1.992634$$

$\vdots$

$\hat{x}_8 = 2.000000$

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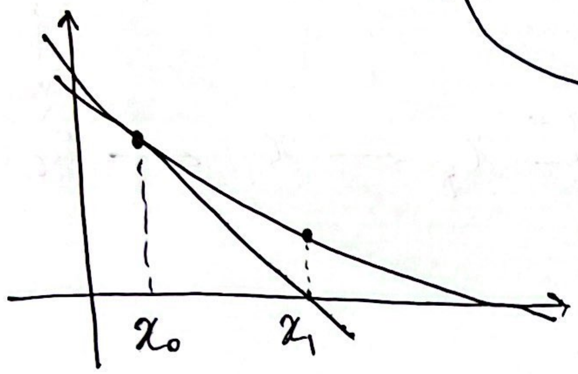
Secant Method / Quasi-Newton Method:

Newton's Method Recap:

$$x_{k+1} = x_k - \underbrace{\frac{f(x_k)}{f'(x_k)}}$$

replace $f'(x_k)$ with backward diff.



$$\text{backward differentiation} = \frac{f(x) - f(x-h)}{h}$$

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

$$= \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \Bigg\}$$ put this part instead of $f'(x_k)$

$\therefore$ Iteration formula for Secant Method:

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}$$

Note: We need 2 starting points for Secant Method (x_0 and x_1).

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Example

$$f(x) = \frac{1}{x} - 0.5 \qquad x_0 = 0.25,\ x_1 = 0.5$$

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}$$

$$= x_k - \frac{\left(\frac{1}{x_k} - 0.5\right)(x_k - x_{k-1})}{\left(\frac{1}{x_k} - 0.5\right) - \left(\frac{1}{x_{k-1}} - 0.5\right)}$$

k	x_k
0	0.25
1	0.5
2	0.6875
3	1.01562
4	1.3540
5	1.68205
6	1.8973
7	1.98367
8	1.99916
⋮	⋮
12	2.00000

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Example:

$$f(x) = x_k^2 - 2x_k e^{-x_k} + e^{-2x_k} \quad \text{— (1)}$$

Newtons Method Iteration Formula:

$$x_{k+1} = x_k - \frac{x_k^2 - 2x_k e^{-x_k} + e^{-2x_k}}{2x_k - 2e^{-x_k} + 2x_k e^{-x_k} - 2e^{-2x_k}} \quad \text{— (2)}$$

Aitken Acceleration:

$$\hat{x}_{k+2} = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k} \quad \text{— (3)}$$

Flow:

check if within error bound, if not, go next

$$x_0 \xrightarrow{eq1} f(x_0) \xrightarrow{eq2} x_1 \xrightarrow{eq1} f(x_1) \xrightarrow{eq2} x_2 \xrightarrow{eq1} f(x_2) \xrightarrow{eq3}$$

$$x_4 \xleftarrow{eq2} f(x_3) \xleftarrow{eq1} x_3 \xleftarrow{eq2} f(\hat{x}_2) \xleftarrow{eq1} \hat{x}_2 \leftarrow$$

$$\xrightarrow{eq1} f(x_4) \xrightarrow{eq3} \hat{x}_4 \xrightarrow{eq1} f(\hat{x}_4) \xrightarrow{eq2} x_5$$

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K	x_k	$f(x_k)$	if $\lvert f(x_k)\rvert < 10^{-5}$?
0	$1 \xrightarrow{eq\,1}$	0.399576	No
	$\downarrow eq\,2$		
1	$0.768941 \xrightarrow{eq\,1}$	0.093292	No
	$\downarrow eq\,2$		
2	$0.664590 \xrightarrow{eq\,1}$	0.022532	No
	$\downarrow eq\,3$		
$\hat{2}$	$0.578651 \xrightarrow{eq\,1}$	3.2×10^{-4}	No
	$\downarrow eq\,2$		
3	$0.572885 \xrightarrow{eq\,1}$	8×10^{-5}	No
	$\downarrow eq\,2$		
4	$0.570011 \xrightarrow{eq\,1}$	2×10^{-5}	No
	$\downarrow eq\,3$		
$\hat{4}$	$0.567154 \xrightarrow{eq\,1}$	2.8×10^{-10}	Yes

Answer: $x_* = 0.56715$ (upto 5 d.p).

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Linear Equations:

→ System of linear equations (exponent of all variables must be 1)

$$a_{11} x_1 + a_{12} x_2 + \cdots + a_{1n} x_n = b_1$$
$$a_{21} x_1 + a_{22} x_2 + \cdots + a_{2n} x_n = b_2$$
$$\vdots \qquad\qquad\qquad \vdots$$
$$a_{n1} x_1 + a_{n2} x_2 + \cdots + a_{nn} x_n = b_n$$

→ Can be represented in a matrix form:

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}}_{(n \times n)\text{ matrix, } A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{(n\times 1)\text{ matrix, } x} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}}_{(n \times 1)\text{ matrix, } b}$$

$$A \cdot x = b$$

Solution:

$$x = A^{-1} \cdot b$$

Basic properties of A:

→ A should be a square matrix of shape $(n \times n)$

→ A must be non-singular [meaning $\det(A) \neq 0$]

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Gaussian Elimination Method:

→ A technique which transforms matrix A into triangular form (upper or lower)

→ Solves $Ax = b$ without finding the inverse.

→ Lower triangular matrix (L), and upper triangular matrix (U) are defined as follows:

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & & & \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \qquad U = \begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1n} \\ 0 & U_{22} & \cdots & U_{2n} \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & U_{nn} \end{bmatrix}$$

Using a (4x4) Lower triangular matrix:

$$\begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

number of operations:

$$l_{11} x_1 + 0 \cdot x_2 + 0 \cdot x_3 + 0 \cdot x_4 = b_1$$

$$\Rightarrow \boxed{x_1 = \frac{b_1}{l_{11}}} \longrightarrow 1 \text{ div}$$

$$l_{21} x_1 + l_{22} x_2 = b_2$$

$$\boxed{x_2 = \frac{b_2 - l_{21} x_1}{l_{22}}} \longrightarrow 1 \text{ div}, 1 \text{ mult}, 1 \text{ sub}$$

number of operations:

$$l_{31} x_1 + l_{32} x_2 + l_{33} x_3 = b_3$$

$$\boxed{x_3 = \frac{b_3 - l_{31}x_1 - l_{32}x_2}{l_{33}}} \longrightarrow 1 \text{ div}, 2 \text{ mult}, 2 \text{ sub}$$

$$l_{41} x_1 + l_{42} x_2 + l_{43} x_3 + l_{44} x_4 = b_4$$

$$\boxed{x_4 = \frac{b_4 - l_{41}x_1 - l_{42}x_2 - l_{43}x_3}{l_{44}}} \longrightarrow 1 \text{ div}, 3 \text{ mult}, 3 \text{ sub}$$

This is a "TOP DOWN" approach because we found x_1 first, then x_2, x_3, x_4.

Total number of operations:

For finding x_n, we need 1 div, $(n-1)$ mult, $(n-1)$ sub.

$$1 + (n-1) + (n-1) = 1 + 2(n-1)$$

$$\therefore \text{total num of operations} = \sum_{j=1}^{n} [1 + 2(j-1)]$$

$$= \sum_{j=1}^{n} (2j - 1)$$

$$= 2\sum_{j=1}^{n} j - \sum_{j=1}^{n} 1$$

$$= n^2 + n - n$$

$$= n^2$$

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Gaussian Elimination Method:

→ To make a matrix into a triangular form, we apply Gaussian Elimination.

→ Need to apply row operations.

→ 1st row operation will make all elements below a_{11} into 0.

Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}' & a_{23}' \\ 0 & a_{32}' & a_{33}' \end{bmatrix} \quad \begin{array}{l} r_2' = r_2 - \underbrace{\boxed{\frac{a_{21}}{a_{11}}}}_{m_{21}} r_1 \\ r_3' = r_3 - \underbrace{\boxed{\frac{a_{31}}{a_{11}}}}_{m_{31}} r_1 \end{array}$$

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$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & x & x \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \end{bmatrix}$$

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Example:

$$x_1 + 2x_2 + x_3 = 0$$

$$x_1 - 2x_2 + 2x_3 = 4$$

$$2x_1 + 12x_2 - 2x_3 = 4$$

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{bmatrix} \qquad b = \begin{bmatrix} 0 \\ 4 \\ 4 \end{bmatrix}$$

Augmented Matrix:

$$\left[\begin{array}{ccc|c} 1 & 2 & 1 & 0 \\ 1 & -2 & 2 & 4 \\ 2 & 12 & -2 & 4 \end{array}\right] \begin{array}{l} \\ \rightarrow r_2' = r_2 - \frac{1}{1} r_1 \quad [X - Y] \\ \rightarrow r_3' = r_3 - \frac{2}{1} r_1 \quad [X - 2Y] \end{array}$$

$$\left[\begin{array}{ccc|c} 1 & 2 & 1 & 0 \\ 0 & -4 & 1 & 4 \\ 0 & 8 & -4 & 4 \end{array}\right] \begin{array}{l} \\ \\ \rightarrow r_3' = r_3 - \frac{8}{-4} r_2 \quad [X + 2Y] \end{array}$$

$$\left[\begin{array}{ccc|c} 1 & 2 & 1 & 0 \\ 0 & -4 & 1 & 4 \\ 0 & 0 & -2 & 12 \end{array}\right]$$

$-2x_3 = 12$	$-4x_2 + x_3 = 4$	$x_1 + 2x_2 + x_3 = 0$
$x_3 = -6$	$-4x_2 - 6 = 4$	$x_1 + 2(-2.5) + (-6) = 0$
	$x_2 = -2.5$	$x_1 = 11$

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LU Decomposition:

→ Need to decompose matrix A into LU

$$A = \begin{bmatrix} 2 & 4 & 3 & 5 \\ -4 & -7 & -5 & -8 \\ 6 & 8 & 2 & 9 \\ 4 & 9 & -2 & 14 \end{bmatrix} \begin{array}{l} \\ \to R_2' = R_2 - \left(-\frac{4}{2}\right) R_1 \\ \to R_3' = R_3 - \left(\frac{6}{2}\right) R_1 \\ \to R_4' = R_4 - \left(\frac{4}{2}\right) R_1 \end{array}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 3 & & 1 & 0 \\ 2 & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & 3 & 5 \\ 0 & 1 & 1 & 2 \\ 0 & -4 & -7 & -6 \\ 0 & 1 & -8 & 4 \end{bmatrix} \begin{array}{l} \\ \\ \to R_3' = R_3 - \left(-\frac{4}{1}\right) R_2 \\ \to R_4' = R_4 - \left(\frac{1}{1}\right) R_2 \end{array}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 3 & -4 & 1 & 0 \\ 2 & 1 & & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & 3 & 5 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & -3 & 2 \\ 0 & 0 & -9 & 2 \end{bmatrix} \begin{array}{l} \\ \\ \\ \to R_4' = R_4 - \left(\frac{-9}{-3}\right) R_3 \end{array}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 3 & -4 & 1 & 0 \\ 2 & 1 & 3 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & 3 & 5 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & -3 & 2 \\ 0 & 0 & 0 & -4 \end{bmatrix}$$

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Steps:

$$\boxed{A}\,x = b$$

$$\boxed{A} \xrightarrow{\text{decompose}} LU$$

$$L\,\underbrace{\boxed{Ux}}_{y} = b$$

$$Ly = b \longrightarrow \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}}_{\text{Solve for } y \text{ [find } y_1,\, y_2,\, y_3]}$$

$$\boxed{Ux = y}$$

$$\underbrace{\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}}_{\text{solve for } x \text{ [find } x_1,\, x_2,\, x_3]}$$

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Example:

$$\begin{bmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \\ 4 \end{bmatrix}$$

$$A \cdot x = b$$

$$A \Downarrow LU$$

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{bmatrix} \begin{matrix} \\ \longrightarrow R_2' = R_2 - \left(\frac{1}{1}\right) R_1 \\ \longrightarrow R_3' = R_3 - \left(\frac{2}{1}\right) R_1 \end{matrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 8 & -4 \end{bmatrix} \begin{matrix} \\ \\ \longrightarrow R_3' = R_3 - \left(\frac{8}{-4}\right) R_2 \end{matrix}$$

$$= \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{bmatrix}}_{U}$$

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$$A \cdot x = b$$

$\Downarrow$ decompose

$$LU$$

$$L\boxed{U \cdot x} = b$$

$\Downarrow$

y

$$L\,y = b$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \\ 4 \end{bmatrix}$$

$$\boxed{y_1 = 0}$$

$$y_1 + y_2 = 4, \quad \boxed{y_2 = 4}$$

$$2y_1 + (-2y_2) + y_3 = 4$$

$$(2\times 0) + (-2\times 4) + y_3 = 4$$

$$\boxed{y_3 = 12}$$

$$U \cdot x = y$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 4 \\ 12 \end{bmatrix}$$

$$-2x_3 = 12$$

$$\boxed{x_3 = -6}$$

$$-4x_2 + x_3 = 4$$

$$-4x_2 - 6 = 4$$

$$\boxed{x_2 = -2.5}$$

$$x_1 + 2x_2 + x_3 = 0$$

$$x_1 + 2(-2.5) + (-6) = 0$$

$$\boxed{x_1 = 11}$$

Advantage:

→ This method can be used to solve linear system that differ by the values of 'b' only. We need to compute L and U only once.

→ But in Gaussian Elimination Method method, if 'b' changes, we need to restart row operations from the very beginning.

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Frobenius Matrix:

$$F^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -m_{21} & 1 & 0 & 0 \\ -m_{31} & 0 & 1 & 0 \\ -m_{41} & 0 & 0 & 1 \end{bmatrix} \quad F^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -m_{32} & 1 & 0 \\ 0 & -m_{42} & 0 & 1 \end{bmatrix} \quad F^{(3)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -m_{43} & 1 \end{bmatrix}$$

$$L = \left(F^{(1)}\right)^{-1} \left(F^{(2)}\right)^{-1} \left(F^{(3)}\right)^{-1}$$

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & 12 & -2 \end{bmatrix} \begin{matrix} \\ \longrightarrow R_2' = R_2 - \left(\frac{1}{1}\right) R_1 \\ \longrightarrow R_3' = R_3 - \left(\frac{2}{1}\right) R_1 \end{matrix}$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 8 & -4 \end{bmatrix} \begin{matrix} \\ \\ \longrightarrow R_3' = R_3 - \left(\frac{8}{-4}\right) R_2 \end{matrix}$$

$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & -4 & 1 \\ 0 & 0 & -2 \end{bmatrix}$$

$$F^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix} \quad F^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix}$$

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$$L = \left(F^{(1)}\right)^{-1}\left(F^{(2)}\right)^{-1}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix}^{-1} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 2 & -2 & 1 \end{bmatrix}$$

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Least Square Approximation:

→ Well defined linear system has equal number of variables & equations.

Example:

$$
\begin{aligned}
x_1 + 2x_2 + x_3 &= 0 \\
x_1 - 9x_2 + 7x_3 &= 2 \\
2x_1 + 3x_2 + 5x_3 &= 5
\end{aligned}
\;\rightarrow\;
\underbrace{\begin{bmatrix} 1 & 2 & 3 \\ 1 & -9 & 7 \\ 2 & 3 & 5 \end{bmatrix}}_{\substack{\text{square matrix} \\ \text{of } \boxed{n}\times n}}
\cdot
\underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{n\times\boxed{1}}
=
\underbrace{\begin{bmatrix} 0 \\ 2 \\ 5 \end{bmatrix}}_{n\times 1}
$$

$$A \cdot x = b$$

→ If we have a system where number of equation > number of variables, it is called an <u>over-determined</u> system.

