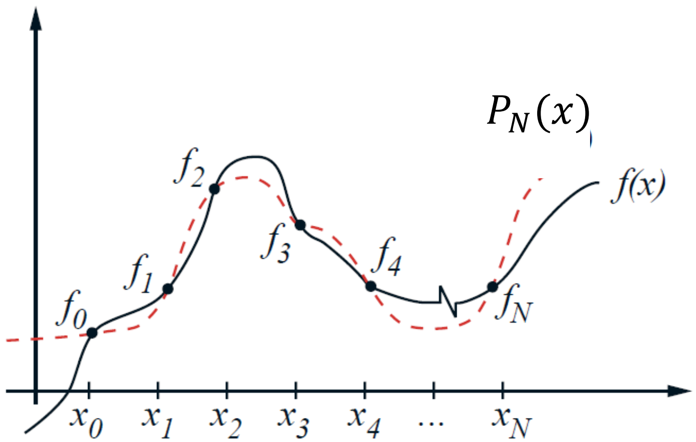
Section 4.3 Numerical Integration

Numerical quadrature: $\int_a^b f(x)dx \approx \sum_{i=0}^{n} f(x_i)a_i$.



The interpolation points are given as:

$$(x_0\,,\quad f(x_0))$$
$$(x_1\,,\quad f(x_1))$$
$$(x_2\,,\quad f(x_2))$$
$$\dots$$
$$(x_N\,,\quad f(x_N))$$

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

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

$$\int_a^b f(x)dx$$

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

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

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

The Trapezoidal Quadrature Rule (obtained by first degree Lagrange interpolating polynomial)

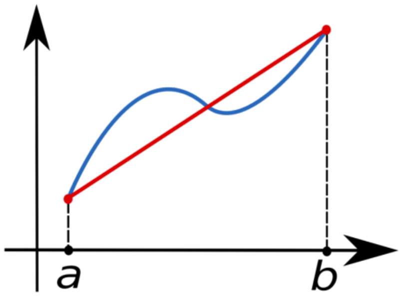


Figure 1 Trapezoidal Rule

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

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

.

Error term

Trapezoidal rule: $\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)]$ with $h = b - a$.

The Simpson's (1/3) Quadrature Rule (Deriving formula by third Taylor polynomial)

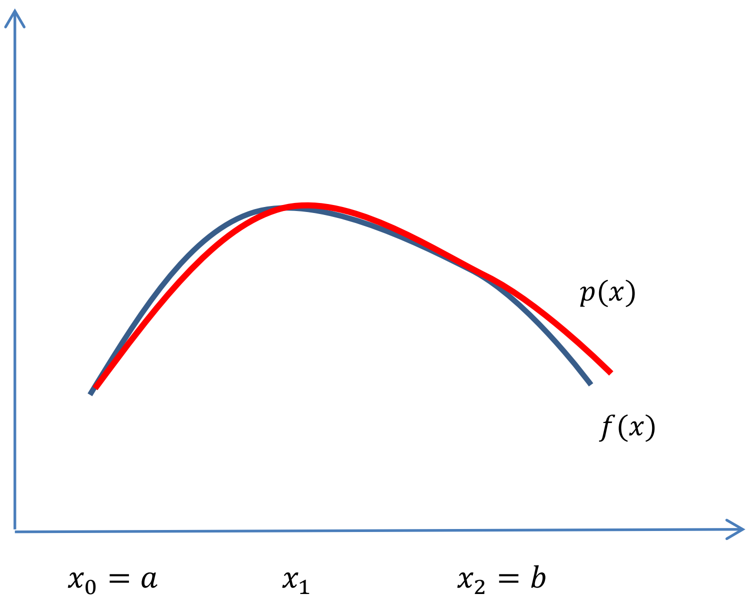


Figure 2 Simpson's Rule

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

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

$$\int_a^b f(x)dx$$

$$= \int_a^b \left(f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 \right.$$

$$\left. + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}\big(\xi(x)\big)}{24}(x - x_1)^4 \right) dx$$

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

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

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

Error term

Simpson's rule: $\boldsymbol{\int_a^b f(x)dx \approx \frac{h}{3}\big(f(x_0) + 4f(x_1) + f(x_2)\big)}$

with $h = \frac{b-a}{2}$.

