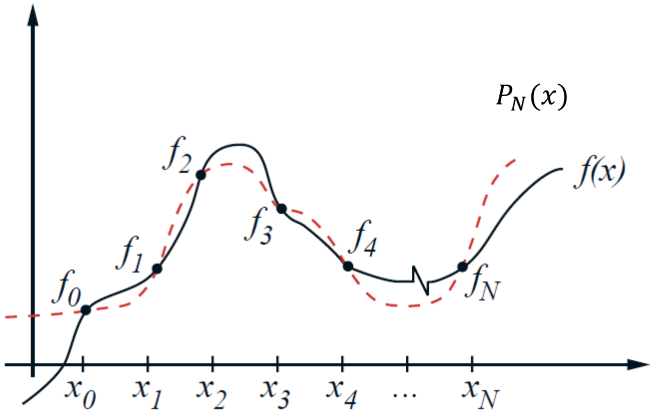
4.3 Numerical Integration

Numerical quadrature: Numerical method to compute $\int_a^b f(x)dx$ approximately by a sum $\sum_{i=0}^{n} f(x_i)a_i$.



The interpolation nodes are given as:

$(x_0\,, \quad f(x_0))$

$(x_1\,, \quad f(x_1))$

$(x_2\,, \quad f(x_2))$

…

$(x_N\,, \quad f(x_N))$

Here $a = x_0$; $b = x_N$. By Lagrange Interpolation Theorem (Thm 3.3):

$$f(x) = \sum_{i=0}^{n} f(x_i)L_{N,i}(x) + \frac{(x-x_0)\cdots(x-x_N)}{(N+1)!} f^{(N+1)}(\xi(x)) \qquad (1)$$

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_{N,i}(x)\,dx + \frac{1}{(N+1)!}\int_a^b (x-x_0)\cdots(x-x_N)f^{(N+1)}(\xi(x))dx$$

Quadrature formula: $\int_a^b f(x)dx \;\approx\; \sum_{i=0}^{n} a_i f(x_i)$ with $a_i = \int_a^b L_{N,i}(x)dx$.

Error: $E(f) = \frac{1}{(N+1)!}\int_a^b (x-x_0)\cdots(x-x_N)f^{(N+1)}(\xi(x))dx$

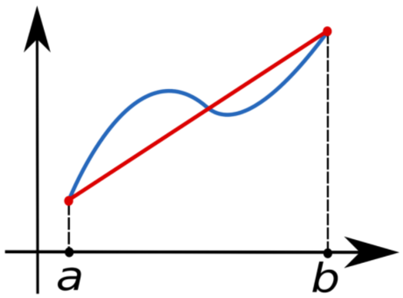


Figure 1 Trapezoidal Rule

The Trapezoidal Rule (obtained by first Lagrange interpolating polynomial)

Let $x_0 = a$; $x_1 = b$; and $h = b - a$. (see Figure 1)

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} \left[f(x_0)\frac{x - x_1}{(x_0 - x_1)} + f(x_1)\frac{x - x_0}{(x_1 - x_0)} \right] dx + \frac{1}{2}\int_{x_0}^{x_1} (x - x_0)(x - x_1) f^{(2)}\big(\xi(x)\big)dx$$

Thus

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

Error term

.

Note: $h = b - a$ for **Trapezoidal rule.**

The Simpson's (1/3) Rule (error obtained by third Taylor polynomial)

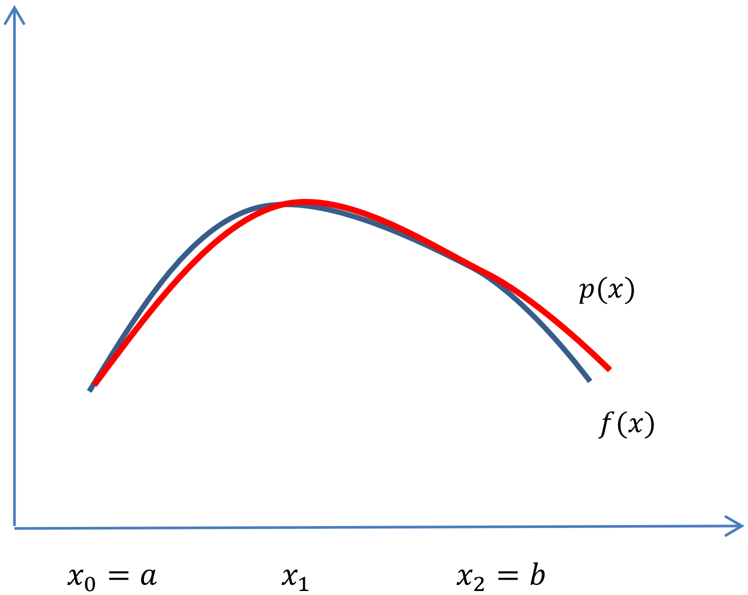


Figure 2 Simpson's Rule

Let $x_0 = a$; $x_1 = \frac{a+b}{2}$; $x_2 = b$; and $h = \frac{b-a}{2}$. (see Figure 2)