How do we solve over-determined system?

Example:

$$
\begin{aligned}
x_1 + 2x_2 + x_3 &= 0 \\
x_1 - 9x_2 + 7x_3 &= 2 \\
x_1 + 3x_2 + 5x_3 &= 4 \\
2x_1 + 11x_2 - 9x_3 &= 5 \\
9x_1 + x_2 - x_3 &= 7
\end{aligned}
\;\rightarrow\;
\underbrace{\begin{bmatrix} 1 & 2 & 1 \\ 1 & -9 & 7 \\ 1 & 3 & 5 \\ 2 & 11 & -9 \\ 9 & 1 & -1 \end{bmatrix}}_{\boxed{m}\times n}
\underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{n\times\boxed{1}}
=
\underbrace{\begin{bmatrix} 0 \\ 2 \\ 4 \\ 5 \\ 7 \end{bmatrix}}_{m\times 1}
$$

$$A \cdot x = b$$

→ Least square approximation method is a way to find an approximate solution of an over-determined system.

$$\underset{(m \times n)}{\overset{\text{over-determined}}{A}} \cdot \underset{(n \times 1)}{x} = \underset{(m \times 1)}{b}$$

<u>How to solve such problems?</u>

→ multiply A^T on both hand sides.

$$\underbrace{\underset{(n \times m)}{A^T} \ \underset{(m \times n)}{A}}_{(n \times n)} \cdot \underset{(n \times 1)}{x} = \underbrace{\underset{(n \times m)}{A^T} \cdot \underset{(m \times 1)}{b}}_{(n \times 1)}$$

$$(n \times n) \quad (n \times 1) \qquad (n \times 1)$$

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Example

From polynomial chapter:

If we had $\underbrace{(n+1) \text{ nodes}}_{x_0, x_1 \cdots x_n}$, we calculated the values of $\underbrace{(n+1) \text{ coefficients}}_{a_0, a_1 \cdots a_n}$

using vandermonde matrix.

Well-defined system

$$\begin{bmatrix} 1 & x_0^1 & x_0^2 & \cdots & x_0^n \\ 1 & x_1^1 & x_1^2 & \cdots & x_1^n \\ \vdots & & & & \\ 1 & x_n^1 & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}$$

But now, lets say

we have $\underbrace{(m+1) \text{ nodes}}_{x_0, x_1 \cdots x_m}$, but we need to calculate $\underbrace{(n+1) \text{ coefficients}}_{a_0, a_1 \cdots a_n}$

[Remember $m > n$]

over-determined system

$$\begin{bmatrix} 1 & x_0^1 & x_0^2 & \cdots & x_0^n \\ 1 & x_1^1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & & & & \\ 1 & x_m^1 & x_m^2 & \cdots & x_m^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_m) \end{bmatrix}$$

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$$\underbrace{a_0 + a_1 x}_{\text{number of coefficients} = 2}$$

Example:

We want to fit a straight line through the following nodes

$x_0 = -3$ $\quad$ $x_1 = 0$ $\quad$ $x_2 = 6$

$f(x_0) = 0$ $\quad$ $f(x_1) = 0$ $\quad$ $f(x_2) = 2$

number of nodes = 3

$$P_1(x_0) = a_0 + a_1(x_0) = f(x_0) \rightarrow a_0 + a_1(-3) = 0$$
$$P_1(x_1) = a_0 + a_1(x_1) = f(x_1) \rightarrow a_0 + a_1(0) = 0$$
$$P_1(x_2) = a_0 + a_1(x_2) = f(x_2) \rightarrow a_0 + a_1(6) = 2$$

$$\begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

$$A \cdot x = b$$

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Multiplying A^T on both sides.

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{bmatrix} \begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix}} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}}$$

$$\begin{bmatrix} 3 & 3 \\ 3 & 45 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 2 \\ 12 \end{bmatrix}$$

Now apply Gaussian elimination/LU/ inverse method to find the values of a_0 and a_1.

Applying inverse method:

$$\begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 3 & 3 \\ 3 & 45 \end{bmatrix}^{-1} \cdot \begin{bmatrix} 2 \\ 12 \end{bmatrix}$$

$$= \begin{bmatrix} 3/7 \\ 5/21 \end{bmatrix}$$

$\therefore a_0 = 3/7, \quad a_1 = 5/21$

$\therefore P_1(x) = \frac{3}{7} + \frac{5}{21} x$

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Orthogonality:

→ To understand orthogonality, we need to understand vector dot product / inner product first.

→ Vector dot product returns a scalar value (a number)

2 types of notations → matrix notation → $x^T \cdot y$
→ vector notation → $\vec{x} \cdot \vec{y}$

$x = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ $y = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$

① Matrix Notation $= x^T \cdot y$

$= \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$

shape → $(\boxed{1} \times 3)$; $(3 \times \boxed{1})$

= ↳ returns a scalar / number

② Vector Notation $= \vec{x} \cdot \vec{y}$

$= (1 \times 4) + (2 \times 5) + (3 \times 6)$

↳ returns a scalar / number

Inner product with itself $= l_2$ - norm

eg. $\vec{x} \cdot \vec{x}$ or $x^T x$

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Dot product:

$$a = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$a \cdot b = a_1 b_1 + a_2 b_2 + a_3 b_3$$

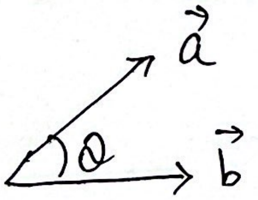
↳ returns a scalar/number.

Length/magnitude of a vector:

$$a = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$$

$$|a| = \sqrt{(a_1)^2 + (a_2)^2 + (a_3)^2}$$

Dot product (Second approach):



$$a \cdot b = |a|\,|b| \cos \theta$$

$$\cos \theta = \frac{a \cdot b}{|a|\,|b|}$$

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Orthogonal Vectors:

If $\angle$ between 2 vectors $= 90^\circ$ or $\frac{\pi}{2}$

In other words, if 2 vectors are perpendicular to each other, the vectors are orthogonal.

For orthogonal vectors, their dot product is 0. Because:

$$\vec{a}\cdot\vec{b} = |\vec{a}|\,|\vec{b}|\,\cos\left(\tfrac{\pi}{2}\right) \rightarrow 0$$

$$\therefore \vec{a}\cdot\vec{b} = 0$$

or $a^T b = 0$

Lets consider a set of vector S.

$$S = \{\vec{a}, \vec{b}, \vec{c}\}$$

Set S is an orthogonal set if

$$\vec{a}\cdot\vec{b} = 0$$
$$\vec{b}\cdot\vec{c} = 0$$
$$\vec{c}\cdot\vec{a} = 0$$

i.e. each vector is perpendicular to each other.

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Orthonormality:

If ① the vectors are orthogonal (dot product = 0)

② the length of the vectors = 1 (unit vectors)

Then the vectors are orthonormal.

$$\vec{a} = \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix} \qquad b = \begin{bmatrix} 1 \\ -3 \\ 2 \end{bmatrix}$$

Checking if orthogonal:

$$\vec{a} \cdot \vec{b} = (4 \times 1) + (2 \times -3) + (1 \times 2) = 0 \quad [\therefore \text{ orthogonal}]$$

Converting into orthonormal (by making length = 1):

$$\hat{a} = \frac{\vec{a}}{|a|} = \frac{1}{\underbrace{\sqrt{21}}_{\sqrt{4^2+2^2+1^2}}} \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 4/\sqrt{21} \\ 2/\sqrt{21} \\ 1/\sqrt{21} \end{bmatrix} \rightarrow |\hat{a}| = \sqrt{\left(\frac{4}{\sqrt{21}}\right)^2 + \left(\frac{2}{\sqrt{21}}\right)^2 + \left(\frac{1}{\sqrt{21}}\right)^2} = 1$$

$$\hat{b} = \frac{\vec{b}}{|b|} = \frac{1}{\sqrt{14}} \begin{bmatrix} 1 \\ -3 \\ 2 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{14} \\ -3/\sqrt{14} \\ 2/\sqrt{14} \end{bmatrix} \rightarrow |\hat{b}| = \sqrt{\left(\frac{1}{\sqrt{14}}\right)^2 + \left(-\frac{3}{\sqrt{14}}\right)^2 + \left(\frac{2}{\sqrt{14}}\right)^2} = 1$$

→ Process of making vectors into unit vectors (length = 1) is called normalization

→ By doing so, we only change the magnitude, not the direction.

