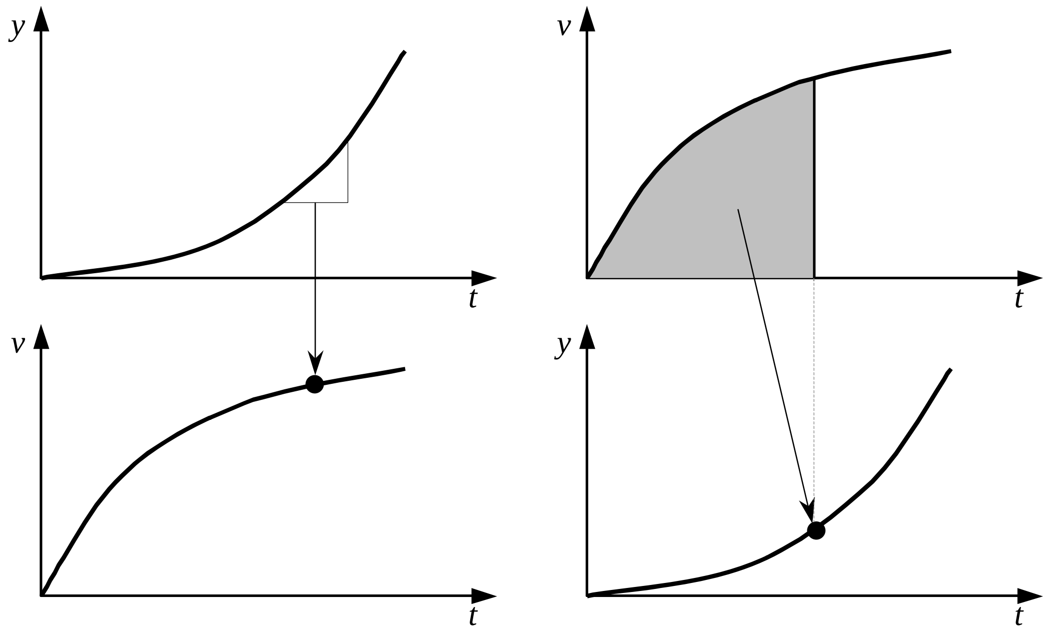
5

NUMERICAL DERIVATIVES & INTEGRALS

- Introduction
- Numerical Derivatives
- Newton-Cotes Integral Formula
- Gauss Quadrature
- Multivariable Integration

5.1 Introduction

- **Derivatives** is a rate of change of a dependent variable against an independent variable, and the process of producing it is known as *differentiation*.
- **Integral** is an inverse to derivative, and the process of producing it is known as *integration*.



(a) Differentiation (b) Integration

FIGURE 5.1 Differentiation and integration of a function

5.2 Numerical Derivatives

- Consider the following Taylor series:

$$
\begin{aligned}
f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 \\
+ \frac{f'''(x_i)}{3!}h + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n
\end{aligned}
\tag{5.1}
$$

where the residual term R_n and the step size h are

$$
R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}
$$
$$
h = x_{i+1} - x_i
$$

Example 5.1

Use the Taylor series of order zero to order four to estimate the following function at $x_{i+1} = 1$ if $x_i = 0$:

$$
f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2
$$

Solution

The step size used is $h = x_{i+1} - x_i = 1$. Hence, the derivatives at $x_i = 0$ are

$$
\begin{aligned}
f'(x_i) &= -0.4x^3 - 0.45x^2 - x - 0.25 = -0.25 \\
f''(x_i) &= -1.2x^2 - 0.9x - 1 = -1 \\
f'''(x_i) &= -2.4x - 0.9 = -0.9 \\
f^{(4)}(x_i) &= -2.4
\end{aligned}
$$

At $x_{i+1} = 1$, the function value is

$$
f(x_{i+1}) = -0.1(1)^4 - 0.15(1)^3 - 0.5(1)^2 - 0.25(1) + 1.2 = 0.2
$$

For $n = 0$:

$$
f(x_{i+1}) = f(x_i) = \underline{1.2}
$$
$$
E_t = 0.2 - 1.2 = \underline{-1}
$$

For $n = 1$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h$$
$$= 1.2 - 0.25(1) = \underline{0.95}$$
$$E_t = 0.2 - 0.95 = \underline{-0.75}$$

For $n = 2$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \tfrac{1}{2} f''(x_i)h^2$$
$$= 1.2 - 0.25(1) + \tfrac{1}{2}(-1)(1)^2 = \underline{0.45}$$
$$E_t = 0.2 - 0.45 = \underline{-0.25}$$

For $n = 3$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \tfrac{1}{2} f''(x_i)h^2 + \tfrac{1}{6} f'''(x_i)h^3$$
$$= 1.2 - 0.25(1) + \tfrac{1}{2}(-1)(1)^2 + \tfrac{1}{6}(-0.9)(1)^3 = \underline{0.3}$$
$$E_t = 0.2 - 0.3 = \underline{-0.1}$$

For $n = 4$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \tfrac{1}{2} f''(x_i)h^2 + \tfrac{1}{6} f'''(x_i)h^3 + \tfrac{1}{24} f''''(x_i)h^4$$
$$= 1.2 - 0.25(1) + \tfrac{1}{2}(-1)(1)^2 + \tfrac{1}{6}(-0.9)(1)^3 + \tfrac{1}{24}(-2.4)(1)^4 = \underline{0.2}$$
$$E_t = 0.2 - 0.2 = \underline{0}$$

