5

Numerical Derivatives & Integrals

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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*.

![Differentiation and integration of a function](image-url)
5.2 Numerical Derivatives

Consider the following Taylor series:

\[
f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n
\]

(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

\[
f'(x_i) = -0.4x^3 - 0.45x^2 - x - 0.25 = -0.25
\]

\[
f''(x_i) = -1.2x^2 - 0.9x - 1 = -1
\]

\[
f'''(x_i) = -2.4x - 0.9 = -0.9
\]

\[
f^{(4)}(x_i) = -2.4
\]

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 \( n = 0 \):

\[
f(x_{i+1}) = f(x_i) = 1.2
\]

\[
E_i = 0.2 - 1.2 = -1
\]
For $n = 1$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h = 1.2 - 0.25(1) = 0.95$$

$$E_t = 0.2 - 0.95 = -0.75$$

For $n = 2$:

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

$$= 1.2 - 0.25(1) + \frac{1}{2}(-1)(1)^2 = 0.45$$

$$E_t = 0.2 - 0.45 = -0.25$$

For $n = 3$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{1}{2} f''(x_i)h^2 + \frac{1}{6} f'''(x_i)h^3$$

$$= 1.2 - 0.25(1) + \frac{1}{2}(-1)(1)^2 + \frac{1}{6}(-0.9)(1)^3 = 0.3$$

$$E_t = 0.2 - 0.3 = -0.1$$

For $n = 4$:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{1}{2} f''(x_i)h^2 + \frac{1}{6} f'''(x_i)h^3 + \frac{1}{24} f''''(x_i)h^4$$

$$= 1.2 - 0.25(1) + \frac{1}{2}(-1)(1)^2 + \frac{1}{6}(-0.9)(1)^3 + \frac{1}{24}(-2.4)(1)^4 = 0.2$$

$$E_t = 0.2 - 0.2 = 0$$

![FIGURE 5.2 Approximation using the Taylor series for Ex. 5.1](image)
• The first derivative is known as the \textit{finite divided difference}:

\[
f''(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)
\]

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

• Similarly, an approximation to backward finite divided difference is

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

\[
= f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!} h^2 - \frac{f'''(x_i)}{3!} h^3 + \cdots.
\]

where the backward difference can be derived as

\[
f'(x_i) \approx \frac{f(x_{i}) - f(x_{i-1})}{h} + O(h)
\]

\[\text{FIGURE 5.3 Forward, Backward and Central Finite Divided Differences}\]
• The central difference can be obtained by combining Eq. (5.1) with Eq. (5.3):

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

\[ f''(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \frac{f'''(x_i)}{6}h^2 + \cdots, \]

\[ \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \] (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 exact 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 \( h = 0.5 \):

\[
x_{i-1} = 0.0 : \quad f(x_{i-1}) = 1.2
\]

\[
x_i = 0.5 : \quad f(x_i) = 0.925
\]

\[
x_{i+1} = 1.0 : \quad f(x_{i+1}) = 0.2
\]

Forward divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-1.45)}{-0.9125} \right| = 58.9\% \]
Backward divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-0.55)}{-0.9125} \right| = 39.7\% \]

Central divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-1.0)}{-0.9125} \right| = 9.6\% \]

For \( h = 0.25 \):

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

\( x_i = 0.5 : \quad f(x_i) = 0.925 \)

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

Forward divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-1.155)}{-0.9125} \right| = 26.5\% \]

Backward divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-0.55)}{-0.9125} \right| = 21.7\% \]

Central divided difference:

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

\[ \varepsilon_i = \left| \frac{(-0.9125) - (-0.934)}{-0.9125} \right| = 2.4\% \]
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

\[ f_n(x) = a_0 + a_1x + a_2x^2 + \cdots + a_{n-1}x^{n-1} + a_nx^n = \sum_{i=0}^{n} a_i x^i \]