→ Hence, they are still orthogonal

→ Since they are orthogonal and has length = 1 (unit vectors), the vectors are orthonormal.

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Example:

Consider the set of vectors, S:

$$S = \left\{ \frac{1}{\sqrt{5}}(2,1)^T , \frac{1}{\sqrt{5}}(1,-2)^T \right\}$$

Show if the set S is orthonormal or not.

Solution:

$$S = \left\{ \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix} , \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ -2 \end{bmatrix} \right\}$$

$$= \left\{ \underbrace{\begin{bmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{bmatrix}}_{\vec{u}_1} , \underbrace{\begin{bmatrix} \frac{1}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} \end{bmatrix}}_{\vec{u}_2} \right\}$$

$$\vec{u}_1 \cdot \vec{u}_2 = \left(\frac{2}{\sqrt{5}} \times \frac{1}{\sqrt{5}}\right) + \left(\frac{1}{\sqrt{5}} \times -\frac{2}{\sqrt{5}}\right) = 0 \quad [\therefore \text{orthogonal}]$$

$$|\vec{u}_1| = \sqrt{\left(\frac{2}{\sqrt{5}}\right)^2 + \left(\frac{1}{\sqrt{5}}\right)^2} = 1$$

$[\therefore$ orthonormal$]$

$$|\vec{u}_2| = \sqrt{\left(\frac{1}{\sqrt{5}}\right)^2 + \left(-\frac{2}{\sqrt{5}}\right)^2} = 1$$

$\therefore$ Yes, the set of vectors are orthonormal.

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Theorem:

Orthogonal / orthonormal matrices are matrices in which the column vectors form an ~~orthogonal~~ orthonormal set (each column vector has length one, and is orthogonal to all other column vectors).

For square orthonormal matrices, the inverse is simply the transpose.

Properties:

$$Q^{-1} = Q^T$$
$$Q Q^T = I$$
$$Q^T Q = I$$

Example:

$$Q = \begin{array}{cc} \vec{a} & \vec{b} \\ \left[\begin{matrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{matrix}\right] \end{array}$$

$$\vec{a} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \qquad \vec{b} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$$

$$\vec{a} \cdot \vec{b} = (1/\sqrt{2} \times 1/\sqrt{2}) + (1/\sqrt{2} \times -1/\sqrt{2}) = 0 \quad [\therefore \text{orthogonal}]$$

$$|\vec{a}| = \sqrt{\left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(\tfrac{1}{\sqrt{2}}\right)^2} = 1$$

$[\therefore$ orthonormal$]$

$$|\vec{b}| = \sqrt{\left(\tfrac{1}{\sqrt{2}}\right)^2 + \left(-\tfrac{1}{\sqrt{2}}\right)^2} = 1$$

→ This makes the columns of the matrix orthonormal to each other.

→ ∴ The matrix Q will have the properties:

1. $Q^{-1} = Q^T$
2. $Q Q^T = I$
3. $Q^T Q = I$

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Gram - Schmidt Process:

Lets have a basis $(u_1, u_2, \ldots u_n)$ from a vector space. Gram - Schmidt process takes the basis $(u_1, u_2 \ldots u_n)$ and forms a new orthogonal basis $(P_1, P_2 \ldots P_n)$. We can later transform these orthogonal basis into orthonormal basis $(q_1, q_2 \ldots q_n)$.

$$
\begin{array}{l}
\text{Original basis : } u_1, u_2, u_3 \\
\quad \Big\downarrow \text{ Gram Schmidt Process} \\
\text{Orthogonal basis : } P_1, P_2, P_3 \\
\quad \Big\downarrow \text{ normalization} \\
\text{Orthonormal basis : } q_1, q_2, q_3
\end{array}
$$

1) $P_1 = u_1$

2) $P_2 = u_2 - \dfrac{u_2 \cdot P_1}{P_1 \cdot P_1} P_1$

3) $P_3 = u_3 - \dfrac{u_3 \cdot P_1}{P_1 \cdot P_1} P_1 - \dfrac{u_3 \cdot P_2}{P_2 \cdot P_2} P_2$

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Example:

$$u_1 = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} \quad u_2 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \quad u_3 = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}$$

1) $P_1 = u_1 = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$

2) $$P_2 = u_2 - \frac{u_2 \cdot P_1}{P_1 \cdot P_1} P_1$$

$$= \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} - \frac{(1\times1) + (0\times-1) + (1\times1)}{(1\times1) + (-1\times-1) + (1\times1)} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} - \frac{2}{3} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$$

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

$$= \begin{bmatrix} 1/3 \\ 2/3 \\ 1/3 \end{bmatrix}$$

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③ $P_3 = U_3 - \dfrac{U_3 \cdot P_1}{P_1 \cdot P_1} P_1 - \dfrac{U_3 \cdot P_2}{P_2 \cdot P_2} P_2$

$$= \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} - \frac{(1\times1)+(1\times-1)+(2\times1)}{(1\times1)+(-1\times-1)+(1\times1)} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} - \frac{(1\times\frac{1}{3})+(1\times\frac{2}{3})+(2\times\frac{1}{3})}{(\frac{1}{3}\times\frac{1}{3})+(\frac{2}{3}\times\frac{2}{3})+(\frac{1}{3}\times\frac{1}{3})} \begin{bmatrix} 1/3 \\ 2/3 \\ 1/3 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} - \frac{2}{3} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} - \frac{5}{2} \begin{bmatrix} 1/3 \\ 2/3 \\ 1/3 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 2/3 \\ -2/3 \\ 2/3 \end{bmatrix} - \begin{bmatrix} 5/6 \\ 5/3 \\ 5/6 \end{bmatrix}$$

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

P_1, P_2, P_3 form an orthogonal basis

If we want orthonormal basis, we can devide each vectors by its length. (normalization).

① $q_1 = \dfrac{P_1}{|P_1|} = \dfrac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} \\ -1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$

② $q_2 = \dfrac{P_2}{|P_2|} = \dfrac{1}{\sqrt{6}/3} \begin{bmatrix} 1/3 \\ 2/3 \\ 1/3 \end{bmatrix} = \begin{bmatrix} \sqrt{6}/6 \\ \sqrt{6}/3 \\ \sqrt{6}/6 \end{bmatrix}$

③ $q_3 = \dfrac{P_3}{|P_3|} = \dfrac{1}{\sqrt{2}/2} \begin{bmatrix} -1/2 \\ 0 \\ 1/2 \end{bmatrix} = \begin{bmatrix} -\sqrt{2}/2 \\ 0 \\ \sqrt{2}/2 \end{bmatrix}$

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QR Decomposition:

Any real $(m\times n)$ matrix "A" with $m>n$ can be written in the form:

$$A = QR$$

Where Q is a $(m\times n)$ matrix with orthonormal columns

R is an upper triangular matrix of shape $(n\times n)$

orthonormal matrix. Therefore has the properties:

$$Q Q^T = I_{nn}$$
$$Q^T Q = I_{nn}$$

$$\underset{m\times n}{A} = \underset{m\times n}{Q}\ \underset{n\times n}{R}$$

→ Multiplying Q^T on both sides.