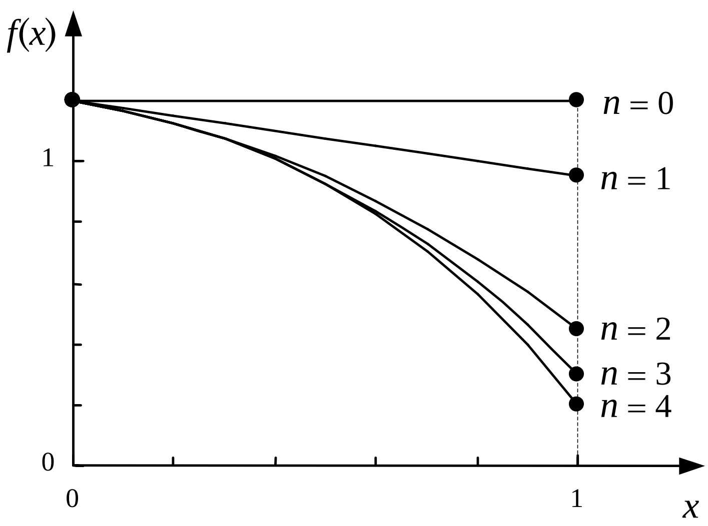


FIGURE 5.2 Approximation using the Taylor series for Ex. 5.1

- The first derivative is known as the *finite divided difference*:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(x_{i+1} - x_i) \equiv \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{5.2}$$

where $O(h)$ is the term representing the first order error.

- Similarly, an approximation to backward finite divided difference is

$$\begin{aligned} f(x_{i-1}) &= f(x_i) + f'(x_i)(-h) + \frac{f''(x_i)}{2!}(-h)^2 + \frac{f'''(x_i)}{3!}(-h)^3 + \cdots, \\ &= f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \cdots. \end{aligned} \tag{5.3}$$

where the backward difference can be derived as

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \tag{5.4}$$

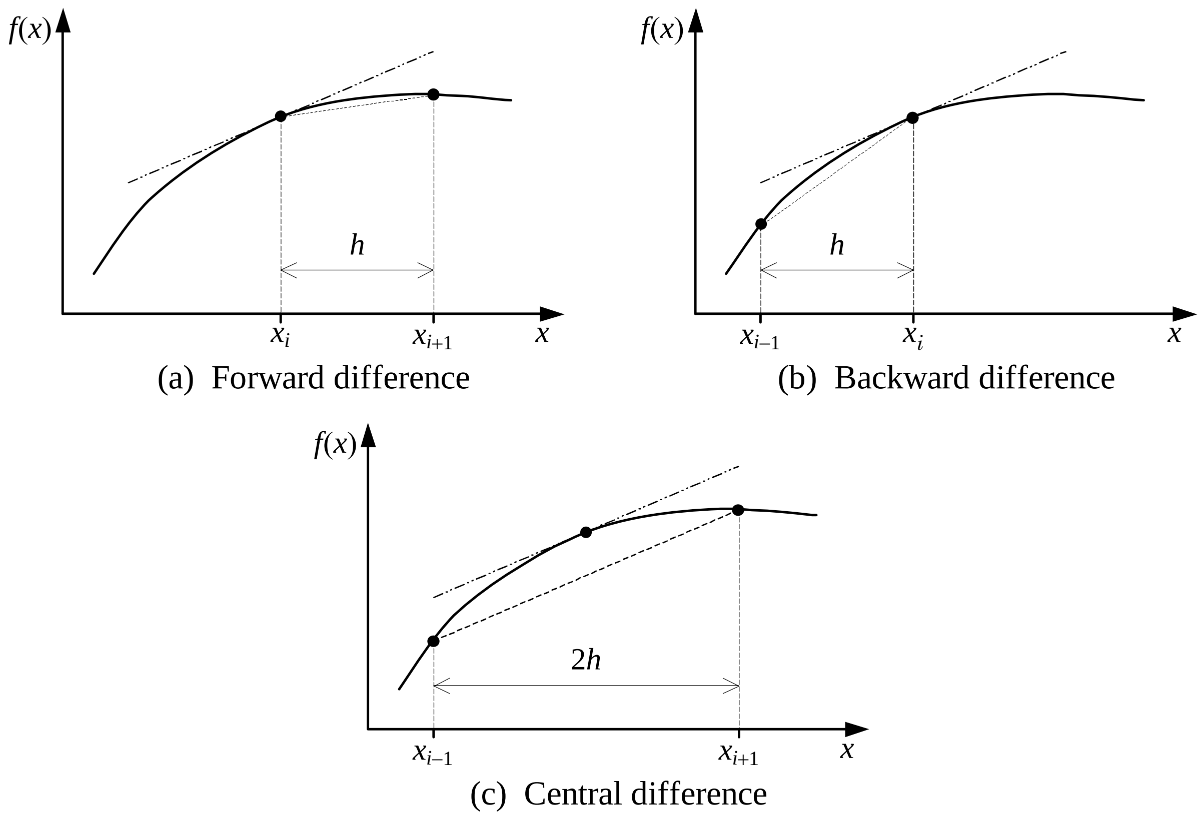


FIGURE 5.3 Forward, Backward and Central Finite Divided Differences

- The central difference can be obtained by combining Eq. (5.1) with Eq. (5.3):

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(x_i)}{3}h^3 + \cdots,$$

$$\begin{aligned} f'(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \frac{f'''(x_i)}{6}h^2 + \cdots, \\ &\approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \end{aligned} \tag{5.5}$$

Example 5.2

Use the forward, backward and central divided differences to approximate the following function:

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ with a step size of $h = 0.5$. Repeat with a step size of $h = 0.25$.

