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Numerical Integration

Newton - Cotes Formula :

- Definite integral,

$$I(f) = \int_a^b \underbrace{f(x)}_{\text{continuous over } [a,b]} dx$$

By definition an integral is an infinite sum. But when we integrate numerically, it is not possible to perform.

⇒ Replace $f(x)$ by n degree polynomial that passes through $(n+1)$ nodes : $x_0, x_1, \dots, x_n$.

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

$$= \int_a^b \sum_{k=0}^{n} \overbrace{l_k(x)}^{\text{lagrange basis}} \underbrace{f(x_k)}_{\text{fixed values of function at nodal points}} dx$$

[Using lagrange basis for n degree polynomial]

$$= \sum_{k=0}^{n} f(x_k) \underbrace{\int_a^b l_k(x)\, dx}_{\text{weight function, } \sigma_k}$$

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

⟵ Quadrature formula

σ_k : coefficients

x_k : quadrature point /abscissas

- If nodes are equidistant, this is Newton-Cotes formula.

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Newton-Cotes Formula

Closed Newton-Cotes

- Nodes $\boxed{\text{equidistant}}$ + interval $[a,b]$ such that

$$\boxed{a = x_0 < x_1 < \dots < x_{n-1} < x_n = b}$$

Using $h = \frac{b-a}{n}$,

$$x_1 = x_0 + h, \quad x_2 = x_1 + h, \dots$$
$$= x_0 + 2h$$

Open Newton-Cotes

- Nodes $\boxed{\text{equidistant}}$ + interval $[a,b]$ such that

$$\boxed{a < x_0 < x_1 < \dots < x_{n-1} < x_n < b}$$

where,

$$x_i = a + (i+1)h \quad ; i = 0, 1, \dots, n$$

and

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

width of function

(?) **Trapezium rule :**

⇒ It is a closed newton-cotes formula with $n = 1$, as there are 2 nodes, $x_0 = a$, $x_1 = b$

interval $[a,b] = [x_0, x_1]$

$$\therefore h = \frac{b-a}{1} = b - a$$

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

[Degree 1 polynomial in lagrange basis]

$$= l_0(x)\, f(a) + l_1(x)\, f(b)$$

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

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$$= \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)$$

Weight factors,

$$\sigma_0 = \int_a^b l_0(x)\, dx = \int_a^b \frac{x-b}{a-b}\, dx = \frac{1}{a-b}\int_a^b (x-b)\, dx$$

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

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

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

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

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

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

$$\sigma_1 = \int_a^b l_1(x)\, dx = \int_a^b \frac{x-a}{b-a}\, dx$$

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

$$= \frac{1}{b-a}\left[\frac{b^2}{2} \cancel{-b^2} - ab - \frac{a^2}{2} + a^2\right]$$

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

$$\therefore I_1(f) = \sigma_0 f(a) + \sigma_1 f(b) = \frac{b-a}{2}\left(f(a) + f(b)\right)$$ Trapezoidal rule

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

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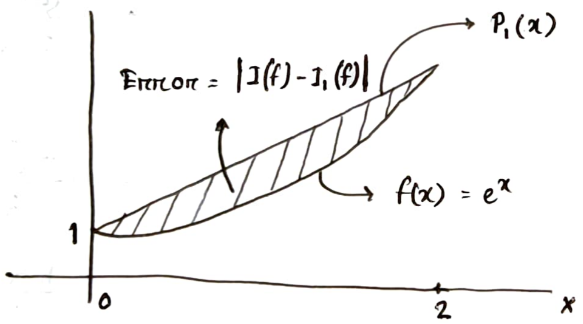
For $a = 0,\ b = 2$ & $f(x) = e^x$:

$$I_1 = \frac{2-0}{2}\left(e^0 + e^2\right) = 8.389 \text{ upto 4 s.f.}$$

Exact result : $I = \int_0^2 e^x\,dx = \left[e^x\right]_0^2 = e^2 - e^0 = 6.389$ upto 4 s.f.