$$Q^T A = \boxed{Q^T Q}\, R$$

$$Q^T A = \overset{1}{\cancel{I}}\, R$$

$$Q^T A = R$$

$$\boxed{R = Q^T A}$$

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Example of QR Decomposition:

$$A = QR$$

Starting with A

$$A = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ u_{21} & u_{22} & \cdots & u_{2n} \\ \vdots & & & \\ u_{m1} & u_{m2} & & u_{mn} \end{bmatrix}$$

$$\downarrow \quad \downarrow \quad \quad \downarrow$$

$$u_1 \quad u_2 \quad \quad u_n$$

convert u into orthogonal vectors p (Gram-Smidt process)

convert p into orthonormal vectors q (normalization)

$$A = \begin{bmatrix} 3 & 1 \\ 6 & 2 \\ 0 & 2 \end{bmatrix}$$

$$\downarrow \quad \downarrow$$

$$u_1 \quad u_2$$

$$p_1 = u_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$$

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$$P_2 = U_2 - \frac{U_2 \cdot P_1}{P_1 \cdot P_1} P_1$$

$$= \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}}{\begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}} \cdot \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{(1 \times 3) + (2 \times 6) + (2 \times 0)}{(3 \times 3) + (6 \times 6) + (0 \times 0)} \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{1}{3} \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

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$\therefore P_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} \quad P_2 = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$

P_1 and P_2 are orthogonal.

→ Now convert P_1 and P_2 into unit vectors. We will call the unit vectors q_1 and q_2.

$$q_1 = \frac{P_1}{|P_1|} = \frac{1}{3\sqrt{5}} \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{5}/5 \\ 2\sqrt{5}/5 \\ 0 \end{bmatrix}$$

$$q_2 = \frac{P_2}{|P_2|} = \frac{1}{2} \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$\therefore q_1 = \begin{bmatrix} \sqrt{5}/5 \\ 2\sqrt{5}/5 \\ 0 \end{bmatrix} \quad q_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

q_1 and q_2 are orthonormal

$\therefore Q = \begin{bmatrix} \sqrt{5}/5 & 0 \\ 2\sqrt{5}/5 & 0 \\ 0 & 1 \end{bmatrix} \quad A = \begin{bmatrix} 3 & 1 \\ 6 & 2 \\ 0 & 2 \end{bmatrix}$

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$$R = Q^T A$$

$$= \begin{bmatrix} \sqrt{5}/5 & 2\sqrt{5}/5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 6 & 2 \\ 0 & 2 \end{bmatrix}$$

$$= \begin{bmatrix} 3\sqrt{5} & \sqrt{5} \\ 0 & 2 \end{bmatrix}$$

$$A = Q \quad R$$

$$\begin{bmatrix} 3 & 1 \\ 6 & 2 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} \sqrt{5}/5 & 0 \\ 2\sqrt{5}/5 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 3\sqrt{5} & \sqrt{5} \\ 0 & 2 \end{bmatrix}$$

Check if $Q \cdot R = A$ in your calculator.

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Example 2

$x_0 = -3$ $\quad x_1 = 0$ $\quad x_2 = 6$

$f(x_0) = 0$ $\quad f(x_1) = 0$ $\quad f(x_2) = 2$

$$\underset{A}{\begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix}} \cdot \underset{x}{\begin{bmatrix} a_0 \\ a_1 \end{bmatrix}} = \underset{b}{\begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}}$$

$$\begin{array}{cc} \downarrow & \downarrow \\ u_1 & u_2 \end{array}$$

$$p_1 = u_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$p_2 = u_2 - \frac{u_2 \cdot p_1}{p_1 \cdot p_1} p_1$$

$$= \begin{bmatrix} -3 \\ 0 \\ 6 \end{bmatrix} - \frac{(-3\times1) + (0\times1) + (6\times1)}{(1\times1) + (1\times1) + (1\times1)} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} -3 \\ 0 \\ 6 \end{bmatrix} - 1 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} -4 \\ -1 \\ 5 \end{bmatrix}$$

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$$P_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \qquad P_2 = \begin{bmatrix} -4 \\ -1 \\ 5 \end{bmatrix}$$

P_1 and P_2 are orthogonal vectors.

$$q_1 = \frac{P_1}{|P_1|} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$$

$$q_2 = \frac{P_2}{|P_2|} = \frac{1}{\sqrt{42}} \begin{bmatrix} -4 \\ -1 \\ 5 \end{bmatrix} = \begin{bmatrix} -4/\sqrt{42} \\ -1/\sqrt{42} \\ 5/\sqrt{42} \end{bmatrix}$$

$$\therefore Q = \begin{bmatrix} 1/\sqrt{3} & -4/\sqrt{42} \\ 1/\sqrt{3} & -1/\sqrt{42} \\ 1/\sqrt{3} & 5/\sqrt{42} \end{bmatrix}$$ $\longrightarrow$ matrix Q has orthonormal columns.

$$R = Q^T A$$

$$= \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ -4/\sqrt{42} & -1/\sqrt{42} & 5/\sqrt{42} \end{bmatrix} \begin{bmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{bmatrix}$$

$$R = \begin{bmatrix} \sqrt{3} & \sqrt{3} \\ 0 & \sqrt{42} \end{bmatrix}$$

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$$Ax = b$$

Applying Least square approximation method by applying A^T on both sides.

$$\begin{array}{ccccc} A^T & A & x & = & A^T \quad b \\ \downarrow & \downarrow & \downarrow & & \downarrow \quad\ \downarrow \\ (QR)^T & (QR) & x & = & (QR)^T \ b \end{array}$$

$$R^T \boxed{Q^T Q} R x = R^T Q^T b$$

$\downarrow$

I_{nn} [because Q = orthonormal matrix]

$$\cancel{R^T} R x = \cancel{R^T} Q^T b$$

$$\boxed{Rx = Q^T b}$$

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$$Rx = Q^T b$$

$$\begin{bmatrix} \sqrt{3} & \sqrt{3} \\ 0 & \sqrt{42} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ -4/\sqrt{42} & -1/\sqrt{42} & 5/\sqrt{42} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

$$\begin{bmatrix} \sqrt{3} & \sqrt{3} \\ 0 & \sqrt{42} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 2/\sqrt{3} \\ 5\sqrt{2}/\sqrt{21} \end{bmatrix}$$

$$\begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 3/7 \\ 5/21 \end{bmatrix}$$

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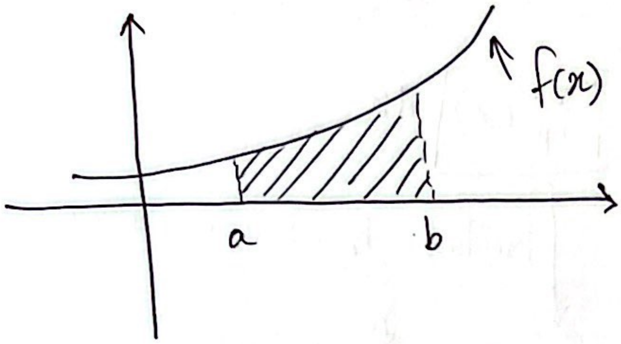
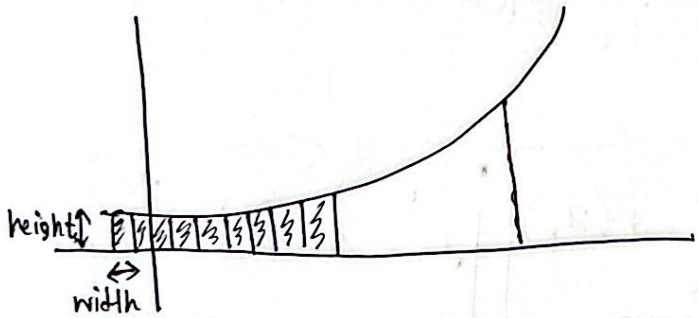
Integration:

$$I(f) = \int_a^b f(x)\,dx$$



→ Integration gives the area under $f(x)$ within the bound a & b.