Solution

The excat value at $x = 0.5$:

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$$

$$f'(0.5) = -0.4(0.5)^3 - 0.45(0.5)^2 - (0.5) - 0.25 = -0.9125$$

For $h = 0.5$:

$$\begin{aligned} x_{i-1} &= 0.0: \quad & f(x_{i-1}) &= 1.2 \\ x_i &= 0.5: \quad & f(x_i) &= 0.925 \\ x_{i+1} &= 1.0: \quad & f(x_{i+1}) &= 0.2 \end{aligned}$$

Forward divided difference:

$$f'(x_i) = \frac{0.2 - 0.925}{0.5} = -1.45$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-1.45)}{-0.9125} \right| = 58.9\%$$

Backward divided difference:

$$f'(x_i) = \frac{0.925 - 1.2}{0.5} = -0.55$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-0.55)}{-0.9125} \right| = 39.7\%$$

Central divided difference:

$$f'(x_i) = \frac{0.2 - 1.2}{2(0.5)} = -1.0$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-1.0)}{-0.9125} \right| = 9.6\%$$

For $h = 0.25$:

$$x_{i-1} = 0.25: \qquad f(x_{i-1}) = 1.10351563$$

$$x_i = 0.5: \qquad f(x_i) = 0.925$$

$$x_{i+1} = 0.75: \qquad f(x_{i+1}) = 0.63632813$$

Forward divided difference:

$$f'(x_i) = \frac{0.63632813 - 0.925}{0.25} = -1.155$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-1.155)}{-0.9125} \right| = 26.5\%$$

Backward divided difference:

$$f'(x_i) = \frac{0.925 - 1.10351563}{0.25} = -0.714$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-0.55)}{-0.9125} \right| = 21.7\%$$

Central divided difference:

$$f'(x_i) = \frac{0.63632813 - 1.10351563}{2(0.25)} = -0.934$$

$$\varepsilon_t = \left| \frac{(-0.9125) - (-0.934)}{-0.9125} \right| = 2.4\%$$

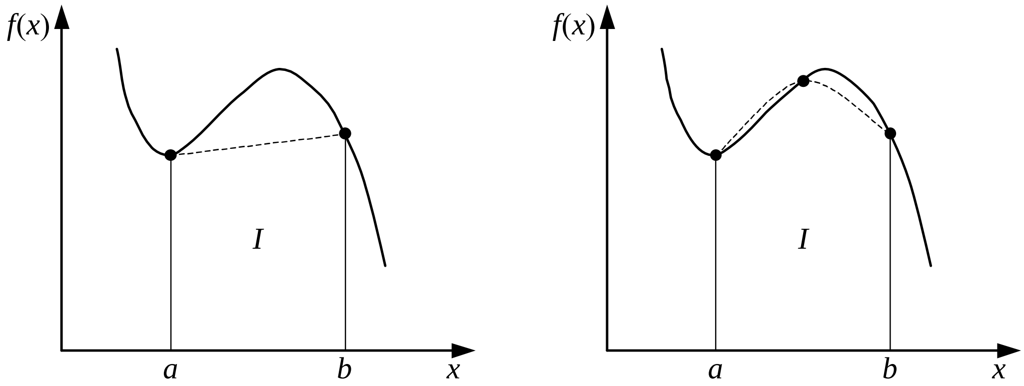
5.3 Newton-Cotes Integral Formula

- A Newton-Cotes integral expression can be written as

$$I = \int_a^b f(x)\,dx \approx \int_a^b f_n(x)\,dx$$

where $f_n(x)$ is an n-th order polynomial function of the form

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1}x^{n-1} + a_n x^n = \sum_{i=0}^{n} a_i x^i$$



(a) Trapezoidal rule (b) Simpson rule

FIGURE 5.4 Numerical integration for linear and quadratic functions

- If $n = 1$, the Newton-Cotes integral is known as the trapezoidal rule

$$I = \int_a^b f(x)\,dx \approx \int_a^b f_1(x)\,dx$$

where $f_1(x)$ is a linear function

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b-a}(x-a)$$

Hence, the integration for the range of a and b is

$$I \approx \int_a^b \left[f(a) + \frac{f(b)-f(a)}{b-a}(x-a) \right] dx \approx (b-a)\frac{f(a)+f(b)}{2} \tag{5.6}$$

and the corresponding approximated error is

$$E_a = -\frac{f''(\xi)}{12}(b-a)^3 \tag{5.7}$$

Example 5.3

Use the trapezoidal rule to estimate the numerical integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$ (exact solution: 1.640533).

Solution

For the value at the edges:

$$x_i = a = 0: \qquad f(0) = 0.2$$

$$x_{i+1} = b = 0.8: \qquad f(0.8) = 0.232$$

Hence, the integration value is

$$I \cong (0.8)\frac{0.2 + 0.232}{2} = 0.1728$$

The associated error

$$E_t = 1.640533 - 0.1728 = 1.467733, \quad \varepsilon_t = \left|\frac{1.467733}{1.640533}\right| = 89.5\%$$