$\therefore$ Actual relative error $= \left|\frac{I - I_n}{I}\right| \times 100\% = 31\%$

Too much error. We need higher order polynomial to reduce the error of numerical integration.



Error Calculation :

If $f(x)$ is interpolated by degree n polynomial $P_n(x)$, Upper bound of interpolation error,

Cauchy's formula →
$$\left|\frac{f^{n+1}(\xi)}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n)\right| \quad \text{where } \xi \in [a,b]$$

$\therefore$ Upper bound of error of numerical integration :

$$|I - I_n| <= \left|\frac{f^{n+1}(\xi)}{(n+1)!}\right|_{\max\ \xi \in [a,b]} \int_a^b \left|(x-x_0)(x-x_1)\cdots(x-x_n)\right| dx$$

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(7) $n=1$, $f(x)=e^{x}$, $a=0$, $b=2$

for Trapezium rule example

$$\left|\frac{f^{n+1}(\xi)}{(n+1)!}\right|_{max}\ \xi\in[a,b] = \left|\frac{f^{2}(\xi)}{2!}\right|_{max}\ \xi\in[0,2]$$

$$=\left[\frac{1}{2}e^{\xi}\right]_{max}\ \xi\in[0,2]$$

$$=\frac{e^{2}}{2}$$

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

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

$$=\left|-\frac{4}{3}\right| = \frac{4}{3}$$

$$\therefore |I-I_n| \le \frac{e^2}{2}\times\frac{4}{3}$$

$$\le 4.926 \quad \text{upto 4 s.f.}$$

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Composite Newton-Cotes formula :

- Improves the result / decrease the error without increasing actual node numbers.

Basic idea

• Divide the interval $[a,b]$ into m-subintervals of equal width. For each one, apply trapezoidal rule and add them up. The sum is denoted by $C_{1,m}(f) \Rightarrow$ composite newton-cotes formula.

$h = \frac{b-a}{m}$ for m-subinterval

$\therefore$ Trapezoidal rule for each interval,

$$I_{1,i} = \frac{h}{2}\left[f(x_i) + f(x_{i+1})\right] \quad ; \; i = 0, 1, 2, \ldots, (m-1)$$

$$\therefore C_{1,m}(f) = \sum_{i=0}^{m-1} I_{1,i}$$

$$= \frac{h}{2}\left[f(x_0) + 2f(x_1) + \cdots + 2f(x_{m-1}) + f(x_m)\right]$$

Will not change with the value of m

(?) $a = 0,\ b = 2,\ f(x) = e^x$

For same example

For $m = 2$:

$h = \frac{b-a}{m} = 1 \quad \therefore a = x_0,\ x_1 = a+h,\ x_2 = b$

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

$$= \frac{1}{2}\left(e^0 + 2e^1 + e^2\right) = 6.91281 \ldots \text{ Upto 6 s.f.}$$

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For $m = 3$:

$h = \frac{b-a}{m} = \frac{2}{3}$, $a = x_0$, $x_1 = a+h$, $x_2 = x_1 + h$, $x_3 = b$

$\Rightarrow x_0 = 0$, $x_1 = 2/3$, $x_2 = 4/3$, $x_3 = 2$

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

$$= \frac{1}{3}\left(e^0 + 2e^{2/3} + 2e^{4/3} + e^2\right)$$

$$= 6.62395 \text{ upto } 6 \text{ s.f.}$$

m	h	$C_{1,m}$	$\lvert I - C_{1,m}\rvert = \lvert 6.389 - C_{1,m}\rvert$
1	2	8.389	2
2	1	6.913	0.524
3	2/3	6.624	0.235
4	1/2	6.522	0.133
8	0.25	6.422	0.033
16	0.125	6.397	0.008
32	0.0625	6.391	0.002

- Error $\downarrow$ as m $\uparrow$

- Here, error decreases by a factor of 4 when we halve the h. $\Rightarrow$ Quadratic convergence, $O(h^2)$

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Exactness :

Upper bound of error,

$$\left| \frac{f^{n+1}(\xi)}{(n+1)!} (x-x_0)(x-x_1)\cdots(x-x_n) \right| \quad \text{where } \xi \in [a,b]$$

$\boxed{\text{If } f^{n+1} = 0}$, error is zero.