- 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

\[ I \approx \int_{a}^{b} \left[ f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] \, dx \approx (b - a) \frac{f(a) + f(b)}{2} \quad (5.6) \]

and the corresponding approximated error is

\[ E_a = -\frac{f''(\xi)}{12} (b - a)^3 \quad (5.7) \]
**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:

\[
\begin{align*}
  f(0) &= 0.2 \\
  f(0.8) &= 0.232
\end{align*}
\]

Hence, the integration value is

\[
I \approx (0.8) \frac{0.2 + 0.232}{2} = 0.1728
\]

The associated error

\[
E_i = 1.640533 - 0.1728 = 1.467733, \quad \varepsilon_i = \left| \frac{1.467733}{1.640533} \right| = 89.5\%
\]

![Figure 5.6](image_url)
• The approximated error can be estimated as followed:

\[ f^{\prime\prime}(x) = -400 + 4050x - 10800x^2 + 8000x^3 \]

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

\[ \bar{f}^{\prime\prime}(x) = \int_0^{0.8} \left(-400 + 4050x - 10800x^2 + 8000x^3\right) dx \]

\[ = -60 \]

\[ E_a = -\frac{f^{\prime\prime}(\xi)}{12} (b-a)^3 = -\frac{(-60)}{12} (0.8)^3 = 2.56 \]

• 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 \( n \) segments

• 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

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

(5.8)

and the associated approximated error is

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

(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 \( h = 0.4 \):

\[
x_0 = a = 0 \quad f(0) = 0.2
\]

\[
x_1 = \frac{1}{2}(a + b) = 0.4 \quad f(0.4) = 2.456
\]

\[
x_2 = b = 0.8 \quad f(0.8) = 0.232
\]

Hence,

\[
I \approx (0.8) \cdot \frac{0.2 + 2(2.456) + 0.232}{2(2)} = 1.0688
\]

\[
E_i = 1.640533 - 1.0688 = 0.57173
\]

\[
\varepsilon_i = \left| \frac{0.57173}{1.640533} \right| = 34.9\%
\]
The second order and the third order Newton-Cotes formula are known as the 1/3- and 3/8-Simpson rules, respectively.

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:

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

### TABLE 5.1 The integration of Ex. 5.4 for \( n \) segment

<table>
<thead>
<tr>
<th>( n )</th>
<th>( h )</th>
<th>( I )</th>
<th>( \epsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.8</td>
<td>0.1728</td>
<td>89.5</td>
</tr>
<tr>
<td>2</td>
<td>0.4</td>
<td>1.0688</td>
<td>34.9</td>
</tr>
<tr>
<td>3</td>
<td>0.2667</td>
<td>1.3695</td>
<td>16.5</td>
</tr>
<tr>
<td>4</td>
<td>0.2</td>
<td>1.4848</td>
<td>9.5</td>
</tr>
<tr>
<td>5</td>
<td>0.16</td>
<td>1.5399</td>
<td>6.1</td>
</tr>
<tr>
<td>6</td>
<td>0.1333</td>
<td>1.5703</td>
<td>4.3</td>
</tr>
<tr>
<td>7</td>
<td>0.1143</td>
<td>1.5887</td>
<td>3.2</td>
</tr>
<tr>
<td>8</td>
<td>0.1</td>
<td>1.6008</td>
<td>2.4</td>
</tr>
<tr>
<td>9</td>
<td>0.0889</td>
<td>1.6091</td>
<td>1.9</td>
</tr>
<tr>
<td>10</td>
<td>0.08</td>
<td>1.6150</td>
<td>1.6</td>
</tr>
</tbody>
</table>
then, the 1/3-Simpson rule becomes:

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

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

\[ I \approx \frac{(b-a)}{6} \left( \frac{f(x_0) + 4f(x_1) + f(x_2)}{\text{width}} \right) \quad (5.11) \]

and the error estimation are

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

**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

\[ I \approx 0.8 \frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467 \]

and the error is

\[ E_i = 1.640533 - 1.367467 = 0.2730667 \]
\[ \varepsilon_i = \left| \frac{0.2730667}{1.640533} \right| = 16.6\% \]
If there are \( n \) segments, the formula for the 1/3-Simpson rule is

\[
I = \frac{1}{6} \left[ f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{n-2}) + f(x_{n}) \right]
\]

or, in a more simplified form

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

(5.13)

and the error estimation are

\[
E_a = -\frac{(b-a)^5}{180n^4} f^{(4)}(c)
\]

