Numerical Integration

* To evaluate the definite integral that has no explicit antiderivative
* Antiderivative is not easy to obtain analytically

The Trapezoidal Rule:

* To find the approximate value of $\int_a^b f(x)\,dx$

Let $x_0 = a$, $x_1 = b$, $h = b - a$

Use the Linear Lagrange polynomial

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

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

$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))\,(x-x_0)(x-x_1)\,dx$$

$$\int_a^b f(x)\,dx = \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1) \right]_{x_0}^{x_1}$$

$$= \frac{(x_1-x_0)^2}{2\cancel{(x_1-x_0)}} f(x_1) - \frac{(x_0-x_1)^2}{2\cancel{(x_0-x_1)}} f(x_0)$$

$$= \frac{x_1-x_0}{2} f(x_1) + \frac{(x_1-x_0)}{2} f(x_0)$$

$$= \frac{b-a}{2} \left[f(x_0) + f(x_1) \right]$$

$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2} \left[f(x_0) + f(x_1) \right]}$$

is called the Trapezoidal rule.

$$\text{Error} = \int_{x_0}^{x_1} \underbrace{f''(\xi(x))}_{\text{Max}} (x-x_0)(x-x_1)\,dx$$

$$\le$$

$$= f''(\xi) \int_{x_0}^{x_1} \underbrace{(x-x_0)(x-x_1)}_{x^2 - x_1 x - x_0 x + x_0 x_1}\,dx$$

$$= f''(\xi)\left[\frac{x^3}{3} - \frac{(x_1+x_0)}{2}x^2 + x_0 x_1 x\right]_{x_0}^{x_1}$$

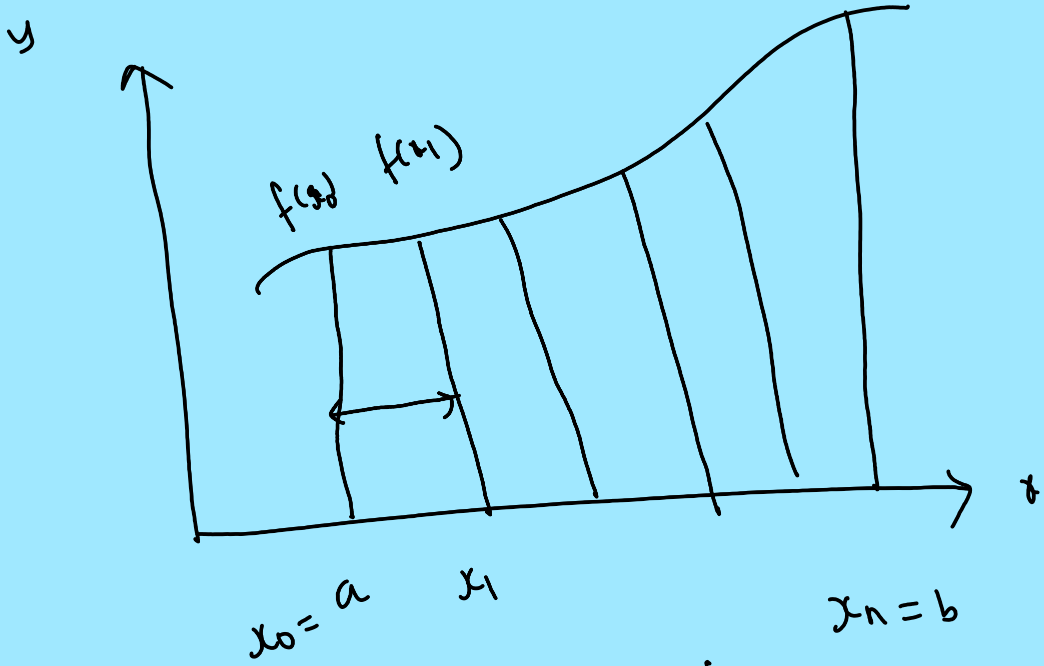
$$= f''(\xi)\left[\left(\frac{x_1^3 - x_0^3}{3}\right) - \frac{(x_1+x_0)(x_1^2 - x_0^2)}{2} + x_0 x_1 (x_1 - x_0)\right]$$