Newton-cotes formula will give exact answer.

$f(x)$ is an n-degree polynomial, $P_n(x)$.

- Trapezium rule $I_1(f)$ is exact for all functions $f(x) = P_1(x)$.

* **Definition :**

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

Meaning

⇒ If we replace $f(x)$ by $P_n(x)$ and compute the exact & numerical result, the error will be zero when both the results are ~~would~~ be equal. So what is the largest integer n for which this equality holds.

↓

Degree of exactness

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- **Check-points :**

  - $n=1 \Rightarrow$ Trapezoidal rule : $\frac{b-a}{2}\left[f(a)+f(b)\right]$

  - $n=2 \Rightarrow$ Simpson's rule : $\frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$

(?) For $n=2$, newton-cotes formula,

$$I_2(f) = \sum_{k=0}^{2} \sigma_k f(x_k)$$

Here, $x_0 = a \quad , \quad x_1 = m \quad , \quad x_2 = b$

$\Downarrow$

as it is a closed form, ~~m~~ ~~mu~~ x_1 must be in the middle

$\therefore \; m-a = b-m$

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

weight factors,

$$\sigma_0 = \int_a^b l_0(x)\,dx = \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= \frac{h}{3}\left[f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right]$$ ← Simpson's rule

(?)	Function	Degree of polynomial	Exact	Newton-Cotes [Simpson's rule]	Result
01.	$f(x) = 1$	Zero	$I(f) = I(1)$ $= \int_a^b 1 \, dx$ $= b-a$	$I_2(1) =$ $\frac{b-a}{6}(1+4+1)$ $= b-a$	Equal
02.	$f(x) = x$	One	$I(f) = I(x) = \int_a^b x \, dx$ $= \frac{1}{2}(b^2-a^2)$	$I_2(x) = \frac{b-a}{6}\left(a + 4 \times \frac{a+b}{2} + b\right)$ $= \frac{1}{2}(b^2-a^2)$	Equal
03.	$f(x) = x^2$	Two	$I(f) = I(x^2) = \int_a^b x^2 \, dx$ $= \frac{1}{3}(b^3-a^3)$	$I_2(x^2) = \frac{b-a}{6}\left[a^2 + 4 \times \left(\frac{a+b}{2}\right)^2 + b^2\right]$ $= \frac{1}{3}(b^3-a^3)$	Equal
04.	$f(x) = x^3$	Three	$I(f) = I(x^3) = \int_a^b x^3 \, dx$ $= \frac{1}{4}(b^4-a^4)$	$I_2(x^3) = \frac{b-a}{6}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right]$ $= \frac{b-a}{12}\left[2a^3 + (a+b)^3 + 2b^3\right]$ $= \frac{b-a}{12} \times 3(b+a)(a^2+b^2)$ $= \frac{1}{4}(b^4-a^4)$	Equal

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	Function	Degree of polynomial	Exact	Newton-cotes	Result
05.	$f(x) = x^4$	Four	$I(f) = I(x^4)$ $= \int_a^b x^4 \, dx$ $= \frac{1}{5}(b^5 - a^5)$	$I_2(x^4) = \frac{b-a}{6}\left[a^4 + 4\left(\frac{a+b}{2}\right)^4 + b^4\right]$ $= \frac{b-a}{24}\left[4a^4 + (a+b)^4 + 4b^4\right]$	Not Equal

$\therefore$ Simpson's formula gives exact result upto degree 3 polynomial and error becomes non-zero from degree four & higher.

$\Rightarrow$ Degree of exactness of simpson rule = 3 (exactly)