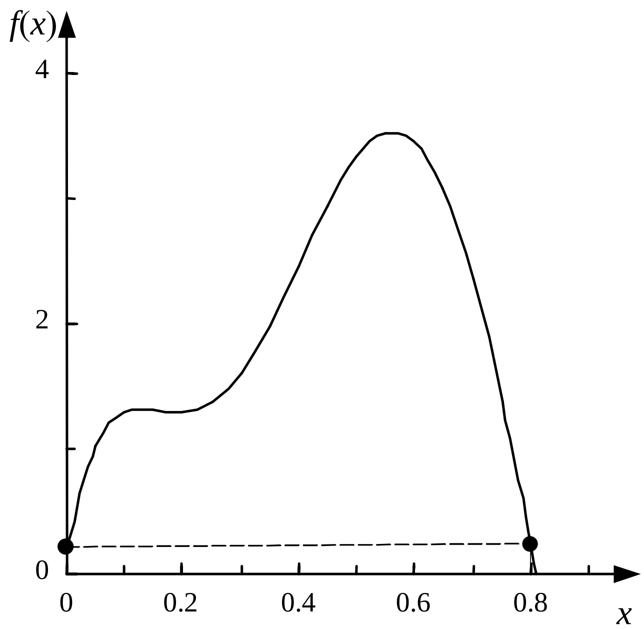


FIGURE 5.6 The curve and the linear approximation of Ex. 5.3

- The approximated error can be estimated as followed:

$$f''(x) = -400 + 4050x - 10800x^2 + 8000x^3$$

The average of the second order derivative and thus the error estimation are

$$\bar{f}''(x) = \frac{\int_0^{0.8}\left(-400 + 4050x - 10800x^2 + 8000x^3\right)dx}{0.8-0} = -60$$

$$E_a = -\frac{f''(\xi)}{12}(b-a)^3 = -\frac{(-60)}{12}(0.8)^3 = 2.56$$

- The accuracy of numerical integration can be improved by using a smaller step size

$$h = \frac{b-a}{n}$$

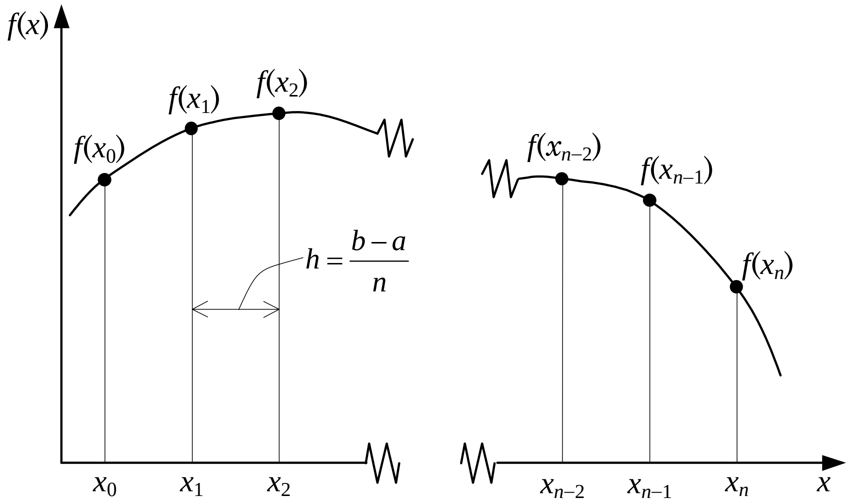


FIGURE 5.7 The trapezoidal rule using *n* segmen

- The total integration is

$$I = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

$$\approx h\cdot\frac{f(x_0)+f(x_1)}{2} + h\cdot\frac{f(x_1)+f(x_2)}{2} + \cdots + h\cdot\frac{f(x_{n-1})+f(x_n)}{2}$$

$$\approx \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

or, in a more simplified form

$$I \approx \underbrace{(b-a)}_{\text{width}} \cdot \underbrace{\frac{\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]}{2n}}_{\text{averaged height}} \tag{5.8}$$

and the associated approximated error is

$$E_a = -\frac{h^3}{12n^3} \sum_{i=1}^{n} f''(\xi_i) \tag{5.9}$$

Example 5.4

Use the trapezoidal rule with two segments to estimate the integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$, and obtain the associated error.

Solution

In this case, $n = 2$ and $h = 0.4$:

$$x_0 = a = 0 \qquad f(0) = 0.2$$

$$x_1 = \tfrac{1}{2}(a+b) = 0.4 \qquad f(0.4) = 2.456$$

$$x_2 = b = 0.8 \qquad f(0.8) = 0.232$$

Hence,

$$I \cong (0.8)\frac{0.2 + 2(2.456) + 0.232}{2(2)} = 1.0688$$

$$E_t = 1.640533 - 1.0688 = 0.57173$$

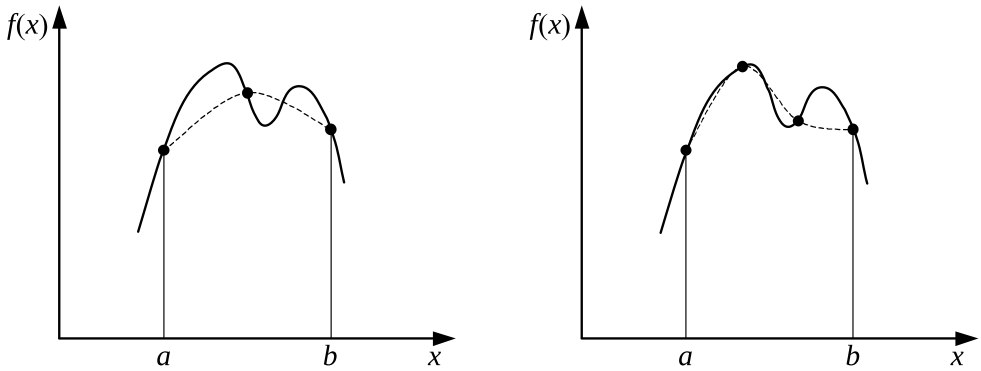
$$\varepsilon_t = \left| \frac{0.57173}{1.640533} \right| = 34.9\%$$

⌂

TABLE 5.1 The integration of Ex. 5.4 for *n* segment

n	h	I	ε_t
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

- The second order and the third order Newton-Cotes formula are known as the **1/3-** and **3/8-Simpson rules**, respectively.