Remark: When the second degree Lagrange interpolating polynomial is used to derive the Simpson's (1/3) quadrature rule, we do not reveal the most accurate information about error of approximation.

Example 1. Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)dx$ when $f(x)$ is:

(a) x^2; (b) $(x+1)^{-1}$; and (c) $\sin(x)$.

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.

$\int_a^b x^0 dx = b - a$; $\int_a^b x^0 dx = \frac{b-a}{2}[1 + 1] = b - a$.

→Trapezoidal rule is exact for 1 (or x^0).

$\int_a^b x dx = \frac{x^2}{2}|_a^b = \frac{b^2-a^2}{2}$; $\int_a^b x dx = \frac{b-a}{2}[a + b] = \frac{b^2-a^2}{2}$.

→Trapezoidal rule is exact for x.

$\int_a^b x^2 dx = \frac{x^3}{3}|_a^b = \frac{b^3-a^3}{3}$; $\int_a^b x^2 dx = \frac{b-a}{2}[a^2 + b^2] \neq \frac{b^3-a^3}{3}$.

→Trapezoidal rule is **NOT** exact for x^2.

Remark:

1. **Simpson's rule has degree of accuracy three.**
2. 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 $n + 1$.

Exercise 20. Let $h = \frac{b-a}{3}, x_0 = a,\ \ x_1 = a + h,\ \ x_2 = b$. Find degree of precision of quadrature formula $\int_a^b f(x)dx = \frac{9}{4}hf(x_1) + \frac{3}{4}hf(x_2)$.

Closed Newton-Cotes Formulas

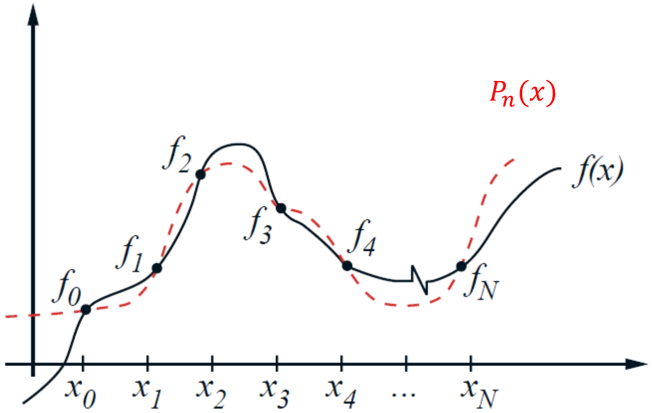


Figure 3 Closed Newton-Cotes Formulas

Let $a = x_0$; $b = x_n$; and $h = \frac{b-a}{n}$.

$x_i = x_0 + ih$, for $i = 0,1,\cdots,n$.

The formula: $\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$

with $a_i = \int_a^b L_{n,i}(x)dx$ is called **Closed Newton-Cotes Formula.** 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

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

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

and

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

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

Remark: Number of nodes n is **even**, **degree of precision** is $n+1$; n is **odd**, **degree of precision** is n.

Examples. degree of precision n=1 for Trapezoidal rule;

degree of precision n=3 for Simpson's rule.

degree of precision n=3 for Simpson's Three-Eighths rule:

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

where $x_0 < \xi < x_3$; $h = \frac{x_3 - x_0}{3}$.