$$= f''(\xi)\left\{-\frac{h^3}{6}\right\}$$

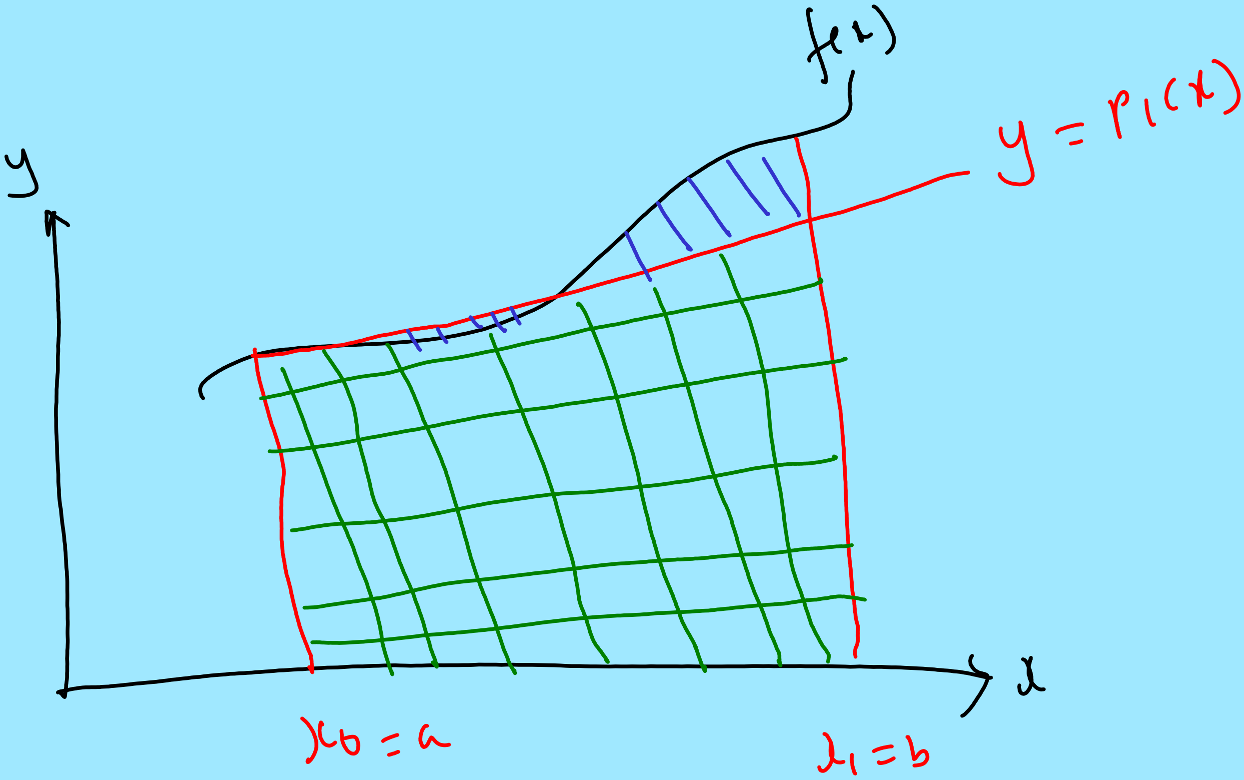
$$\boxed{\text{Error} = -\frac{h^3}{6} f''(\xi)}$$

(or)

