CHAPTER 4

Differentiation and Integration

4.1 INTRODUCTION

Given a function \( f(x) \) explicitly or defined at a set of \( n + 1 \) distinct tabular points, we discuss methods to obtain the approximate value of the \( r \)th order derivative \( f^{(r)}(x) \), \( r \geq 1 \), at a tabular or a non-tabular point and to evaluate

\[
\int_{a}^{b} w(x) f(x) \, dx,
\]

where \( w(x) > 0 \) is the weight function and \( a \) and / or \( b \) may be finite or infinite.

4.2 NUMERICAL DIFFERENTIATION

Numerical differentiation methods can be obtained by using any one of the following three techniques:

(i) methods based on interpolation,
(ii) methods based on finite differences,
(iii) methods based on undetermined coefficients.

Methods Based on Interpolation

Given the value of \( f(x) \) at a set of \( n + 1 \) distinct tabular points \( x_0, x_1, \ldots, x_n \), we first write the interpolating polynomial \( P_n(x) \) and then differentiate \( P_n(x) \), \( r \) times, \( 1 \leq r \leq n \), to obtain \( P_n^{(r)}(x) \). The value of \( P_n^{(r)}(x) \) at the point \( x^* \), which may be a tabular point or a non-tabular point gives the approximate value of \( f^{(r)}(x) \) at the point \( x = x^* \). If we use the Lagrange interpolating polynomial

\[
P_n(x) = \sum_{i=0}^{n} l_i(x) f(x_i)
\]

having the error term

\[
E_n(x) = f(x) - P_n(x)
= \frac{(x-x_0)(x-x_1)\ldots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi)
\]

we obtain

\[
f^{(r)}(x^*) = P_n^{(r)}(x^*), \quad 1 \leq r \leq n
\]

and

\[
E_n^{(r)}(x^*) = f^{(r)}(x^*) - P_n^{(r)}(x^*)
\]

is the error of differentiation. The error term (4.3) can be obtained by using the formula
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\[ \frac{1}{(n+1)!} \frac{d^j}{dx^j} [f^{(n+1)}(\xi)] = \frac{j!}{(n+j+1)!} f^{(n+j+1)}(\eta_j) \]

where \( \min(x_0, x_1, \ldots, x_n, x) < \eta_j < \max(x_0, x_1, \ldots, x_n, x) \).

When the tabular points are equispaced, we may use Newton’s forward or backward difference formulas.

For \( n = 1 \), we obtain

\[ f(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 \quad \ldots \text{[4.4 (i)]} \]

and

\[ f'(x_k) = \frac{f_1 - f_0}{x_1 - x_0} k = 0, 1 \quad \ldots \text{[4.4 (ii)]} \]

Differentiating the expression for the error of interpolation

\[ E_1(x) = \frac{1}{2} (x - x_0)(x - x_1) f^{(\prime\prime)}(\xi), \quad x_0 < \xi < x_1 \]

we get, at \( x = x_0 \) and \( x = x_1 \)

\[ E_1^{(1)}(x_0) = -E_1^{(1)}(x_1) = \frac{x_0 - x_1}{2} f^{(\prime\prime)}(\xi), \quad x_0 < \xi < x_1. \]

For \( n = 2 \), we obtain

\[ f(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f_2 \quad \ldots \text{[4.5 (i)]} \]

\[ E_2(x) = \frac{1}{6} (x - x_0)(x - x_1)(x - x_2) f^{(\prime\prime\prime)}(\xi), \quad x_0 < \xi < x_2 \quad \ldots \text{[4.5 (ii)]} \]

\[ f'(x_k) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f_2 \quad \ldots \text{[4.5 (iii)]} \]

with the error of differentiation

\[ E_2^{(1)}(x_0) = \frac{1}{6} (x_0 - x_1)(x_0 - x_2) f^{(\prime\prime\prime)}(\xi), \quad x_0 < \xi < x_2. \]

Differentiating (4.5 (i)) and (4.5 (ii)) two times and setting \( x = x_0 \), we get

\[ f^{(\prime\prime)}(x_0) = 2 \left[ \frac{f_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{f_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{f_2}{(x_2 - x_0)(x_2 - x_1)} \right] \quad (4.6) \]

with the error of differentiation

\[ E_2^{(2)}(x_0) = \frac{1}{3} (2x_0 - x_1 - x_2) f^{(\prime\prime\prime)}(\xi) + \frac{1}{24} (x_0 - x_1)(x_1 - x_2) [f^{(iv)}(\eta_1) + f^{(iv)}(\eta_2)] \]

where \( x_0 < \xi, \eta_1, \eta_2 < x_2 \).