(a) The 1/3-Simpson rule (b) The 3/8-Simpson rule

FIGURE 5.8 The 1/3- and 3/8-Simpson rules

- For the 1/3-Simpson rule:

$$I = \int_a^b f(x)\,dx \approx \int_a^b f_2(x)\,dx$$

Using the second order Lagrange interpolation:

$$I \approx \int \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_1)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

then, the 1/3-Simpson rule becomes:

$$I \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] \tag{5.10}$$

where the step size is $h = \frac{1}{2}(b-a)$. It can be represented by

$$I \approx \underbrace{(b-a)}_{\text{width}} \cdot \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{averaged height}} \tag{5.11}$$

and the error estimation are

$$E_a = -\frac{1}{90} h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \tag{5.12}$$

Example 5.5

Use the 1/3-Simpson rule to obtain the integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$.

Solution

The value of the function at x_i:

$$f(0) = 0.2$$
$$f(0.4) = 2.456$$
$$f(0.8) = 0.232$$

Hence, the integration is

$$I \cong 0.8 \frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

and the error is

$$E_t = 1.640533 - 1.367467 = 0.2730667$$

$$\varepsilon_t = \left|\frac{0.2730667}{1.640533}\right| = 16.6\%$$

⌂

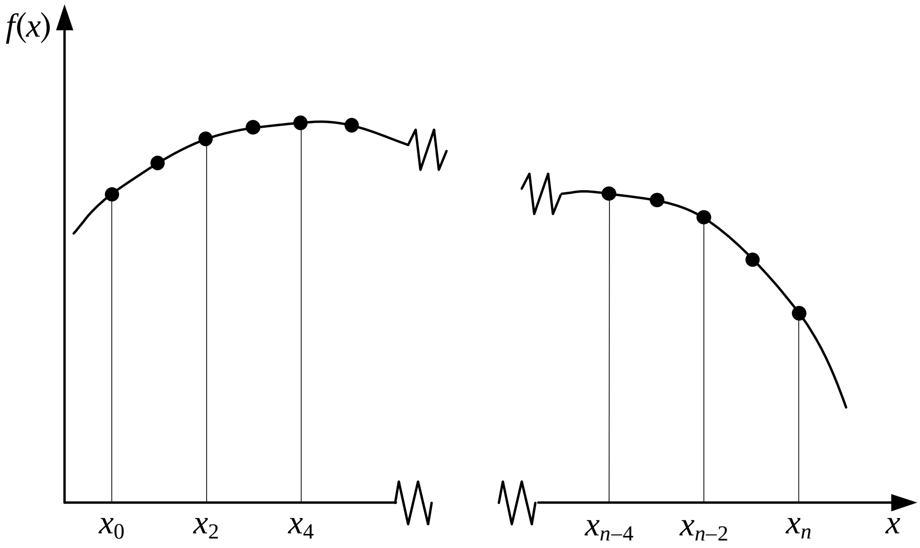


FIGURE 5.9 The 1/3-Simpson rule using *n* segment

- If there are *n* segments, the formula for the 1/3-Simpson rule is

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

$$I \approx 2h \cdot \frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h \cdot \frac{f(x_2) + 4f(x_3) + f(x_4)}{6} + \cdots$$
$$+ 2h \cdot \frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

or, in a more simplified form

$$I \approx (b-a) \cdot \frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n} \quad (5.13)$$

and the error estimation are

$$E_a = -\frac{(b-a)^5}{180 n^4} \bar{f}^{(4)} \quad (5.14)$$

Example 5.6

Use the 1/3-Simpson rule with four segment to obtain the integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$.

Penyelesaian

The value of the function at each node x_i:

$$f(0) = 0.2$$
$$f(0.2) = 1.288$$
$$f(0.4) = 2.456$$
$$f(0.6) = 3.464$$
$$f(0.8) = 0.232$$

Hence, the integration io

$$I = 0.8\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

and the error is

$$E_t = 1.640533 - 1.623467 = 0.017067$$

$$\varepsilon_t = \left|\frac{0.017067}{1.640533}\right| = 1.04\%$$

$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

⌂

- In the 3/8-Simpson rule, the third order Lagrange polynomial is used:

$$I = \int_a^b f(x)\,dx \approx \int_a^b f_3(x)\,dx$$

to yield

$$I \approx \frac{3}{8}h\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \qquad (5.15)$$

where the step size is $h = \frac{1}{3}(b-a)$. It can be represented by

$$I \approx (b-a)\cdot \frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8} \tag{5.16}$$

and the associated error is

$$E_a = -\frac{3}{80}h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480} f^{(4)}(\xi) \tag{5.17}$$

Example 5.7

Use the 3/8-Simpson rule to obtain the integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$.

Solution

The value of function at each node x_i:

$$f(0) = 0.2$$
$$f(0.2667) = 1.432724$$
$$f(0.5333) = 3.487177$$
$$f(0.8) = 0.232$$

Hence, the integration is

$$I = 0.8\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.519170$$

and the error is

$$E_t = 1.640533 - 1.519170 = 0.1213630$$

$$\varepsilon_t = \left|\frac{0.1213630}{1.640533}\right| = 7.40\%$$

$$E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.1213630$$

□

- In general, the Newton-Cotes Integral formula can be written as

$$I = \int_a^b f(x)dx = \alpha h\left[w_0 f_0 + w_1 f_1 + w_2 f_2 + \cdots + w_n f_n\right] + E \qquad (5.18)$$

where $f_n = f(x_n)$, $x_n = a + nh$ and $h = (b-a)/n$, and α and w are coefficients as listed in Table 5.2.

