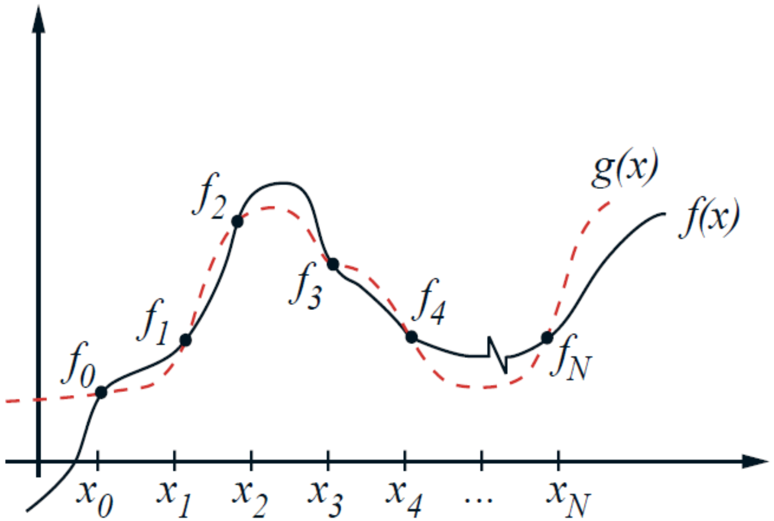
Section 4.3 Elements of Numerical Integration

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

$\sum_{i=0}^{N} f(x_i)a_i$ is the quadrature formula.

Idea for deriving quadrature formula

1. Let the interpolation points be given as:
$(x_0, f(x_0)), (x_1, f(x_1)), \ldots (x_N, f(x_N))$. Here $a = x_0$; $b = x_N$.



2. By Lagrange Interpolation Theorem (Thm 3.3):

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

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

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

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

Definition (quadrature formula)

Let $f(x)$ be an arbitrary continuous function in $[a, b]$, then a

$(N+1)$-point quadrature formula for the integral $\int_a^b f(x)dx$ is an

approximation of the form $\sum_{i=0}^{N} f(x_i)a_i$.

Here the x_i are called the *quadrature nodes* (abscissas) and the a_i are

the *quadrature weights.*

Remark: For a given set of quadrature nodes $\{x_i\}$, the quadrature

weights are uniquely determined via $a_i = \int_a^b L_{N,i}(x)dx$

The (2-pts) Trapezoidal Quadrature Rule

- Obtained by first degree Lagrange interpolating polynomial. (Figure 1)
- Let $x_0 = a$; $x_1 = b$; and $h = b - a$.

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

Error term

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

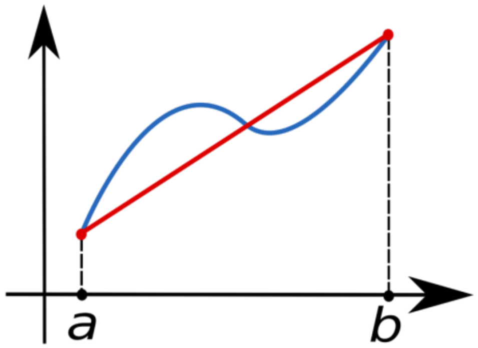


Figure 1
Trapezoidal Rule

Example 1. Derive the 3-pts quadrature formula for

$$\int_0^1 f(x)dx$$

using quadrature nodes $x_0 = 0;\ \ x_1 = \frac{1}{2}, x_2 = 1.$

Answer: $\int_0^1 f(x)dx \approx \frac{1}{6}\left[f(0) + 4f\left(\frac{1}{2}\right) + f(1)\right]$

The (3-pts) Simpson's Quadrature Rule

- Obtained by second degree Lagrange interpolating polynomial.
- Let $x_0 = a;\ \ x_1 = \frac{a+b}{2}, x_2 = b$; and $h = \frac{b-a}{2}$.