Open Newton-Cotes Formula

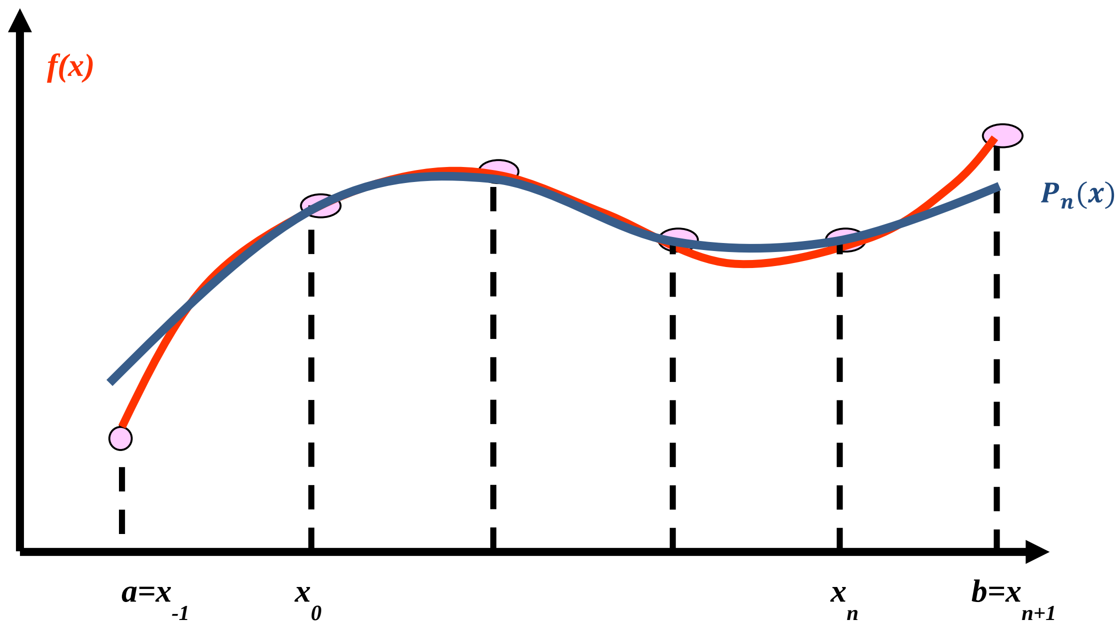


Figure 4 Open Newton-Cotes Formula

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 $x_{-1} = a$; and $x_n = b - h$.

The formula: $\int_a^b f(x)dx \approx \sum_{i=0}^{N} a_i f(x_i)$

with $a_i = \int_{x_{-1}}^{x_{n+1}} L_{n,i}(x)dx$ is called **open Newton-Cotes Formula.** $L_{n,i}(x)$ is the ith Lagrange basis polynomial using nodes $x_0, \ldots, x_n$.

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

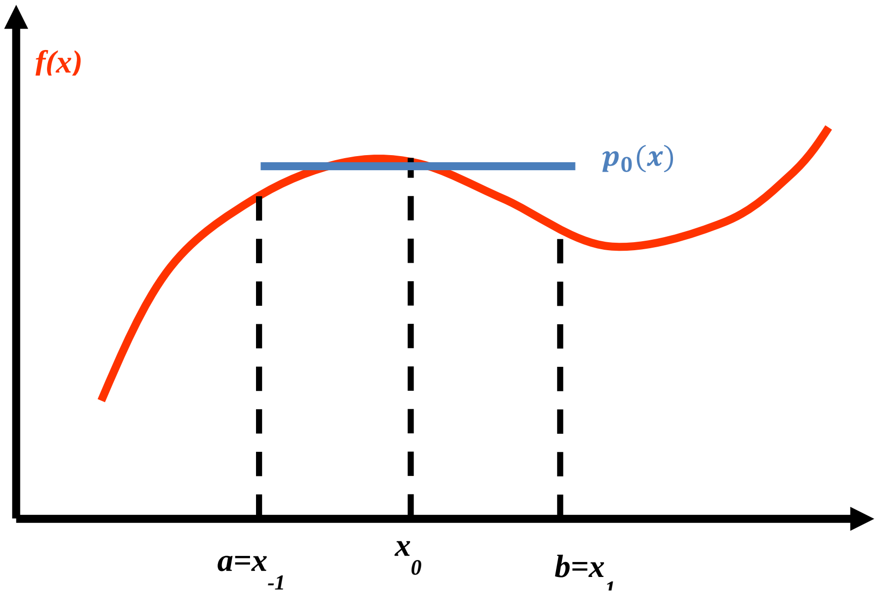


Figure 5 Midpoint rule

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

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 $x_{-1} < \xi < x_3$. $h = \frac{b-a}{4}$.

n=3: $\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95h^5}{144} f^{(4)}(\xi)$;
where $x_{-1} < \xi < x_4$. $h = \frac{b-a}{5}$.

Example 2. Use closed and open Newton-Cotes with $n = 3$ respectively to approximate $\int_0^{\frac{\pi}{4}} \sin(x)\, dx$ respectively, and compare abs. errors.