→ By definition, integration is an infinite sum.



$$\int_a^b f(x)\,dx = \lim_{n\to\infty} \sum_{i=1}^{n} \underbrace{f_i(x)}_{\text{height}} \underbrace{\Delta x}_{\text{width}}$$

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→ Numerical integration replace function $f(x)$ with interpolating polynomial of degree n that passes through $(n+1)$ nodes

Actual Integration $= I(f) = \int_a^b f(x)\,dx$

Numerical Integration $= I_n(f) = \int_a^b \boxed{P_n(x)}\,dx$

$\downarrow$ writing $P_n(x)$ using lagrange basis

This polynomial $P_n(x)$ must be interpolated with equidistant nodes $x_0, x_1, \dots x_n$ ← $P_n(x) = \sum_{i=0}^{n} l_k(x) \cdot f(x_k)$

$\downarrow$ equally spaced.

$$\therefore \quad I_n(f) = \int_a^b \sum_{i=0}^{n} l_k(x) \cdot f(x_k)\,dx$$

$$= \boxed{\sum_{k=0}^{n} f(x_k)} \boxed{\int_a^b l_k(x)\,dx}$$

$\downarrow$

σ_k (~~weight function~~)
(weighted factors)

$$\therefore \quad \boxed{I_n(f) = \sum_{k=0}^{n} \sigma_k \cdot f(x_k)}$$

↑

Newton cote's Formula.

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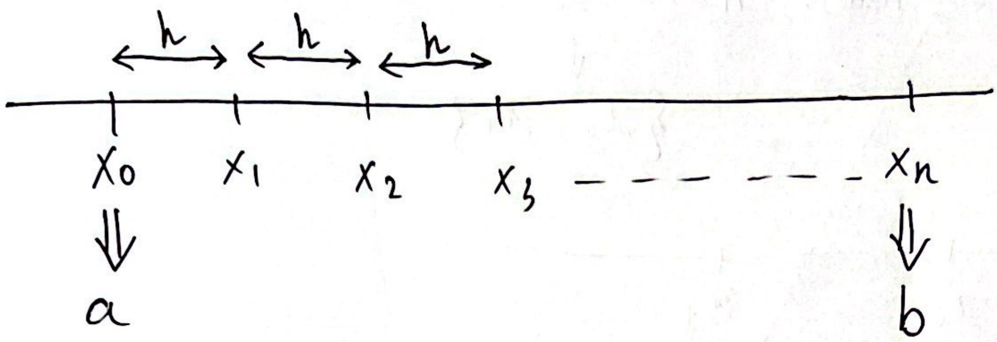
Newton Cote's Formula → Closed, open

Finding $x_0, x_1 \dots x_n$ Using closed Newton cote's Formula:



→ 'a' and 'b' are integration intervals.

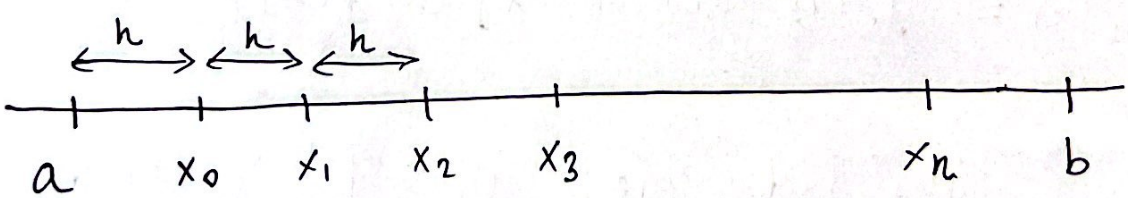
→ $\boxed{h = \dfrac{b-a}{n}}$

$x_0 = a$

$x_1 = x_0 + h$

$x_2 = x_1 + h = x_0 + 2h$

Finding $x_0, x_1 \dots x_n$ using open Newton cote's Formula:



$\boxed{h = \dfrac{b-a}{n+2}}$

$x_0 = a + h$

$x_1 = a + 2h$

$x_2 = a + 3h$

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Trapezium / Trapezoidal Rule:

→ Closed Newton Cotes formula with $n=1$

$n =$ degree of polynomial $= 1$

$\therefore$ number of nodes $= n+1 = 2$

$$2 \downarrow \{x_0, x_1\}$$

$$x_0 \Downarrow a \qquad x_1 \Downarrow b$$

[because closed newton cote's]

$$I_n(f) = \int_a^b P_n(x)\,dx$$

$$I_1(f) = \int_a^b P_1(x)\,dx$$

$$P_1(x) = l_0(x) f(x_0) + l_1(x) f(x_1)$$

$$I_1(f) = \int_a^b \left[l_0(x) f(x_0) + l_1(x) f(x_1) \right] dx$$

$$= \underbrace{\int_a^b l_0(x)\,dx}_{\sigma_0} \cdot f(x_0) + \underbrace{\int_a^b l_1(x)\,dx}_{\sigma_1} \cdot f(x_1)$$

$$\therefore \; I_1(f) = \sigma_0 f(x_0) + \sigma_1 f(x_1)$$

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$$\sigma_0 = \int_a^b l_0(x)\,dx$$

$$= \int_a^b \frac{x - x_1}{x_0 - x_1}\,dx$$

$$= \int_a^b \frac{x-b}{a-b}\,dx$$

$$= \frac{1}{a-b}\int_a^b (x-b)\,dx$$

$$= \frac{1}{a-b}\left[\frac{x^2}{2} - bx\right]_a^b$$

$$= \frac{1}{a-b}\left(\frac{b^2}{2} - b^2 - \frac{a^2}{2} + ab\right)$$

$$= \frac{b-a}{2}$$

$$\sigma_1 = \int_a^b l_1(x)\,dx$$

$$= \frac{1}{b-a}\int_a^b (x-a)\,dx$$

$\vdots$

$$= \frac{b-a}{2}$$

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$$\therefore I_1(f) = \int_a^b P_1(x)\,dx$$
$$= \sigma_0 f(x_0) + \sigma_1 f(x_1)$$
$$= \sigma_0 f(a) + \sigma_1 f(b)$$
$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$
$$= \frac{b-a}{2}\left(f(a) + f(b)\right)$$

$$\therefore \boxed{I_1(f) = \frac{b-a}{2}\left[f(a) + f(b)\right]}$$

Example:

Find $\underbrace{I(f)}_{\text{Actual}}$ and $\underbrace{I_1(f)}_{\text{Numerical}}$ of the function e^x on interval $[0,2]$.

Solution:

$$I(f) = \int_0^2 e^x\,dx = \left[e^x\right]_0^2 = e^2 - e^0 = 6.389 \text{ [Actual]}$$

$$I_1(f) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$
$$= \frac{2-0}{2}\left[e^0 + e^2\right] = 8.389 \text{ [numerical approx]}$$

$$\% \text{ error} = \frac{I - I_1}{I} \times 100 = 31.3\,\%$$ [error is large bcz degree 1 polynomial is used].

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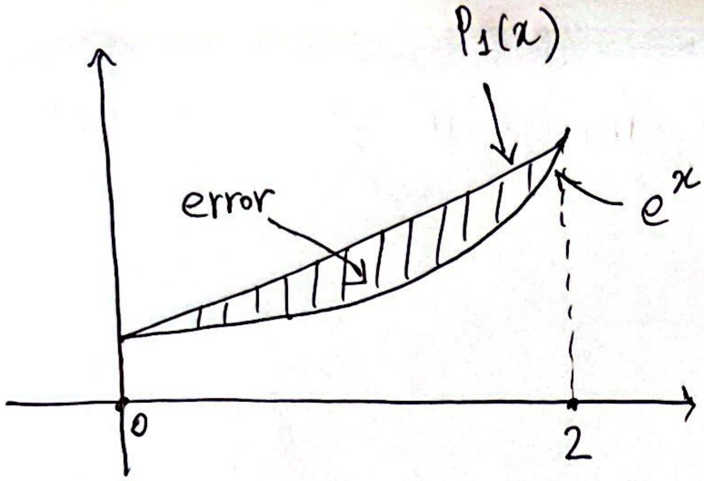

→ We can find the upper bound of the error.