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

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

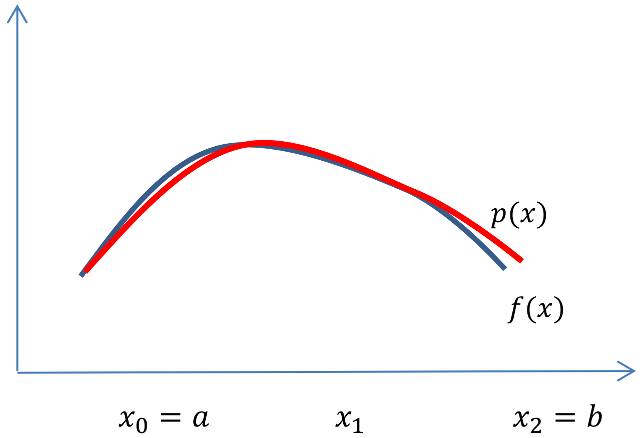


Figure 2 Simpson's Rule

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

(a) x^2; (b) $(x+1)^{-1}$.

Measuring Precision

Definition 4.1. 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 $k = 0, 1, \cdots, n$.

Remark: If a quadrature formula has degree of accuracy n, then the error of approximation is zero for all polynomials of degree $\leq n$. But is not zero for some polynomial of degree $n + 1$.

- **Trapezoidal rule has degree of accuracy one.**

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

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

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

→Trapezoidal rule is exact for x.

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

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

Example 3. approximate $\int_0^1 x^3 dx$ using Simpson's rule.

Remark: Simpson's rule has degree of accuracy three.

Example 4. 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

- 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.

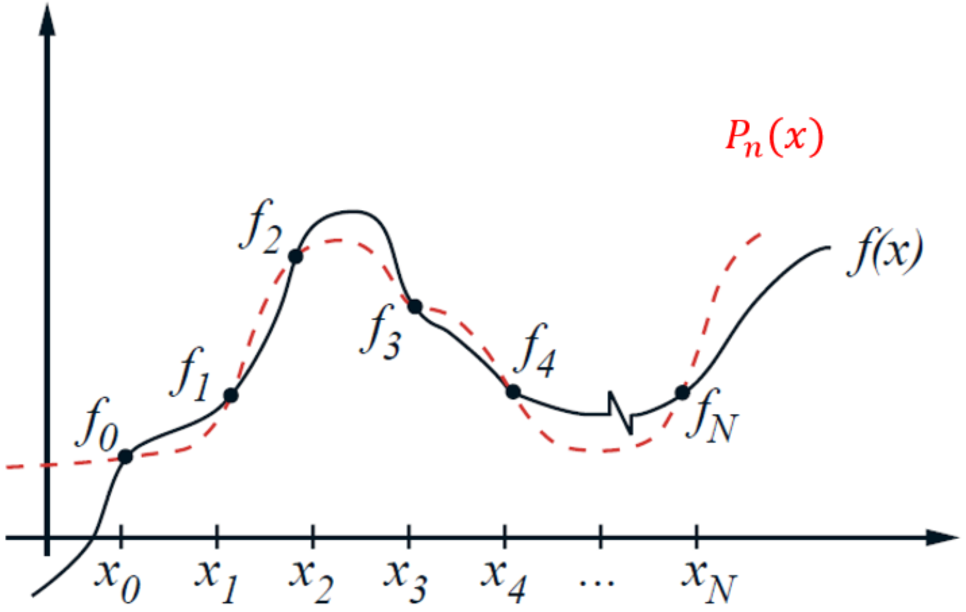


Figure 3 Closed Newton-Cotes Formulas

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

(4-pts) 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 $x_0 < \xi < x_3$; $h = \frac{x_3 - x_0}{3}$.

- Degree of precision is 3 for Simpson's three-eighths rule, which is the same as Simpson's rule.

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 $x_{n+1} = b$.

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 $x_0, \ldots, x_n$.

