V - Numerical Integration

1. Introduction

(*) **Task**: Compute $\int_a^b f(x)\,dx$ where

- $f(x)$ has a difficult functional form
- One wants to fit an area under a curve which does not have a known functional form (for instance, data)

(Remember: a definite integral yields an area under a curve)

2 - Basic methods (Quadrature):

(*) **Procedure**: $\int_a^b f(x)\,dx \simeq \sum_{i=0}^{n} a_i f(x_i)$

(one approximates the integral by a sum)

- Step 1: We select a set of nodes $\{x_0, \dots, x_n\}$ from $[a, b]$

Step 2: We integrate the n-th Lagrange interpolati[on] polynomial

$$\int_a^b f(x)\,dx \approx \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x)\,dx = \sum_{i=0}^{n} \int_a^b f(x_i) L_i(x)\,d[x]$$

$$\Rightarrow a_i = \int_a^b L_i(x)\,dx \qquad i = 0, 1, \dots, n$$

Error : $E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i) f^{(n+1)}(\xi(x))\, dx$

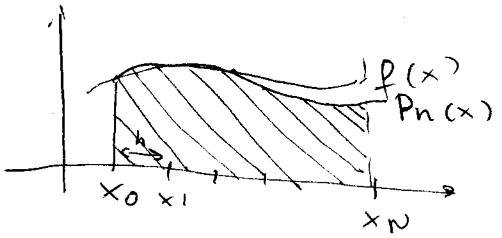
(from the Lagrange error formula)

2.1 - Newton-Cotes formulae

2.1.1 (n+1)-point closed Newton-cotes formula:

Nodes : $x_i = x_0 + ih$, $i = 0, 1, \dots, n$ with $x_0 = a$, $x_n = b$, $h = \frac{(b-a)}{n}$

$\int_a^b f(x)\, dx \approx \int_a^b P_n(x)\, dx$ passing through the n nodes (equally spaced)



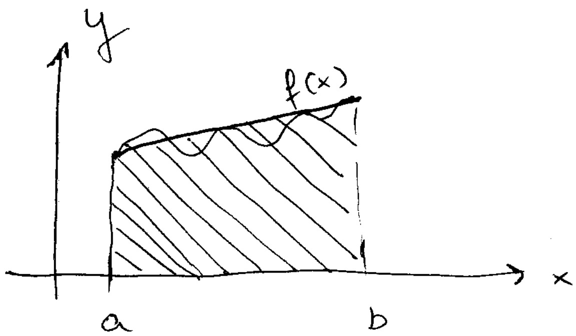
Specific cases:

* Trapezoidal rule ($n = 1$) : $\int_a^b f(x)dx \approx \int_a^b \underbrace{P_1(x)}_{\text{1st Lagrange interpolating polynomial}} dx$

$$\int_a^b P_1(x)\, dx = \frac{f(b)}{b-a} \int_a^b (x-a)\, dx + - \frac{f(a)}{b-a} \int_a^b (x-b)\, dx = \frac{f(b)}{b-a} \left[\left[\frac{x^2}{2} - ax \right] \right]_a^b - \frac{f(a)}{b-a} \left[\frac{x^2}{2} - bx \right]_a^b =$$

$$= \frac{1}{2} (f(b) + f(a)) \underbrace{(b-a)}_{h}$$

Error: $\frac{1}{2}\int_a^b f''(\xi)(x-a)(x-b)\,dx = \frac{1}{2} f''(\xi)\int_a^b (x^2-(a+b)x+ab)\,dx$



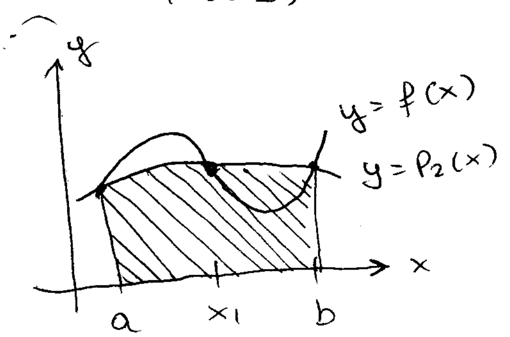
$= \frac{1}{2} f''(\xi)\left[\frac{x^3}{3} - \frac{(a+b)}{2}x^2 + abx\right]_a^b$

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

⊛ Simpson's rule: $\int_a^b f(x)\,dx \approx \int_a^b P_2(x)\,dx \approx \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] + \frac{h^5}{90} f^{(4)}(\xi)$

$(n=2)$

$P_2(x)$ → 2nd Lagrange interpolating polynomial



Nodes: $x_0 = a$
$x_1 = a+h$
$x_2 = b$

Increment: $h = \frac{b-a}{2}$

Proof: $P_2(x) = \frac{f(x_0)(x-x_1)(x-x_2)}{\underbrace{(x_0-x_1)}_{-h}\underbrace{(x_0-x_2)}_{-2h}} + \frac{f(x_1)(x-x_0)(x-x_2)}{\underbrace{(x_1-x_0)}_{h}\underbrace{(x_1-x_2)}_{-h}}$

$+ \frac{f(x_2)(x-x_0)(x-x_1)}{\underbrace{(x_2-x_0)}_{2h}\underbrace{(x_2-x_1)}_{h}}$

$\int P_2(x)\,dx = \frac{f(x_0)}{2h^2}\int_a^b (x-x_1)(x-x_2)\,dx - \frac{f(x_1)}{h^2}\int_a^b (x-x_0)(x-x_2)\,dx$