TABLE 5.2 Coefficients and errors for the Newton-Cotes integration formula

n	α	$w_i \; \forall \; i = 0,1,2,\ldots,n$	E_t
1	$\frac{1}{2}$	1 1	$-\frac{1}{2}h^3 f''(\xi)$
2	$\frac{1}{3}$	1 4 1	$-\frac{1}{90}h^5 f^{(4)}(\xi)$
3	$\frac{3}{8}$	1 3 3 1	$-\frac{3}{80}h^5 f^{(4)}(\xi)$
4	$\frac{2}{45}$	7 32 12 32 7	$-\frac{8}{945}h^7 f^{(6)}(\xi)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

5.4 Gauss Quadrature

- The error in the trapeziodal rule can be improved by using a weighted approach for the node value used

$$I = (b-a)\frac{f(a)+f(b)}{2}$$

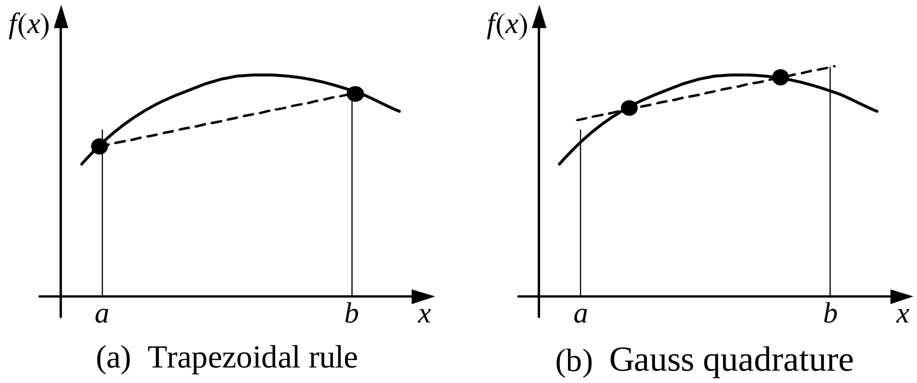


FIGURE 5.10 Comparison between the trapezoidal rule and the Gauss quadrature

- This method is known as the *Gauss (-Legendre) quadrature approximation* and its nodes are known as *Gauss points*.

- The general formula for the range [–1, 1]:

$$\int_{-1}^{1} f(x)\,dx \cong \sum_{i=1}^{n} w_i f(x_i) \qquad (5.19)$$

where n is the number of Gauss points, w_i is the weight for each Gauss point and x_i is the coordinate for the Gauss point.

- For $n = 2$, it can be mapped into a cubic polynomial having four unknowns:

$$I \cong w_1 f(x_1) + w_2 f(x_2) = \int_{-1}^{1} f(x)\,dx$$

$$\begin{aligned} w_1\left(a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3\right) + w_2\left(a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3\right) \\ = \int_{-1}^{1}\left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)dx \\ = \int_{-1}^{1} a_0\,dx + \int_{-1}^{1} a_1 x\,dx + \int_{-1}^{1} a_2 x^2\,dx + \int_{-1}^{1} a_3 x^3\,dx, \\ = 2a_0 + \tfrac{3}{2} a_2 . \end{aligned}$$

Hence, four equations can be formed as followed:

Coefficent a_0: $w_1 + w_2 = 2$

Coefficent a_1: $w_1 x_1 + w_2 x_2 = 0$

Coefficent a_2: $w_1 x_1^2 + w_2 x_2^2 = \frac{3}{2}$

Coefficent a_2: $w_1 x_1^3 + w_2 x_2^3 = 0$

which can be solved to give

$$w_1 = w_2 = 1, \quad x_1 = -1/\sqrt{3}, \quad x_2 = +1/\sqrt{3}.$$

- For any number of Gauss points, the *Legendre polynomial* $P_n(x)$ can be used to evaluate such points:

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0 \quad \text{where} \quad P_0(x) = 1, \quad P_1(x) = x. \tag{5.20}$$

- The *Legendre polynomial* $P_n(x)$ has several important characteristics:

1. It is orthogonal in the range [–1, 1]:

$$\int_{-1}^{1} P_n(x) \cdot P_m(x)\, dx \begin{cases} = 0 & \text{if} \quad n \neq m \\ > 0 & \text{if} \quad n = m \end{cases}$$

2. Any polynomial of n-th order $f_n(x)$ can be formed as an arithmetic combination of Legendre polynomials:

$$f_n(x) = \sum_{i=0}^{n} c_i P_i(x)$$

3. For $P_n(x) = 0$, there are n roots in the range [–1, 1].

- The Gauss-Legendre quadrature with n points is accurate at polynomials of order ($2n$–1) or lower.

- The parameters for the Gauss-Legendre quadrature is listed in Table 5.3.