→ If a function $f(x)$ is interpolated by a degree n polynomial, error ~~is~~ ~~for~~ can be found using cauchy's Theorem.

upper bound error
$$|f(x) - P_n(x)| \leq \left| \frac{f^{(n+1)}(\xi)}{(n+1)!} (x-x_0)(x-x_1)\cdots(x-x_n) \right|$$

For integration, upper bound error =

$$|I - I_n| \leq \underbrace{\left| \frac{f^{(n+1)}(\xi)}{(n+1)!} \right|}_{\text{Need to find max value within } [a;b]} \int_a^b \left| (x-x_0)(x-x_1)\cdots(x-x_n) \right| dx$$

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Example:

Computing the upper bound of error for the previous example.

$\rightarrow n = 1$

$f(x) = e^{x}$

$a = 0$

$b = 2$

Solution:

Finding the max of $\left| \frac{f^{(n+1)}(\xi)}{(n+1)!} \right|$ within $[0,2]$

$$= \left| \frac{f^{(2)}(\xi)}{2!} \right|$$

$$= \left| \frac{e^{\xi}}{2!} \right|$$

$f(x) = e^{x}$

$f^{(1)}(x) = e^{x}$

$f^{(2)}(x) = e^{x}$

$\therefore f^{(2)}(\xi) = e^{\xi}$

Max of $\frac{e^{\xi}}{2!}$ within $[0,2] = \frac{e^{2}}{2!}$

$$\rightarrow \int_a^b |(x-x_0)(x-x_1)|\,dx$$

$$= \int_a^b |(x-a)(x-b)|\,dx = \int_0^2 |(x^2-2x)|\,dx$$

$$= \left| \left[\frac{x^3}{3} - \frac{2x^2}{2} \right]_0^2 \right| = \frac{4}{3}$$

$\therefore$ upper bound of error $\leq \frac{e^2}{2!} \times \frac{4}{3} \approx 4.926.$

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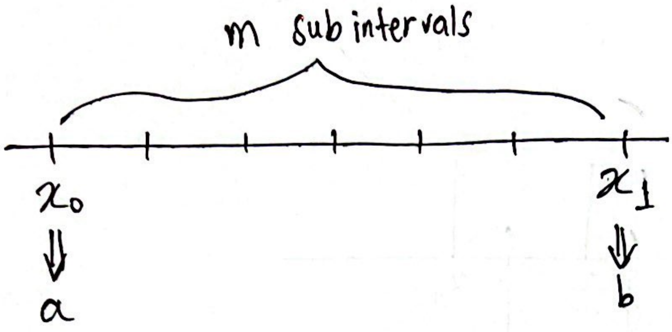
Composite Newton - Cotes Formula:

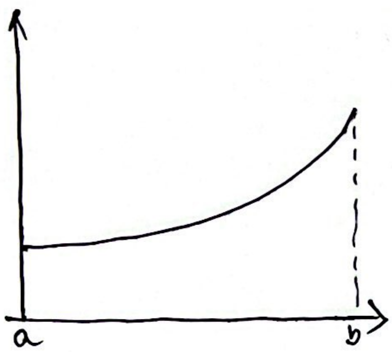
→ This method improves result without increasing num. of nodes.

→ Basic idea is to divide the interval $[a, b]$ into m sub intervals.

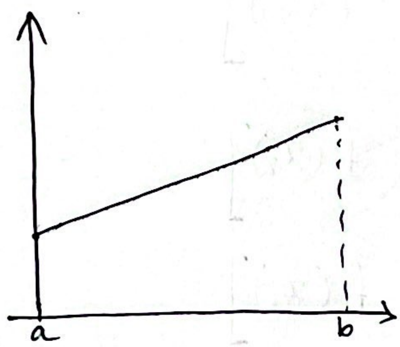
when $n = 1$:



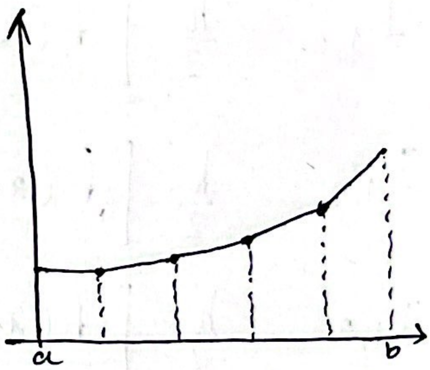
→ For each sub interval, we apply trapezium rule, then add them up.



Actual integration
$I(f)$



Newton-cotes with $n=1$
$I_1(f)$



Composite Newton Cotes with $n = 1$
$C_{1,m}(f)$

→ Total sum is denoted by $C_{1,m}(f)$ and called composite Newton Cote's.

for degree 1   for m sub interval

→ For m sub intervals, we define

$$\boxed{h = \frac{b-a}{m}}$$

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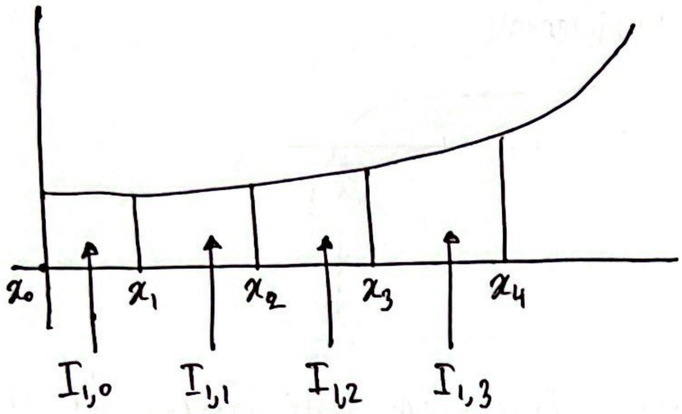
Apply Trapezium Rule for each sub interval

$$I_1(f) = \text{Trapezium Rule} = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$= \frac{h}{2}\left[f(a) + f(b)\right]$$



$$I_{1,0} = \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$

$$I_{1,1} = \frac{h}{2}\left[f(x_1) + f(x_2)\right]$$

$$I_{1,2} = \frac{h}{2}\left[f(x_2) + f(x_3)\right]$$

$$\vdots$$

$$I_{1,m-1} = \frac{h}{2}\left[f(x_{m-2}) + f(x_{m-1})\right]$$

$$I_{1,m} = \frac{h}{2}\left[f(x_{m-1}) + f(x_m)\right]$$

$$C_{1,m}(f) = \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + \dots + 2f(x_{m-1}) + f(x_m)\right]$$

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Example:

$f(x) = e^x$

$a = 0$
$b = 2$

→ Exact result $= I(f) = \int_0^2 e^x \, dx = 6.389056$

→ Composite Newton Cotes with ~~m~~ num of subintervals $= 2$ $(m=2)$:

Step 1: Find h

$$h = \frac{b-a}{m} = \frac{2-0}{2} = 1$$

Step 2: Find $x_0, x_1, x_2 \cdots x_m$

→ Remember: If $m=2$, find x_0 to x_2
If $m=3$, find x_0 to x_3
If $m=4$, find x_0 to x_4.