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

$$\int_a^b f(x)dx = \int_a^b \left(f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4 \right) dx$$

$$= 2hf(x_1) + \frac{h^3}{3} f''(x_1) + \frac{f^{(4)}(\xi_1)}{60} h^5$$

Now approximate $f''(x_1) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi_2)$

Thus

$$\boldsymbol{\int_a^b f(x)dx = \frac{h}{3}\big(f(x_0) + 4f(x_1) + f(x_2)\big) - \frac{h^5}{90} f^{(4)}(\xi)}$$

Error term

Note: $h = \frac{b-a}{2}$ for **Simpson's rule.**

Precision

Definition: The **degree of accuracy** or **precision** of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \cdots, n$.

Trapezoidal rule has degree of accuracy one.

$\int_a^b x^0 dx = b - a;$ $\quad \int_a^b x^0 dx = \frac{b-a}{2}[1+1] = b - a.$ Trapezoidal rule is exact for 1 (or x^0).

$\int_a^b x dx = \frac{x^2}{2}|_a^b = \frac{b^2-a^2}{2}.$ $\quad \int_a^b x dx = \frac{b-a}{2}[a+b] = \frac{b^2-a^2}{2}.$ Trapezoidal rule is exact for x.

$\int_a^b x^2 dx = \frac{x^3}{3}|_a^b = \frac{b^3-a^3}{3}.$ $\quad \int_a^b x^2 dx = \frac{b-a}{2}[a^2+b^2] \neq \frac{b^3-a^3}{3}$ Trapezoidal rule is **NOT** exact for x^2.

Simpson's rule has degree of accuracy three.

Remark: The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \cdots, n$, but is NOT zero for some polynomial of degree $n + 1$.

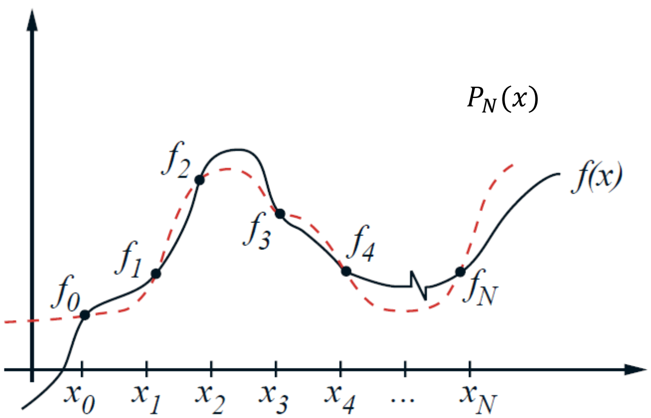


Figure 3 Closed Newton-Cotes Formulas

Closed Newton-Cotes Formulas

Let $a = x_0$; $b = x_N$; and $h = \frac{b-a}{N}$. $\quad x_i = x_0 + ih$, for $i = 0, 1, \cdots, N$.

$\int_a^b f(x)dx \approx \sum_{i=0}^N a_i f(x_i)$ with $a_i = \int_a^b L_{N,i}(x)dx$.

Here $L_{N,i}(x)$ is the ith Lagrange base polynomial of degree N.

Theorem 4.2 Suppose that $\sum_{i=0}^{N} a_i f(x_i)$ is the (n+1)-point closed Newton-Cotes formula with $a = x_0$; $b = x_N$; and $h = \frac{b-a}{N}$. There exists $\xi \in (a,b)$ for which $\int_a^b f(x)dx \approx \sum_{i=0}^{N} a_i f(x_i) + \frac{h^{N+3} f^{(N+2)}(\xi)}{(N+2)!} \int_0^N t^2(t-1)\cdots(t-N)dt$,

if N is even and $f \in C^{N+2}[a,b]$, and

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

if N is odd and $f \in C^{N+1}[a,b]$.

Remark: N is **even**, **degree of precision** is $N+1$. N is **odd**, **degree of precision** is N.

Examples. N=1: Trapezoidal rule; N=2: Simpson's rule.