TABLE 5.3 Parameters for the Gauss-Legendre quadrature

No. of points n	Coordinates x_i or ξ_i	Weights w_i	Error E_t
1	0	2	$\cong f^{(2)}(\xi)$
2	−0.577350269	1	$\cong f^{(4)}(\xi)$
	+0.577350269	1	
3	−0.774596669	0.555555555	$\cong f^{(6)}(\xi)$
	0	0.888888889	
	+0.774596669	0.555555555	
4	−0.861136312	0.347854845	$\cong f^{(8)}(\xi)$
	−0.339981044	0.652145155	
	+0.339981044	0.652145155	
	+0.861136312	0.347854845	
5	−0.906179846	0.236926885	$\cong f^{(10)}(\xi)$
	−0.538469310	0.478628670	
	0	0.568888889	
	+0.538469310	0.478628670	
	+0.906179846	0.236926885	
6	−0.932469514	0.171324492	$\cong f^{(12)}(\xi)$
	−0.661209386	0.360761573	
	−0.238619186	0.467913935	
	+0.238619186	0.467913935	
	+0.661209386	0.360761573	
	+0.932469514	0.171324492	

- The Gauss-Legendre quadrature can be used in the range $[a, b]$ using a transformation linear as followed:

$$I = \int_a^b f(x)\,dx = \int_{-1}^{1} \tilde{f}(\xi)\cdot\left(\frac{dx}{d\xi}\right)d\xi$$

$$I \cong \frac{b-a}{2}\sum_{i=1}^{n} w_i \tilde{f}(\xi_i) \cong \frac{b-a}{2}\sum_{i=1}^{n} w_i f(x_i) \tag{5.23}$$

- In Eq. (5.23), $dx/d\xi = \frac{1}{2}(b-a)$, and the actual coordinate x_i can be obtained from

$$x_i = \frac{(b-a)\xi_i + a + b}{2} \tag{5.24}$$

Example 5.8

Use the Gauss quadrature to obtained the integration of:

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

in a range from 0 to 0.8.

Solution

The Gauss quadrature formula:

$$I = \int_0^{0.8} f(x)\,dx = \int_{-1}^{1} \tilde{f}(\xi)\cdot\left(\frac{dx}{d\xi}\right)d\xi \cong \frac{0.8-0}{2}\sum_{i=1}^{n} w_i f(x_i)$$

where $\xi_i = \pm 0.577350$ and,

$$x_i = \frac{(0.8-0)(\pm 0.577350) + 0 + 0.8}{2},$$

$$= 0.169060, 0.630940.$$

Thus the values of function at the Gauss points are

$$f(0.169060) = 1.291851$$

$$f(0.630940) = 3.264593$$

Hence,

$$I = 0.4[(1)(1.291851) + (1)(3.264593)],$$

$$= 1.822578.$$

The error for this integration is

$$E_t = 1.640533 - 1.82243 = -0.182045$$

$$\varepsilon_t = \left|\frac{-0.182045}{1.640533}\right| = 11.1\%$$

Ex. 5.8 can be repeated for other number of points (see Table 5.4).

TABLE 5.4 Integration results of Ex. 5.8 for n points

n	I	ε_t
1	1.9648	19.8
2	1.822578	11.1
3	1.640533	0.0

5.5 Multivariable Integration

- For multi-variable cases, the Newton-Cotes integration formula can be modified for the 2-D and 3-D cases as followed:

$$\iint f(x,y)\,dx\,dy \cong \sum_{i=1}^{l}\sum_{j=1}^{m} u_i v_j f_{ij} \tag{5.25}$$

$$\iiint f(x,y,z)\,dx\,dy\,dz \cong \sum_{i=1}^{l}\sum_{j=1}^{m}\sum_{k=1}^{n} u_i v_j w_j f_{ijk} \tag{5.26}$$

- where the coefficients u_i, v_j dan w_k are integral coefficients in the x, y and z direction, and l, m and n are the numbers of points in the respective direction.

- For an example, if the following 2-D integration uses the trapezoidal rule with 3 points in the x direction and the 1/3-Simpson rule with 5 points in the y direction, the formula becomes

$$\begin{aligned}\iint f(x,y)\,dx\,dy \cong \frac{\Delta x}{2}\frac{\Delta y}{3}\big[&\left(f_{11}+4f_{12}+2f_{13}+4f_{14}+f_{15}\right)\\ &+2\left(f_{21}+4f_{22}+2f_{23}+4f_{24}+f_{25}\right)\\ &+\left(f_{31}+4f_{32}+2f_{33}+4f_{34}+f_{35}\right)\big]\end{aligned}$$

or, in a more visible pattern,

$$\iint f(x,y)\,dx\,dy \cong \frac{\Delta x}{2}\frac{\Delta y}{3}\begin{bmatrix}1 & 4 & 2 & 4 & 1\\ 2 & 8 & 4 & 8 & 2\\ 1 & 4 & 2 & 4 & 1\end{bmatrix} f_{ij}$$

- If the Gauss quadrature is used, then the 2-D and 3-D cases become:

$$\int_{-1}^{1}\int_{-1}^{1} f(x,y)\,dx\,dy \cong \sum_{i=1}^{l}\sum_{j=1}^{m} u_i v_j f(x_i, y_j) \tag{5.27}$$