(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 \(x_i\):

\[
\begin{align*}
    f(0) &= 0.2 \\
    f(0.2) &= 1.288 \\
    f(0.4) &= 2.456 \\
    f(0.6) &= 3.464 \\
    f(0.8) &= 0.232
\end{align*}
\]

Hence, the integration is

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

and the error is

\[
E_t = 1.640533 - 1.623467 = 0.017067
\]

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

- 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

\[
I \approx \frac{3}{8} h[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] \tag{5.15}
\]
where the step size is \( h = \frac{1}{3}(b - a) \). It can be represented by

\[
I \approx (b - a) \frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}
\]

(5.16)

and the associated error is

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

(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

\[
E_t = 1.640533 - 1.519170 = 0.1213630
\]

\[
E_t = \frac{0.1213630}{1.640533} = 7.40\%
\]

\[
E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.1213630
\]
In general, the Newton-Cotes Integral formula can be written as

\[ I = \int_a^b f(x)dx = \alpha h[w_0f_0 + w_1f_1 + w_2f_2 + \cdots + w_nf_n] + E \quad (5.18) \]

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

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \alpha )</th>
<th>( w_i \forall i = 0,1,2,\ldots,n )</th>
<th>( E_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \frac{1}{2} )</td>
<td>1 1</td>
<td>(-\frac{1}{2} h^3 f''(\xi))</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{1}{3} )</td>
<td>1 4 1</td>
<td>(-\frac{1}{30} h^5 f^{(4)}(\xi))</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{1}{8} )</td>
<td>1 3 3 1</td>
<td>(-\frac{1}{96} h^5 f^{(4)}(\xi))</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{2}{45} )</td>
<td>7 32 12 32 7</td>
<td>(-\frac{1}{3600} h^7 f^{(6)}(\xi))</td>
</tr>
<tr>
<td>( \vdots )</td>
<td>( \vdots )</td>
<td>( \vdots )</td>
<td>( \vdots )</td>
</tr>
</tbody>
</table>
5.4 Gauss Quadrature

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

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

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

- The general formula for the range \([-1, 1]\):

\[ \int_{-1}^{1} f(x) \, dx \approx \sum_{i=1}^{n} w_i f(x_i) \tag{5.19} \]

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:

\[
I \approx w_1 f(x_1) + w_2 f(x_2) = \int_{-1}^{1} f(x) \, dx \\
w_1 \left(a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3\right) + w_2 \left(a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3\right) \\
= \int_{-1}^{1} \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right) \, dx \\
= \int_{-1}^{1} a_0 \, dx + \int_{-1}^{1} a_1 x \, dx + \int_{-1}^{1} a_2 x^2 \, dx + \int_{-1}^{1} a_3 x^3 \, dx, \\
= 2a_0 + \frac{3}{2} a_2.
\]
Hence, four equations can be formed as followed:

Coefficient $a_0$: \[ w_1 + w_2 = 2 \]
Coefficient $a_1$: \[ w_1x_1 + w_2x_2 = 0 \]
Coefficient $a_2$: \[ w_1x_1^2 + w_2x_2^2 = \frac{3}{2} \]
Coefficient $a_2$: \[ w_1x_1^3 + w_2x_2^3 = 0 \]

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:

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

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

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

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

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

<table>
<thead>
<tr>
<th>No. of points $n$</th>
<th>Coordinates $x_i$ or $\xi_i$</th>
<th>Weights $w_i$</th>
<th>Error $E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>$\approx f^{(2)}(\xi)$</td>
</tr>
<tr>
<td>2</td>
<td>$-0.577350269$</td>
<td>1</td>
<td>$\approx f^{(4)}(\xi)$</td>
</tr>
<tr>
<td></td>
<td>$+0.577350269$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$-0.774596669$</td>
<td>0.5555555555</td>
<td>$\approx f^{(6)}(\xi)$</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0.888888889</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.774596669$</td>
<td>0.5555555555</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$-0.861136312$</td>
<td>0.347854845</td>
<td>$\approx f^{(8)}(\xi)$</td>
</tr>
<tr>
<td></td>
<td>$-0.339981044$</td>
<td>0.652145155</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.339981044$</td>
<td>0.652145155</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.861136312$</td>
<td>0.347854845</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$-0.906179846$</td>
<td>0.236926885</td>
<td>$\approx f^{(10)}(\xi)$</td>
</tr>
<tr>
<td></td>
<td>$-0.538469310$</td>
<td>0.478628670</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0.568888889</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.538469310$</td>
<td>0.478628670</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.906179846$</td>
<td>0.236926885</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$-0.932469514$</td>
<td>0.171324492</td>
<td>$\approx f^{(12)}(\xi)$</td>
</tr>
<tr>
<td></td>
<td>$-0.661209386$</td>
<td>0.360761573</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$-0.238619186$</td>
<td>0.467913935</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.238619186$</td>
<td>0.467913935</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.661209386$</td>
<td>0.360761573</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$+0.932469514$</td>
<td>0.171324492</td>
<td></td>
</tr>
</tbody>
</table>

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

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

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

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

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

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

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

\[ E_I = 1.640533 - 1.82243 = -0.182045 \]
\[ \varepsilon_i = \frac{-0.182045}{1.640533} = 11.1\% \]

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

<table>
<thead>
<tr>
<th>TABLE 5.4</th>
<th>Integration results of Ex. 5.8 for n points</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>I</td>
</tr>
<tr>
<td>1</td>
<td>1.9648</td>
</tr>
<tr>
<td>2</td>
<td>1.822578</td>
</tr>
<tr>
<td>3</td>
<td>1.640533</td>
</tr>
</tbody>
</table>
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:

\[
\iint f(x, y) \, dx \, dy \approx \sum_{i=1}^{l} \sum_{j=1}^{m} u_i v_j f_{ij} \\
\iiint f(x, y, z) \, dx \, dy \, dz \approx \sum_{i=1}^{l} \sum_{j=1}^{m} \sum_{k=1}^{n} u_i v_j w_k f_{ijk}
\]

(5.25)  (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

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

or, in a more visible pattern,

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

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

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

(5.27)  (5.28)
and its transformation to a general range can be performed using

\[
\int_{a_1}^{b_2} \int_{a_1}^{b_2} f(x, y) \, dx \, dy = \int_{-1}^{1} \int_{-1}^{1} \tilde{f}(\xi, \eta) \left( \frac{\partial x}{\partial \xi} \cdot \frac{\partial y}{\partial \eta} \right) \, d\xi \, d\eta
\]

\[
\cong \frac{b_2 - a_2}{2} \sum_{i=1}^{m} u_i v_j f(x_i, y_j)
\]

(5.29)

\[
\int_{a_1}^{b_2} \int_{a_1}^{b_2} \int_{a_1}^{b_2} f(x, y, z) \, dx \, dy \, dz = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \tilde{f}(\xi, \eta, \zeta) \left( \frac{\partial x}{\partial \xi} \cdot \frac{\partial y}{\partial \eta} \cdot \frac{\partial z}{\partial \zeta} \right) \, d\xi \, d\eta \, d\zeta
\]

\[
\cong \frac{b_2 - a_2}{2} \sum_{i=1}^{m} u_i v_j w_k f(x_i, y_j, z_k)
\]

(5.30)

where the transformed variable system \((\xi, \eta)\) or \((\xi, \eta, \zeta)\) is known as the isoparametric coordinate system.