$+ \frac{f(x_2)}{2h^2}\int_a^b (x-x_0)(x-x_1)\,dx$

Change of variable: $x = x_0 + ht \Rightarrow dx = h\,dt$

$$\int_{x_0=a}^{x_2=b} f(x)\,dx \approx \frac{f(x_0)}{2h^2}\int_0^2 h^3 \overbrace{(t-1)(t-2)}^{t^2-3t+2}\,dt - \frac{h^3}{h^2}\int_0^2 \overbrace{t(t-2)}^{t^2-2t}\,dt +$$

$$+\frac{f(x_2)}{2h^2}\int_0^2 h^3 (t^2-t)\,dt$$

$$= \frac{f(x_0)h}{2}\left(\frac{t^3}{3}-\frac{3t^2}{2}+2t\right)\Bigg|_0^2 - h f(x_1)\left(\frac{t^3}{3}-t^2\right)\Bigg|_0^2 +$$

$$+\frac{h f(x_2)}{2}\left(\frac{t^3}{3}-\frac{t^2}{2}\right)\Bigg|_0^2$$

$$= \frac{h}{3}\left(f_0 + 4f_1 + f_2\right)$$

$n=3$: Simpson's Three-Eights rule ($f(x) \approx P_3(x)$)

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] - \frac{3h^5}{80} f^{(4)}(\xi)$$

$$(x_0<\xi<x_3)$$

$n=4$:

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)\right.$$
$$\left.+7f(x_4)\right] - \frac{8h^7}{945} f^{(6)}(\xi) \quad (x_0<\xi<x_4)$$

(*) **Error** ((n+1)-point closed Newton-Cotes formula).

- n even:

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!}\int_0^n t^2(t-1)\cdots(t-n)\,dt$$

- n odd:

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt$$

2.1.2 - Open Newton-Cotes formulae

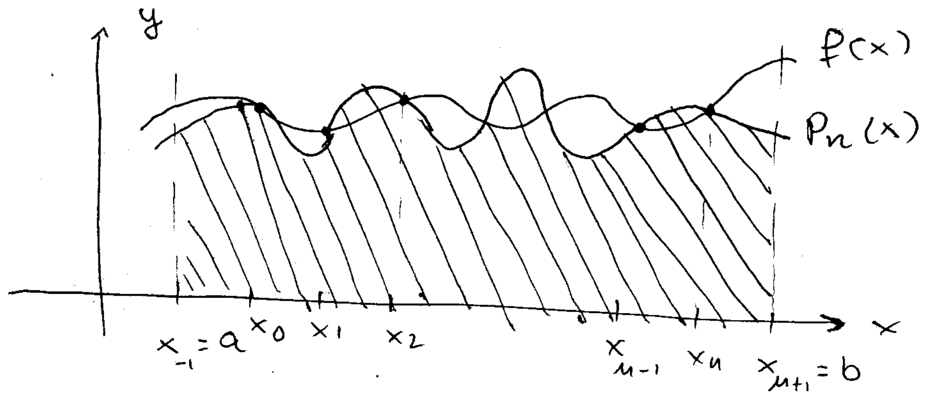
Nodes: $x_i = x_0 + ih$, $i = 0, 1, \ldots, n$ with $h = \frac{(b-a)}{n+2}$

$x_0 = a + h$

$x_n = b - h$

Hence $x_{-1} = a$, $x_{n+1} = b$

$f(x) \approx P_n(x)$ on the open interval (a, b)



$$\int_a^b f(x)\,dx = \int_{x_{-1}}^{x_{n+1}} f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

$$a_i = \int_a^b L_i(x)\,dx$$

Error: • n even:

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt$$

• n odd:

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt$$

Specific cases:

$n=0$ (midpoint rule)

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

$$\approx \int_{x_0-h}^{x_0+h} f(x_0)\,dx = 2h f(x_0)$$

zeroth Lagrange polynomial

$n = 1$

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

$n = 2$

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

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

(*) DRAWBACK: Newton-Cotes formulae are unsuitable over large integration intervals (one would need high-degree formulae)

3 - Composite numerical integration

(*) One uses low-order Newton Cotes formula on consecutive subintervals of $[a,b]$

Step 1: Choose an integer N

Step 2: Subdivide $[a,b]$ into N subintervals

Step 3: Apply the Newton-Cotes formula in question on each consecutive pair of subinterval

(*) 3.1 - Composite Simpson's rule

$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx \approx \sum_{j=1}^{n/2} \left\{ \frac{h}{3} \left[f(x_{2j-2}) + 4 f(x_{2j-1}) + f(x_{2j}) \right] \right\}$$

with $h = \frac{b-a}{n}$, $x_j = a + jh$, $j = 0, 1, \dots, n$

$\frac{n}{2} \equiv$ number of subintervals (n must be even)

Examples

Compute $\int_0^4 e^x dx$ by applying Simpson's rule to the subintervals $[0,2]$ and $[2,4]$

$\frac{n}{2} = 2 \Rightarrow n = 4$; $h = \frac{4}{4} = 1$

$$\int_0^4 e^x dx = \int_0^2 e^x dx + \int_2^4 e^x dx \approx \sum_{j=1}^{2} \left\{ \frac{1}{3} \left[f(x_{2j-2}) + 4 f(x_{2j-1}) + f(x_{2j}) \right] \right\} = \frac{1}{3}\left[e^0 + 4e + e^2 + e^2 + 4e^3 + e^4 \right] = 53.86385$$

3.2 - Composite Trapezoidal rule

$$\int_a^b f(x)\, dx = \frac{h}{2} \left[f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right]$$