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(x,y,z)\,dx\,dy\,dz \cong \sum_{i=1}^{l}\sum_{j=1}^{m}\sum_{k=1}^{n} u_i v_j w_k f(x_i, y_j, z_k) \tag{5.28}$$

and its transformation to a general range can be performed using

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x,y)\,dx\,dy = \int_{-1}^{1}\int_{-1}^{1}\tilde{f}(\xi,\eta)\left(\frac{\partial x}{\partial \xi}\cdot\frac{\partial y}{\partial \eta}\right)d\xi\,d\eta$$
$$\cong \frac{b_1-a_1}{2}\cdot\frac{b_2-a_2}{2}\sum_{i=1}^{l}\sum_{j=1}^{m}u_i v_j f(x_i,y_j) \tag{5.29}$$

$$\int_{a_3}^{b_3}\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x,y,z)\,dx\,dy\,dz = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\tilde{f}(\xi,\eta,\zeta)\left(\frac{\partial x}{\partial \xi}\cdot\frac{\partial y}{\partial \eta}\cdot\frac{\partial z}{\partial \zeta}\right)d\xi\,d\eta\,d\zeta$$
$$\cong \frac{b_1-a_1}{2}\cdot\frac{b_2-a_2}{2}\cdot\frac{b_3-a_3}{2}\times \tag{5.30}$$
$$\sum_{i=1}^{l}\sum_{j=1}^{m}\sum_{k=1}^{n}u_i v_j w_k f(x_i,y_j,z_k)$$

where the transformed variable system (ξ,η) or (ξ,η,ζ) is known as the *isoparametric* coordinate system.

Example 5.9

Evaluate:

$$\int_{-\pi/2}^{\pi/2}\int_{1}^{3}\int_{0}^{1}\frac{e^{-x}\cos z}{y}\,dx\,dy\,dz$$

using the Gauss quadrature with two points in all directions. Compare the result with the analytical value of 1.38891.

Solution

The 3-D Gauss quadrature formula can be written as

$$I = \int_{-\pi/2}^{\pi/2}\int_{1}^{3}\int_{0}^{1} f(x)\,dx\,dy\,dz = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\tilde{f}(\xi,\eta,\zeta)\left(\frac{\partial x}{\partial \xi}\cdot\frac{\partial y}{\partial \eta}\cdot\frac{\partial z}{\partial \zeta}\right)d\xi\,d\eta\,d\zeta\,,$$
$$\cong \frac{1-0}{2}\cdot\frac{3-1}{2}\cdot\frac{\pi/2-(-\pi/2)}{2}\sum_{i=1}^{l}\sum_{j=1}^{m}\sum_{k=1}^{n}u_i v_j w_k f(x_i,y_j,z_k),$$
$$\cong \frac{\pi}{4}\sum_{i=1}^{l}\sum_{j=1}^{m}\sum_{k=1}^{n}u_i v_j w_k f(x_i,y_j,z_k).$$

By taking $n = 2$ in all directions, $\xi_i = \eta_j = \zeta_k = \pm 0.57735$:

i, j, k	x_i	y_j	z_k	$u_i v_j w_k$	$f(u_i,v_j,w_k)$	$u_i v_j w_k \times f(u_i,v_j,w_k)$
1,1,1	0.21132	1.42265	–0.90690	1	0.35062	0.35062
1,1,2	0.21132	1.42265	0.90690	1	0.35062	0.35062
1,2,1	0.21132	2.57735	–0.90690	1	0.19354	0.19354
1,2,2	0.21132	2.57735	0.90690	1	0.19354	0.19354
2,1,1	0.78868	1.42265	–0.90690	1	0.19683	0.19683
2,1,2	0.78868	1.42265	0.90690	1	0.19683	0.19683
2,2,1	0.78868	2.57735	–0.90690	1	0.10865	0.10865
2,2,2	0.78868	2.57735	0.90690	1	0.10865	0.10865
					Jumlah	1.69928

Therefore,

$$I = \frac{\pi}{4}\left(1.69928\right) = 1.33462.$$

giving an error of

$$E_t = 1.38891 - 1.33462 = 0.05430$$

$$\varepsilon_t = \left|\frac{0.05430}{1.38891}\right| = 3.91\%$$

Exercises

1. It is known that the following integration has a solution as followed:

$$\int_0^{\pi} x \sin x \, dx = \pi$$

Evaluate this integration using the following methods and calculate the corresponding relative errors:

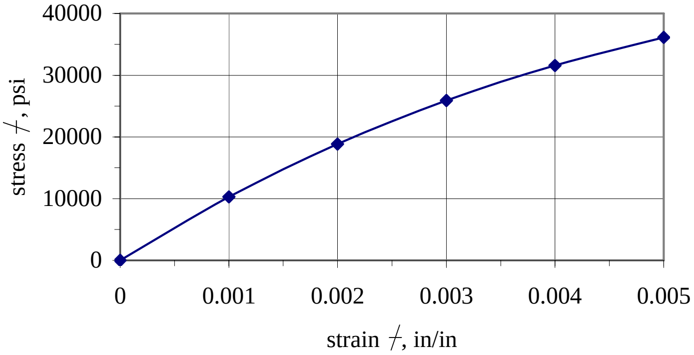
a. The trapezoidal rule with four steps.
b. The 1/3-Simpson rule with four steps.
c. The Gauss quadrature with four points in a step.

2. Estimate the following integration using the Gauss quadrature with two and four points and compare the results with the analytical solution as given below:

$$\int_a^b f(x) \, dx = \int_2^4 x^3 \ln x \, dx = 124 \ln 2 - 14$$

3. A stress-strain test has been conducted on an aircraft component and the result is tabulated as followed:

ε, in/in	σ, psi
0.000	0
0.001	10298
0.002	18852
0.003	25882
0.004	31586
0.005	36137



In this test, it is found that the component fails at the strain of 0.005 in/in. Use the trapezoidal rule and the Gauss quadrature to estimate the strain energy of the component which is required to assess the reability of the aircraft wing system. As a guidance, the curve for the test is given by:

$$\sigma = 11.2514 \times 10^6 \, \varepsilon \, e^{-88.52\varepsilon}$$