**Example 5.9**

Evaluate:

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

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

\[
I = \int_{-\pi/2}^{\pi/2} \int_{0}^{3} \int_{0}^{1} f(x) \, dx \, dy \, dz = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \tilde{f}(\xi, \eta, \zeta) \left( \frac{\partial x}{\partial \xi} \cdot \frac{\partial y}{\partial \eta} \cdot \frac{\partial z}{\partial \zeta} \right) \, d\xi \, d\eta \, d\zeta,
\]

\[
\cong \frac{1}{2} \cdot \frac{3 - 1}{2} \cdot \frac{\pi/2 - (-\pi/2)}{2} \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{n} u_i v_j w_k f(x_i, y_j, z_k),
\]

\[
\cong \frac{\pi}{4} \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{n} u_i v_j w_k f(x_i, y_j, z_k).
\]
By taking \( n = 2 \) in all directions, \( \xi_i = \eta_j = \zeta_k = \pm 0.57735 \):

<table>
<thead>
<tr>
<th>( i,j,k )</th>
<th>( x_i )</th>
<th>( y_j )</th>
<th>( z_k )</th>
<th>( u_ivjw_k )</th>
<th>( f(u_i,v_j,w_k) )</th>
<th>( \frac{u_ivjw_k \times f(u_i,v_j,w_k)}{f(u_i,v_j,w_k)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,1,1</td>
<td>0.21132</td>
<td>1.42265</td>
<td>(-0.90690)</td>
<td>1</td>
<td>0.35062</td>
<td>0.35062</td>
</tr>
<tr>
<td>1,1,2</td>
<td>0.21132</td>
<td>1.42265</td>
<td>0.90690</td>
<td>1</td>
<td>0.35062</td>
<td>0.35062</td>
</tr>
<tr>
<td>1,2,1</td>
<td>0.21132</td>
<td>2.57735</td>
<td>(-0.90690)</td>
<td>1</td>
<td>0.19354</td>
<td>0.19354</td>
</tr>
<tr>
<td>1,2,2</td>
<td>0.21132</td>
<td>2.57735</td>
<td>0.90690</td>
<td>1</td>
<td>0.19354</td>
<td>0.19354</td>
</tr>
<tr>
<td>2,1,1</td>
<td>0.78868</td>
<td>1.42265</td>
<td>(-0.90690)</td>
<td>1</td>
<td>0.19683</td>
<td>0.19683</td>
</tr>
<tr>
<td>2,1,2</td>
<td>0.78868</td>
<td>1.42265</td>
<td>0.90690</td>
<td>1</td>
<td>0.19683</td>
<td>0.19683</td>
</tr>
<tr>
<td>2,2,1</td>
<td>0.78868</td>
<td>2.57735</td>
<td>(-0.90690)</td>
<td>1</td>
<td>0.10865</td>
<td>0.10865</td>
</tr>
<tr>
<td>2,2,2</td>
<td>0.78868</td>
<td>2.57735</td>
<td>0.90690</td>
<td>1</td>
<td>0.10865</td>
<td>0.10865</td>
</tr>
<tr>
<td><strong>Jumlah</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.69928</td>
<td></td>
</tr>
</tbody>
</table>

Therefore,

\[
I = \frac{\pi}{4} (1.69928) = 1.33462.
\]

giving an error of

\[
E_i = 1.38891 - 1.33462 = 0.05430
\]

\[
\varepsilon_i = \frac{0.05430}{1.38891} = 3.91\%
\]
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:

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

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

<table>
<thead>
<tr>
<th>( \varepsilon ), in/in</th>
<th>( \sigma ), psi</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0</td>
</tr>
<tr>
<td>0.001</td>
<td>10298</td>
</tr>
<tr>
<td>0.002</td>
<td>18852</td>
</tr>
<tr>
<td>0.003</td>
<td>25882</td>
</tr>
<tr>
<td>0.004</td>
<td>31586</td>
</tr>
<tr>
<td>0.005</td>
<td>36137</td>
</tr>
</tbody>
</table>

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 reliability of the aircraft wing system. As a guidance, the curve for the test is given by:

\[ \sigma = 11.2514 \times 10^6 \varepsilon e^{-88.52\varepsilon} \]