$O(h^3)$



$$h\left(\frac{f(x_1)+f(x_0)}{2}\right)$$

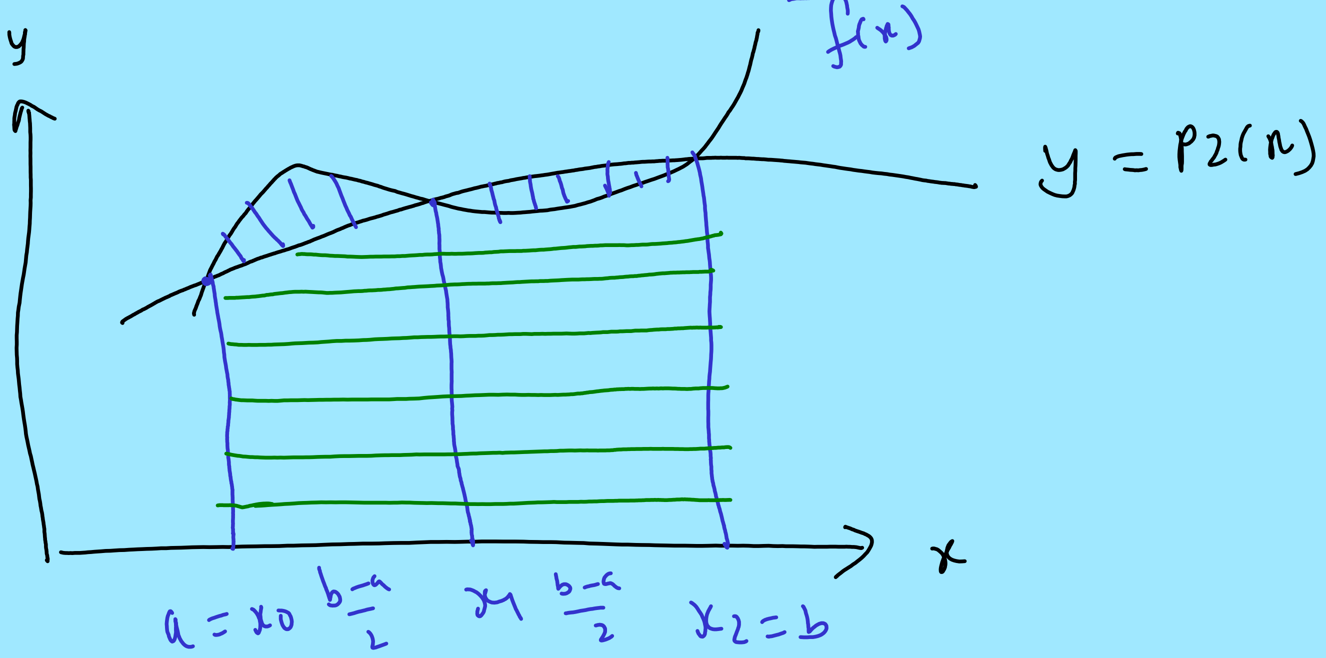


Simpson Rule

* Integrating the second Lagrange polynomial with equally-spaced nodes over $[a,b]$

* $x_0 = a$, $x_2 = b$, $x_1 = a + h$

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



$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \left(\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

$$+\underbrace{\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx}_{\text{Error}}$$

* If we derive Simpson's rule, it provide $O(h^4)$ error involving $f^{(3)}(\xi)$.

* We will use third Taylor polynomial about x_1 to derive Simpson's rule.

Then for x in (x_0, x_2)

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(iv)}(\xi(x))}{24}(x-x_1)^4$$

$$\int_{x_0}^{x_2} f(x)\,dx = \Bigg[f(x_1)\,x + f'(x_1)\frac{(x-x_1)^2}{2} + f''(x_1)\frac{(x-x_1)^3}{6} + f'''(x_1)\frac{(x-x_1)^4}{24} \Bigg]_{x_0}^{x_2}$$

$$= f(x_1)(x_2-x_0) + f'(x_1)\left\{ \underbrace{\frac{(x_2-x_1)^2 - (x_0-x_1)^2}{2}}_{=0} \right\}$$

$$+ f''(x_1)\left\{ \frac{(x_2-x_1)^3 - (x_0-x_1)^3}{6} \right\}$$

$$+ f'''(x_1)\left\{ \underbrace{\frac{(x_2-x_1)^4 - (x_0-x_1)^4}{24}}_{=0} \right\}$$

$$x_2 - x_1 = h = x_1 - x_0$$

$$\therefore \quad x_2 - x_0 = x_2 - x_1 + x_1 - x_0 = 2h$$

$$(x_2-x_1)^2 - (x_0-x_1)^2 = h^2 - h^2 = 0$$

$$(x_2-x_1)^3 - (x_0-x_1)^3 = h^3 - (-h^3) = 2h^3$$

$$(x_2-x_1)^4-(x_0-x_1)^4 = h^4-h^4=0$$

$$\therefore \int_a^b f(x)\,dx = 2h\,f(x_1)+2h^3 f''(x_1) \quad \text{Ⓐ}$$

Using mid-point formula of $f''(x)$, we get

$$f''(x_0) = \frac{1}{h^2}\left[f(\underbrace{x_0-h}_{x_0})-2f(\underbrace{x_0}_{x_1})+f(\underbrace{x_0+h}_{x_2})\right]-\frac{h^2}{12}f^{(4)}(\xi)$$

$\ast$ x_0 $\quad$ $\underline{\underline{x_1}}$ $\quad$ $\ast$ x_2

$$\therefore f''(x_1) = \frac{1}{h^2}\left[f(x_0)-2f(x_1)+f(x_2)\right] - \frac{h^2}{12}f^{(4)}(\xi)$$

Error

Sub. in Ⓐ, we get

$$\int_a^b f(x)\,dx = 2h\,f(x_1)+\frac{h^{\cancel{3}}}{3}\times\frac{1}{\cancel{h^2}}\left[f(x_0)-2f(x_1)+f(x_2)\right] - \frac{h^3}{3}\cdot\frac{h^2}{12}f^{(IV)}(\xi)$$

$$= \frac{h}{3}f(x_0)+\left(2h-2\,h/3\right)f(x_1) + h/3\; f(x_2)$$

$$= \frac{h}{3} f(x_0) + \frac{4h}{3} f(x_1) + \frac{h}{3} f(x_2)$$

$$\boxed{\therefore \int_a^b f(x)\, dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]}$$

is called <u>Simpson's $\frac{1}{3}$ Rule</u>

<u>Error</u>

$$E_1 = \int_{x_0}^{x_2} \underbrace{f^{(IV)}(\xi(x))}_{\text{Max}} \frac{(x-x_1)^4}{24} dx$$

$$= f^{(IV)}(\xi) \int_{x_0}^{x_2} \frac{(x - x_1)^4}{24} dx$$

$$= f^{(IV)}(\xi) \left[\frac{(x-x_1)^5}{120} \right]_{x_0}^{x_2}$$

$$= f^{(IV)}(\xi)\left[\frac{(x_2-x_1)^5-(x_0-x_1)^5}{120}\right]$$

$$= f^{(IV)}(\xi)\,\frac{\cancel{2}h^5}{\cancel{120}\,60}$$

$$E_2 = -\frac{h^2}{12}\times\frac{h^3}{3}f^{(IV)}(\xi)$$

$$\therefore \text{Error} = E_1 + E_2$$

$$= f^{(IV)}(\xi)\left[\frac{h^5}{60}-\frac{h^5}{36}\right]$$

$$\boxed{\text{Error} = -\frac{h^5}{90}f^{(IV)}(\xi)}$$

Trapezoidal Rule: $n=1$

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right] - \frac{h^3}{12} f^{(11)}(\xi)$$