N=3: Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}\big(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\big) - \frac{3h^5}{80} f^{(4)}(\xi) \quad \text{where } x_0 < \xi < x_3;\ h = \frac{x_3 - x_0}{3}.$$

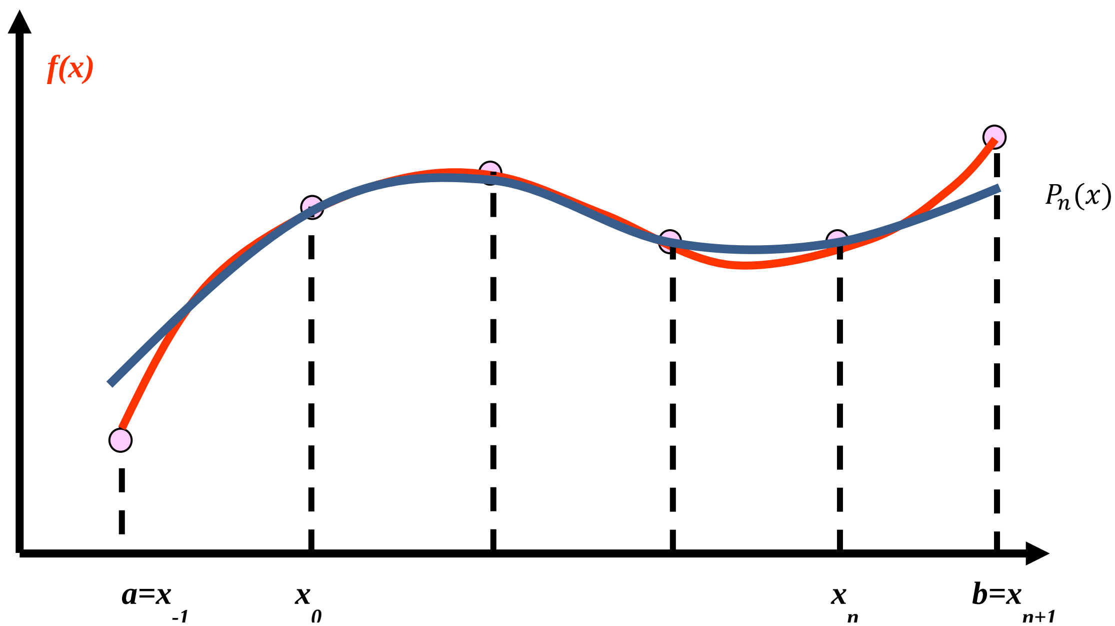


Figure 4 Open Newton-Cotes Formula

Open Newton-Cotes Formula

See Figure 4. Let $h = \frac{b-a}{n+2}$; and $x_0 = a + h$. $x_i = x_0 + ih$, for $i = 0,1,\cdots,n$. This implies $x_n = b - h$.

Theorem 4.3 Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ is the (n+1)-point open Newton-Cotes formula with $a = x_{-1}$; $b = x_{n+1}$; and $h = \frac{b-a}{n+2}$. There exists $\xi \in (a,b)$ for which $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)dt$,

if n is even and $f \in C^{n+2}[a,b]$, and

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

if n is odd and $f \in C^{n+1}[a,b]$.

Examples of open Newton-Cotes formulas

n=0: Midpoint rule (Figure 5)

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

where $x_{-1} < \xi < x_1$. $h = \frac{b-a}{2}$

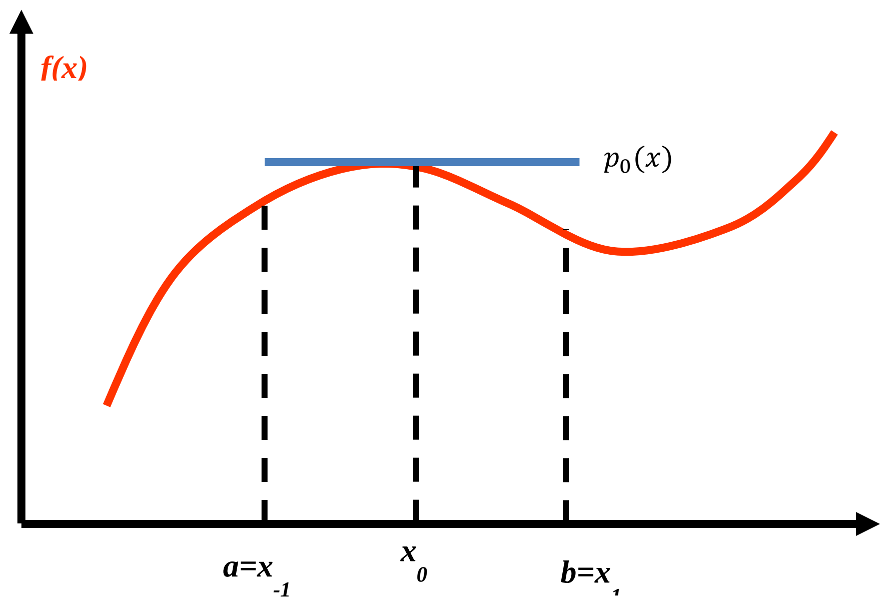


Figure 5 Midpoint rule

n=1: $\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4} f^{(2)}(\xi)$ where $x_{-1} < \xi < x_2$. $h = \frac{b-a}{3}$

n=2: $\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi)$ where $x_{-1} < \xi < x_3$. $h = \frac{b-a}{4}$