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:

\[
(x_0, f(x_0)) \\
(x_1, f(x_1)) \\
(x_2, f(x_2)) \\
\vdots \\
(x_N, f(x_N))
\]

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

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

**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)

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

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

Thus

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

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)

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

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

Figure 2 Simpson's Rule
\[
\int_a^b f(x)dx \\
= \int_a^b \left(f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4\right)dx \\
= 2hf(x_1) + \frac{h^3}{3} f''(x_1) + \frac{f^{(4)}(\xi_1)}{60} h^5
\]

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

Thus

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

Simpson’s rule: \( \int_a^b f(x)dx \approx \frac{h}{3} \left(f(x_0) + 4f(x_1) + f(x_2)\right) \)

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.**

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

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

\[
\int_a^b x \, dx = \frac{x^2}{2} \bigg|_{a}^{b} = \frac{b^2-a^2}{2}; \quad \int_a^b x \, dx = \frac{b-a}{2} [a + b] = \frac{b^2-a^2}{2}.
\]

→ Trapezoidal rule is exact for $x$.

\[
\int_a^b x^2 \, dx = \frac{x^3}{3} \bigg|_{a}^{b} = \frac{b^3-a^3}{3}; \quad \int_a^b x^2 \, dx = \frac{b-a}{2} [a^2 + b^2] \neq \frac{b^3-a^3}{3}.
\]

→ Trapezoidal rule is **NOT** exact for $x^2$. 
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 $k = 0, 1, \ldots, n$, 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

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

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

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 $i$th 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 $x_0 < \xi < x_3; h = \frac{x_3-x_0}{3}$.
See Figure 4. Let \( h = \frac{b-a}{n+2} \); and \( x_0 = a + h \). \( x_i = x_0 + ith \), for \( i = 0, 1, \ldots, n \). 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 \( a_i = \int_{x_{i-1}}^{x_{i+1}} L_{n,i}(x)dx \) is called open Newton-Cotes Formula. \( L_{n,i}(x) \) is the \( i \)th 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

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

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](image)

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

**n=2**: \[ \int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3} [2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi); \quad \text{where} \quad x_{-1} < \xi < x_3. \quad h = \frac{b-a}{4}. \]
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 $\int_{0}^{\pi/4} \sin(x) dx$ respectively, and compare abs. errors.