Simpson's $\frac{1}{3}$ Rule. $n=2$

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1) + f(x_2)\right] - \frac{h^5}{90} f^{(IV)}(\xi)$$

Simpson's $\frac{3}{8}$ Rule: [3rd Lagrange polynomials)

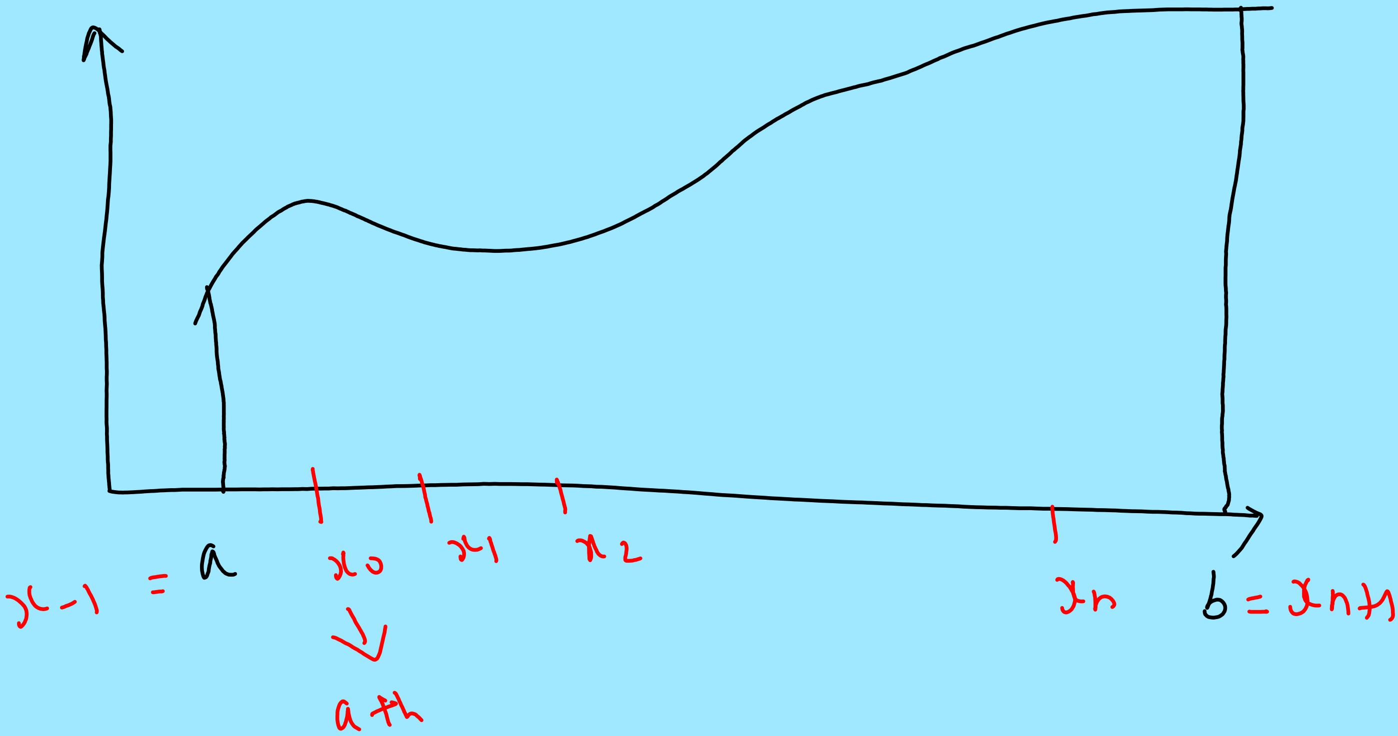
$n=3$

$$\int_a^b f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2) + f(x_3)\right] - \frac{3h^5}{80} f^{(IV)}(\xi)$$

All the above formula's are called as Closed Newton-Cotes formula.