$X_0 = a = 0$ [since trapezium rule follows closed newton cotes]

$X_1 = X_0 + h = 0 + 1 = 1$

$X_2 = X_1 + h = 1 + 1 = 2$

Step 3: Find $C_{1,m}(f)$

$$C_{1,2}(f) = \frac{h}{2}\left[f(x_0) + 2f(x_1) + f(x_2)\right]$$

$$= \frac{1}{2}\left[e^0 + 2e^1 + e^2\right]$$

$$= 6.91281$$

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→ Composite Newton Cotes with num of sub intervals = 3 $(m=3)$:

$$h = \frac{b-a}{m} = \frac{2-0}{3} = \frac{2}{3}$$

Find x_0 to x_3:

$x_0 = a = 0$

$x_1 = x_0 + h = 0 + \frac{2}{3} = \frac{2}{3}$

$x_2 = x_1 + h = \frac{2}{3} + \frac{2}{3} = \frac{4}{3}$

$x_3 = x_2 + h = \frac{4}{3} + \frac{2}{3} = 2$

$$C_{1,3}(f) = \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + f(x_3)\right]$$

$$= \frac{2/3}{2}\left[e^{0} + 2e^{2/3} + 2e^{4/3} + e^{2}\right]$$

$$= 6.62395$$

→ Composite Newton Cotes with $m=4$:

$$C_{1,4} = \frac{0.5}{2}\left[e^{0} + 2e^{0.5} + 2e^{1} + 2e^{1.5} + e^{2}\right] = 6.52161$$

$\boxed{\text{Error decreases as } m \text{ increases}}$

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Simpcon's Rule:

Trapezium Rule $= \int_a^b P_1(x)\,dx$

Simpson's Rule $= \int_a^b P_2(x)\,dx$

$$I_2(f) = \int_a^b P_2(x)\,dx$$

$$\downarrow$$

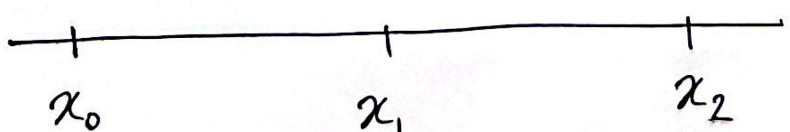
$$P_2(x) = l_0(x)\,f(x_0) + l_1(x)\,f(x_1) + l_2(x)\,f(x_2)$$

$$I_2(f) = \int_a^b \left[l_0(x)\,f(x_0) + l_1(x)\,f(x_1) + l_2(x)\,f(x_2) \right] dx$$

$$= \underbrace{\int_a^b l_0(x)\,dx}_{\sigma_0} \cdot f(x_0) + \underbrace{\int_a^b l_1(x)\,dx}_{\sigma_1} \cdot f(x_1) + \underbrace{\int_a^b l_2(x)\,dx}_{\sigma_2} \cdot f(x_2)$$

$$\therefore\ I_2(f) = \sigma_0\,f(x_0) + \sigma_1\,f(x_1) + \sigma_2\,f(x_2)$$

Here, since $n=2$, number of nodes $= n+1 = 3 \rightarrow \{x_0, x_1, x_2\}$



$x_0 \Downarrow a$

$x_1 \Downarrow x_1 = x_0 + h$

$m = x_1 = \frac{a+b}{2}$

$x_2 \Downarrow b$

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$$\sigma_0 = \int_a^b l_0(x)\,dx$$

$$= \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx$$

$$= \int_a^b \frac{(x-m)(x-b)}{(a-m)(a-b)}\,dx$$

$$= \frac{1}{(a-m)(a-b)} \int_a^b (x-m)(x-b)\,dx$$

$$= \frac{1}{6}(b-a)$$

$$\sigma_1 = \int_a^b l_1(x)\,dx$$

$$= \vdots$$

$$= \frac{2}{3}(b-a)$$

$$\sigma_2 = \int_a^b l_2(x)\,dx$$

$$= \vdots$$

$$= \frac{1}{6}(b-a)$$

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$$I_2(f) = \sigma_0 f(x_0) + \sigma_1 f(x_1) + \sigma_2 f(x_2)$$

$$= \sigma_0 f(a) + \sigma_1 f(m) + \sigma_2 f(b)$$

$$= \frac{1}{6}(b-a) f(a) + \frac{2}{3}(b-a) f(m) + \frac{1}{6}(b-a) f(b)$$

$$= \frac{b-a}{6}\left[f(a) + 4f(m) + f(b) \right]$$

$$= \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

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Exactness:

For numerical integration, upper bound of error =

$$|I - I_n| = \left|\frac{1}{(n+1)!} f^{(n+1)}(\xi)\right| \int_a^b |(x-x_0)(x-x_1)\dots(x-x_n)|\, dx$$

→ If $f^{(n+1)}(\xi) = 0$, error $= 0$

→ In that case, Newton Cotes will give exact answers

→ The above formula was derived using <u>Cauchy's Theorem</u>.

<u>Cauchy's Theorem</u>:

$$|f(x) - P_n(x)| = \underbrace{\left|\frac{1}{(n+1)!} f^{(n+1)}(\xi)\; (x-x_0)(x-x_1)\dots(x-x_n)\right|}_{\text{error}}$$

$$f(x) - P_n(x) = \text{error}$$

$$f(x) = P_n(x) + \text{error}$$

→ If error $= 0$,

$$\boxed{f(x) = P_n(x)}$$

→ $f(x)$ is a n-degree polynomial

→ $f(x)$ is a polynomial itself.

→ If $f(x)$ itself is a polynomial, $I_n(f)$ will give <u>exact result</u> since error $= 0$.

→ ~~The~~ This implies that trapezium rule $I_1(f)$ is <u>exact</u> for all functions $f(x) = P_1(x)$

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→ In other words, if we have a degree 1 polynomial, $P_1(x)$ and we apply both the actual integration, $I(f)$, and numerical integration, $I_1(f)$, we will get the exact result.

Definition:

The degree of exactness is the largest integer, n, for which the formula is exact for all polynomials, $P_n(x)$.

Example:

Find (a) Actual integration, $I(f)$

(b) Newton Cote's integral using $n=2$, $I_2(f)$

for the following functions:

① $f(x) = 1$

② $f(x) = x$

③ $f(x) = x^2$

④ $f(x) = x^3$

⑤ $f(x) = x^4$

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① $f(x) = 1$

(a) Exact $= I(f) = \int_a^b 1 \, dx = b-a$

match / zero error

(b) Newton cotes $= I_2(f) = \frac{b-a}{6}\left[1+4+1\right] = b-a$

---

② $f(x) = x$

(a) Exact $= I(f) = \int_a^b x \, dx = \frac{1}{2}(b^2 - a^2)$

match/ zero error

(b) Newton Cotes $= I_2(f) = \frac{b-a}{6}\left[a + 4\left(\frac{a+b}{2}\right) + b\right] = \frac{1}{2}(b^2 - a^2)$

---

③ $f(x) = x^2$

(a) Exact $= I(f) = \int_a^b x^2 \, dx = \frac{1}{3}(b^3 - a^3)$

match

(b) Newton Cotes $= I_2(f) = \frac{b-a}{2}\left[a^2 + 4\left(\frac{a+b}{2}\right)^2 + b^2\right] = \frac{1}{3}(b^3 - a^3)$

---

④ $f(x) = x^3$

(a) Exact $= I(f) = \int_a^b x^3 \, dx = \frac{1}{4}(b^4 - a^4)$

Match

(b) Newton cotes $= I_2(f) = \frac{b-a}{6}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right] = \frac{1}{4}(b^4 - a^4)$

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

(a) Exact $= I(f) = \int_a^b x^4 \, dx = \frac{1}{5}(b^5 - a^5)$

(b) Newton Cotes $= I_2(f) = \frac{b-a}{6}\left[a^4 + 4\left(\frac{a+b}{2}\right)^4 + b^4\right] \neq \frac{1}{5}(b^5 - a^5)$

$\therefore$ Above result shows that simpson's formula, $I_2(f)$, gives exact result upto degree 3 polynomial, and error becomes non-zero from degree 4 polynomial and higher.

$\rightarrow$ Degree of exactness is exactly 3 for Simpson's Rule, $I_2(f)$.

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