Endpoints are not included as nodes

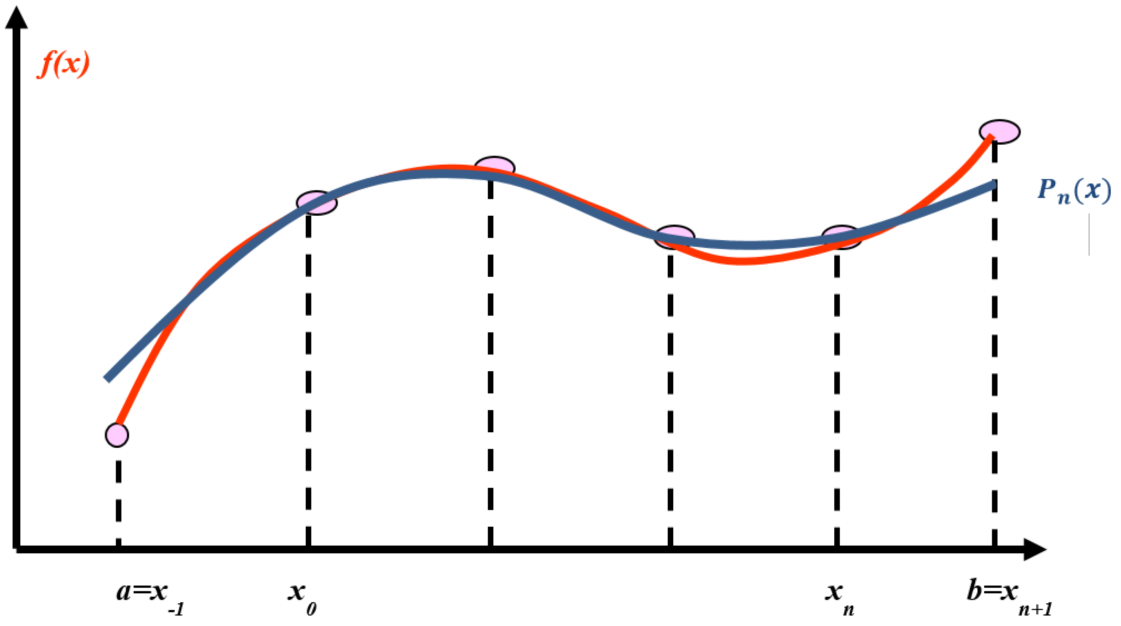


Figure 4 Open Newton-Cotes Formula

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

- $\boldsymbol{n = 0}$: **Midpoint rule (Figure 5)**

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

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

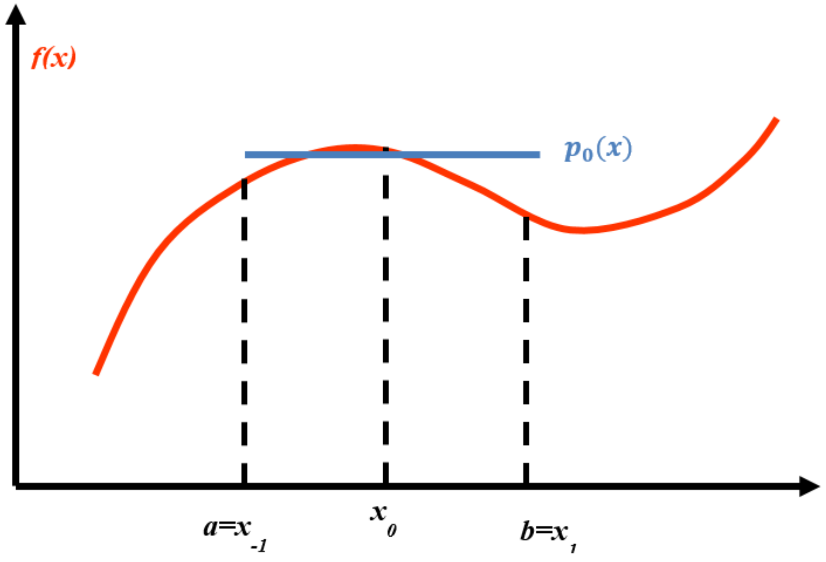


Figure 5 Midpoint rule