Open Newton-Cotes formulas

* The open Newton-Cotes formula do not includes the endpoints of $[a,b]$



$$x_i = x_0 + ih, \quad i = 0, 1, 2, \ldots n$$

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

$$x_0 = a+h$$

$$x_n = b-h$$

Most common open Newton-Cotes formulas:

n = 0 Mid point rule

$$\int_{a=x_{-1}}^{b=x_1} f(x)\,dx = 2h\, f(x_0) + \frac{h^3}{3} f''(\xi)$$

$$x_{-1} < \xi < x_1$$

n = 1

$$\int_{a=x_{-1}}^{b=x_2} f(x)\,dx = \frac{3h}{2}\left[f(x_0) + f(x_1) \right] + \frac{3h^3}{4} f''(\xi)$$

$$x_{-1} < \xi < x_2$$

n = 2

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2) \right] + \frac{14h^5}{45} f^{(iv)}(\xi)$$

$x_{-1} < \xi < x_3$

$\underline{\underline{n=3}}$

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}\Big[11 f(x_0) + f(x_1) + f(x_2) + 11 f(x_3)\Big] + \frac{95}{144} h^5 f^{(IV)}(\xi)$$

where $x_{-1} < \xi < x_4$

1) Compare the results of closed and open Newton-Cotes formula with exact

Exact value

Solution $\int_0^{\pi/4} \sin x \, dx = 0.29289322$

$\underline{\underline{\text{Sol:}}}$

<u>Closed formula:</u>

<u>$n=1$ Trapezoidal rule</u>

$$h = \frac{b-a}{n} = \frac{\pi/4 - 0}{1} = \pi/4$$

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(x_0) + f(x_1) \right]$$

$$x_0 = 0 \; ; \quad x_1 = \pi/4$$

$$\int_0^{\pi/4} \sin x \, dx = \frac{\pi/4}{2}\left[f(0) + f(\pi/4) \right]$$

$$= 0.27768018$$

$n = 2$ Simpson's $\frac{1}{3}$ Rule:

$$h = \frac{b-a}{n} = \pi/8$$

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2) \right]$$

$$x_0 = 0 \; ; \quad x_1 = x_0 + h = \pi/8$$

$$x_2 = x_0 + 2h = \pi/4$$

$$\int_0^{\pi/4} \sin x \, dx = 0.2929326\text{4}$$

$n = 3$ Simpson's $\frac{3}{8}$ Rule

$$h = \frac{b-a}{n} = \frac{\pi}{12}$$

$x_0 = 0; \quad x_1 = \frac{\pi}{12}; \quad x_2 = \frac{\pi}{6}; \quad x_3 = \frac{\pi}{4}$

$$\int_a^b f(x)\,dx = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right]$$

$$\int_0^{\pi/4} \sin x \, dx = 0.29291070$$

n	App value	Exact value	|Error|
1	0.27768018	0.29289322	10^{-2} 0.015213
2	0.29293264	"	10^{-5} 0.0000394
3	0.29291070	"	10^{-5} 0.00001748

Open Newton-Cotes formula:

$n=0$

$$\int_a^b f(x) = 2h\, f(x_0)$$

$$h = \frac{b-a}{n+2} = \frac{\pi/4}{2} = \frac{\pi}{8}$$

$$x_0 = a+h = 0+\pi/8 = \pi/8$$

$$\int_0^{\pi/4} \sin x\, dx = 2\left(\frac{\pi}{8}\right) f(x_0)$$

$$= 0.30055887$$

$n=1$

$$\int_a^b f(x)\, dx = \frac{3h}{2}\left[f(x_0) + f(x_1)\right]$$

$$h = \frac{b-a}{n+2} = \frac{\pi/4}{3} = \frac{\pi}{12}$$

$$x_0 = a+h = \frac{\pi}{12}$$

$$x_1 = a+2h = \pi/6$$

$$\int_0^{\pi/4} \sin x\, dx = 0.29798754$$

$\underline{\underline{n=2}}$

$$\int_a^b f(x)\,dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right]$$

$$h = \frac{b-a}{n+2} = \frac{\pi/4}{4} = \frac{\pi}{16}$$

$$x_0 = a + h = \frac{\pi}{16}$$

$$x_1 = \pi/8 \;; \quad x_2 = \frac{3\pi}{16}$$

$$\int_0^{\pi/4} \sin x \, dx = 0.29285866$$

$\underline{\underline{n=3}}$

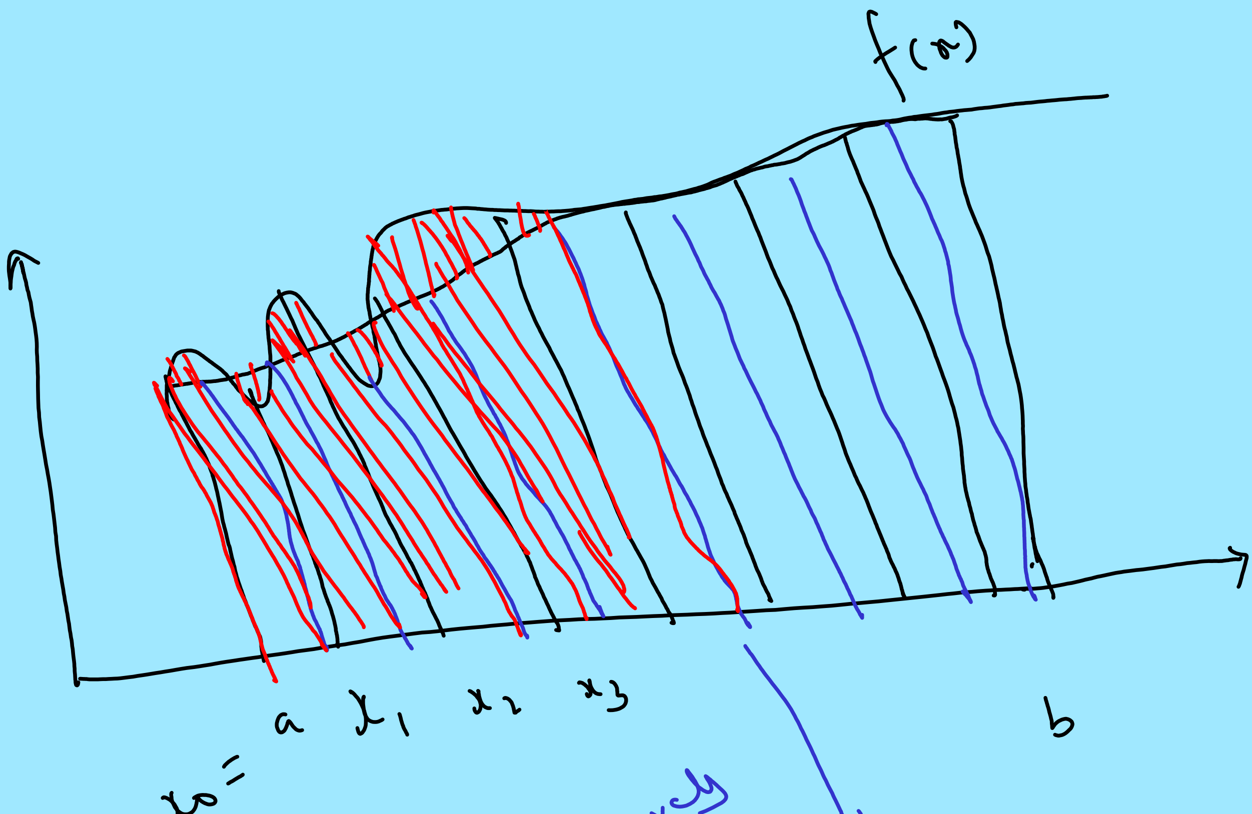
$$\int_a^b f(x)\,dx = \frac{5h}{24}\left[11 f(x_0) + f(x_1) + f(x_2) + 11 f(x_3)\right]$$

$$h = \frac{b-a}{n+2} = \frac{\pi}{20} \qquad x_0 = \pi/20 \;; \quad x_1 = \frac{\pi}{10}$$

$$x_2 = \frac{3\pi}{20} \;; \quad x_4 = \frac{\pi}{5}$$

$$\int_0^{\pi/4} \sin x \, dx = 0.29286923$$

n	App. Value	Exact Value		|Error|
0	0.3005587	0.29289322	$O(h^3)$	0.007665 (10^{-3})
1	0.29798754	"	$O(h^3)$	0.00509432 (10^{-3})
2	0.29285866	"	$O(h^5)$	0.00003456 (10^{-5})
3	0.29286923	"	$O(h^5)$	0.00002399 (10^{-5})

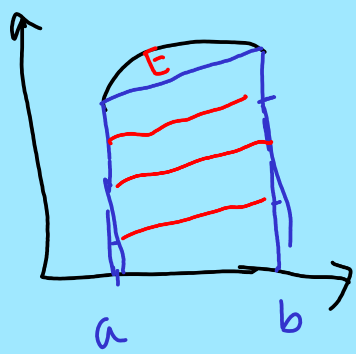


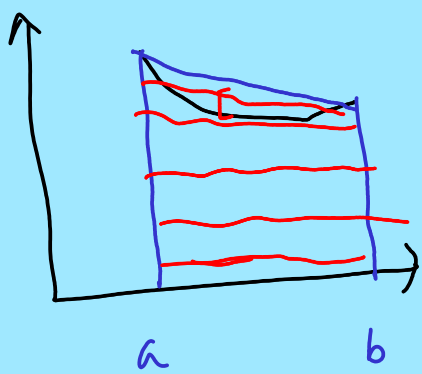
Equally spaced intervals → n large → computational time is too high

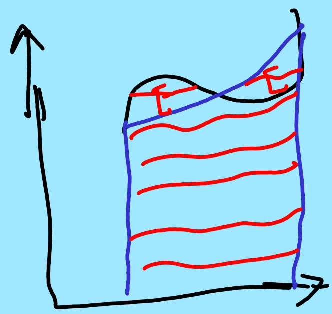
Gaussian Quadrature:

* Newton cotes formula is exact when app. the integral of any polynomial of degree less than (or) equal n.

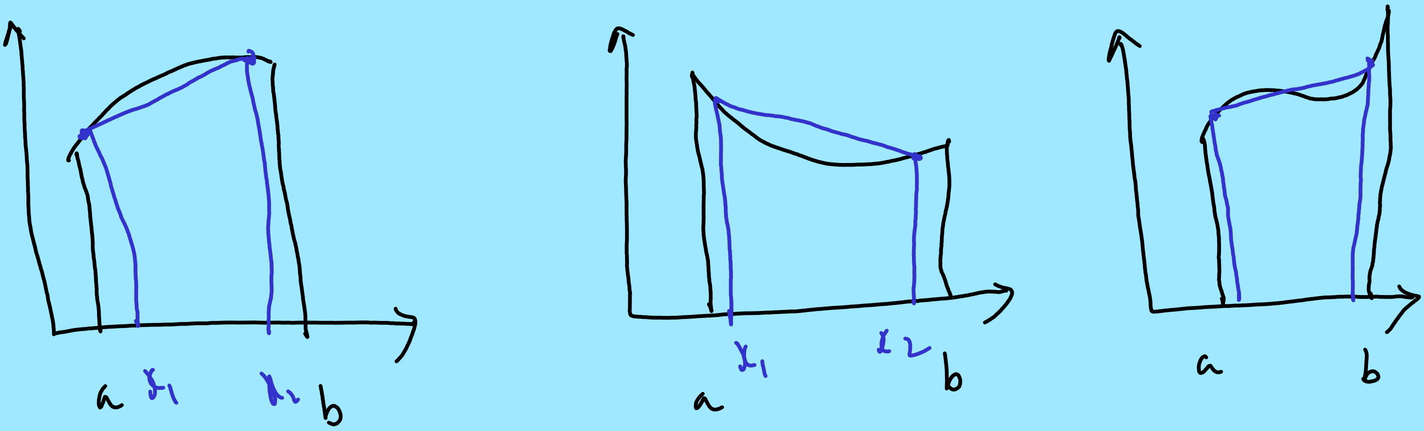
* Newton cotes formulas use values of the function at equally spaced points.







Trapezoidal Rule



Gaussian Quadrature

* The Trapezoidal rule approximating the integral of $f(x)$ by integrating <u>the linear function</u> that joins endpoints of the graph of function.

* It is not likely the best approximation.

* Gaussian Quadrature chooses the pts for evaluation in an optimal rather than equally spaced way.

The nodes $x_1, x_2, \ldots x_n$ in $[a,b]$ and co-efficients $c_1, c_2, \ldots c_n$ are to be chosen to minimize the expected error

$$\int_a^b f(x)\,dx \simeq \sum_{i=1}^{n} c_i f(x_i)$$

* $c_1, c_2, \ldots c_n$ are arbitrary
* $x_1, x_2, \ldots x_n$ are restricted only by the fact that they lie in $[a,b]$
* $2n$ parameters to choose
* If the co-effs of a polynomial are considered parameters, then polynomial of degree at most $2n-1$ contains $2n$ parameters

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0$$

$n+1$

* Procedure for choosing the appropriate parameters when $\underline{\underline{n=2}}$ in $[-1,1]$

Suppose we want to find

c_1, c_2, x_1, x_2 so that

$$\int_{-1}^{1} f(x)\,dx \simeq c_1 f(x_1) + c_2 f(x_2)$$

gives exact result whenever

$f(x)$ is a polynomial of degree

$2(2)-1 = 3$. (or) less

It means

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

$$\int f(x)\,dx = \int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\,dx$$

$$= c_1 f(x_1) + c_2 f(x_2)$$

It will give exact result when

$f(x)$ is $1, x, x^2, x^3$.

$\therefore$ we need c_1, c_2, x_1, x_2 such that

$f(x)=1 \Rightarrow \quad c_1 + c_2 = \int_{-1}^{1} 1\,dx = 2$ — (1)

$f(x)=x \Rightarrow \quad c_1 x_1 + c_2 x_2 = \int_{-1}^{1} x\,dx = 0$ — (2)

$f(x)=x^2 \Rightarrow \quad c_1 x_1^2 + c_2 x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}$ — (3)

$f(x)=x^3 \Rightarrow \quad c_1 x_1^3 + c_2 x_2^3 = \int_{-1}^{1} x^3\,dx = 0$ — (4)

Solve (1), (2), (3), (4)

$c_1 = 1$

$c_2 = 1$

$x_1 = -\frac{\sqrt{3}}{3} = \frac{-1}{\sqrt{3}}$

$x_2 = \frac{\sqrt{3}}{3} = \frac{1}{\sqrt{3}}$

$$\therefore \boxed{\int_{-1}^{1} f(x)\,dx \simeq f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

n	x_i	c_i
2	0.5773502692	1
	-0.5773502692	1
3	0.7745966692	0.5555556
	0	0.8888889
	-0.774596692	0.5555556

* Above tabule values are calculated using the Legendre polynomial.

1) Approximate $\int_{-1}^{1} e^{x} \cos x \, dx$ with $n=2$, $n=3$.

Sol:

$$\int_{-1}^{1} f(x) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

$n=2$

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

$$\therefore \int_{-1}^{1} e^{x} \cos x = e^{-1/\sqrt{3}} \cos \frac{-1}{\sqrt{3}} + e^{1/\sqrt{3}} \cos \frac{1}{\sqrt{3}}$$

$$= 1.96297$$

$n=3$

$$\int_{-1}^{1} f(x)\, dx = (0.55556)\, f(+0.7745967)$$

$$+ (0.88889)\, f(0)$$

$$+ (0.55556)\, f(-0.7745967)$$

$$= 1.9334$$

$$\int_{-1}^{1} e^{x} \cos x \, dx = R.P \int_{-1}^{1} e^{(x+ix)} \, dx$$

$$\frac{e^{i\theta}+e^{-i\theta}}{2}=\cos\theta$$

$$= R.P \int_{-1}^{1} e^{(1+i)x}\,dx$$

$$= R.P \left[\frac{e^{(1+i)x}}{1+i}\right]_{-1}^{1}$$

$$= R.P \left[\frac{e^{(1+i)} - e^{-(1+i)}}{1+i}\right]$$

$$= R.P \quad \frac{e(\cos 1 + i\sin 1) - e^{-1}(\cos 1 - i\sin 1)}{1+i}$$

$$= R.P \quad \frac{(e\cos 1 - e^{-1}\cos 1) + i(e\sin 1 + e^{-1}\sin 1)}{1+i}$$

$$= \frac{R.P}{2} \quad (e\cos 1 - e^{-1}\cos 1) + i(e\sin 1 + e^{-1}\sin 1)\,(1-i)$$

$$= \frac{(e\cos 1 - e^{-1}\cos 1) + (e\sin 1 + e^{-1}\sin 1)}{2}$$

$$= (e - e^{-1})\cos 1 + (e+e^{-1})\sin 1 \Big|_{2}$$

$$= 1.933\,4214$$

$\therefore$ Absolute Error $= \underline{\underline{3.2 \times 10^{-5}}}$

1) Evaluate $\displaystyle\int_1^3 x^6 - x^2 \sin 2x \, dx = 317.3442466$

Closed Newton-Cotes Formula $n=2$

$h=1$

1 3

(Simpson's 1/3 Rule)

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

$$h = \frac{b-a}{n} = \frac{3-1}{2} = 1$$

$x_0 = 1$

$x_1 = 2$

$x_2 = 3$

$$\int_1^3 x^6 - x^2 \sin 2x \, dx = \frac{1}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

$$= \frac{1}{3}\left[f(1) + 4f(2) + f(3)\right]$$

$$= 333.23809$$

Open Newton-Cotes formula. $\underline{\underline{n=2}}$

$$\int_a^b f(x)\,dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right]$$

$$h = \frac{b-a}{n+2} = \frac{3-1}{4} = \frac{1}{2}$$

$x_0 = 1+h$
$= 1.5$
$x_1 = 2$
$x_2 = 2.5$

$$\therefore \int_1^3 x^6 - x^2 \sin 2x\,dx = \frac{4(1/2)}{3}\left[2f(1.5) - f(2) + 2f(2.5)\right]$$

$$= 303.5912$$

Gaussian Quadrature when $n=3$

$$\int_{-1}^{1} f(x)\,dx = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3)$$

$$\int_1^3 x^6 - x^2 \sin 2x\,dx$$

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)t + (b+a)}{2}\right)\left(\frac{b-a}{2}\right)dt$$

$a = 1\,;\ b = 3$

$$x = \frac{2t + \cancel{4}}{2} = t + 2$$

$x = 1 \Rightarrow t = -1$

$x = 3 \Rightarrow t = 1$

$$\therefore \int_1^3 x^6 - x^2 \sin 2x \, dx = \int_{-1}^{1} f(t+2)\left(\frac{3-1}{2}\right)dt$$

$$= \int_{-1}^{1} (t+2)^6 - (t+2)^2 \sin 2(t+2)\,dt$$

$$\int_{-1}^{1} f(t+2)\,dt = (0.55556)\, f(-0.7745967+2)$$

$$+ (0.88889)\, f(0+2)$$

$$+ (0.55556)\, f(0.7745967+2)$$

$= 317.2641$

Error

Closed NCF: $n = 2$ $|E_1| = 15.8938$

Open NCF $n = 2$ $|E_2| = 13.7534$

Gauss Qua $n = 3$ $|E_3| = 0.080096$

10^{-2}