For equispaced tabular points, the formulas [4.4 (ii)], [4.5 (iii)], and (4.6) become, respectively

\[ f'(x_0) = \frac{f_1 - f_0}{h}, \quad (4.7) \]

\[ f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h}, \quad (4.8) \]

\[ f''(x_0) = \frac{f_0 - 2f_1 + f_2}{2h}, \quad (4.9) \]

with the respective error terms.
If we write
\[ E_n^{(r)}(x_k) = | f^{(r)}(x_k) - P_n^{(r)}(x_k) | \]

\[ = c h^p + O(h^{p+1}) \]

where \( c \) is a constant independent of \( h \), then the method is said to be of order \( p \). Hence, the methods (4.7) and (4.9) are of order 1, whereas the method (4.8) is of order 2.

**Methods Based on Finite Differences**

Consider the relation

\[ Ef(x) = f(x + h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + ... \]

\[ = \left( 1 + hD + \frac{h^2D^2}{2!} + ... \right) f(x) = e^{hD} f(x) \] (4.10)

where \( D = d / dx \) is the differential operator.

Symbolically, we get from (4.10)

\[ E = e^{hD}, \text{ or } hD = \ln E. \]

We have

\[ \delta = E^{1/2} - E^{-1/2} = e^{hD/2} - e^{-hD/2} \]

\[ = 2 \sinh (hD / 2). \]

Hence, \( hD = 2 \sinh^{-1} (\delta / 2). \)

Thus, we have

\[ hD = \ln \left( \frac{1 + \Delta}{1 - \Delta} \right) = \Delta - \frac{1}{2} \Delta^2 + \frac{1}{3} \Delta^3 - ... \]

\[ - \ln (1 - \nabla) = \nabla + \frac{1}{2} \nabla^2 + \frac{1}{3} \nabla^3 + ... \]

\[ 2 \sinh^{-1} \left( \frac{\delta}{2} \right) = \delta - \frac{1^2}{2^2} \delta^3 + ... \] (4.11)

Similarly, we obtain

\[ \Delta^r = \frac{1}{2} r \Delta^{r+1} + \frac{r(3r + 5)}{24} \Delta^{r+2} - ... \]

\[ \nabla^r = \frac{1}{2} r \nabla^{r+1} + \frac{r(3r + 5)}{24} \nabla^{r+2} + ... \]

\[ h^r D^r = \]

\[ \mu \delta^r = \frac{r + 3}{24} \mu \delta^{r+2} + \frac{5r^2 + 52r + 135}{5760} \mu \delta^{r+4} - ..., \quad (r \text{ odd}) \]

\[ \delta^r = \frac{r}{24} \delta^{r+2} + \frac{r(5r + 22)}{5760} \delta^{r+4} - ..., \quad (r \text{ even}) \] (4.12)
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where, \( \mu = \sqrt{1 + \frac{\delta^2}{4}} \) is the averaging operator and is used to avoid off-step points in the method.

Retaining various order differences in (4.12), we obtain different order methods for a given value of \( r \). Keeping only one term in (4.12), we obtain for \( r = 1 \)

\[
\begin{align*}
  f'(x_k) &= \frac{(f_{k+1} - f_k)}{h}, \quad \text{...}[4.13 \ (i)] \\
  &\quad \frac{(f_k - f_{k-1})}{h}, \quad \text{...}[4.13 \ (ii)] \\
  &\quad \frac{(f_{k+1} - f_{k-1})}{2h}, \quad \text{...}[4.13 \ (iii)]
\end{align*}
\]

and for \( r = 2 \)

\[
\begin{align*}
  f''(x_k) &= \frac{(f_{k+2} - 2f_{k+1} + f_k)}{h^2}, \quad \text{...}[4.14 \ (i)] \\
  &\quad \frac{(f_k - 2f_{k-1} + f_{k-2})}{h^2}, \quad \text{...}[4.14 \ (ii)] \\
  &\quad \frac{(f_{k+1} - 2f_{k} + f_{k-1})}{h^2}. \quad \text{...}[4.14 \ (iii)]
\end{align*}
\]

The methods (4.13 \( i \)), (4.13 \( ii \)), (4.14 \( i \)), (4.14 \( ii \)) are of first order, whereas the methods (4.13 \( iii \)) and (4.14 \( iii \)) are of second order.

**Methods Based on Undetermined Coefficients**

We write

\[
h^r f^{(r)}(x_k) = \sum_{i=-m}^{m} a_i f(x_{k+i})
\]

for symmetric arrangement of tabular points and

\[
h^r f^{(r)}(x_k) = \sum_{i=-m}^{m} a_i f(x_{k+i})
\]

for non-symmetric arrangement of tabular points.

The error term is obtained as

\[
E_r(x_k) = \frac{1}{h^r} \left[ h^r f^{(r)}(x_k) - \sum a_i f(x_{k+i}) \right].
\]

The coefficients \( a_j \)'s in (4.15) or (4.16) are determined by requiring the method to be of a particular order. We expand each term in the right side of (4.15) or (4.16) in Taylor series about the point \( x_k \) and on equating the coefficients of various order derivatives on both sides, we obtain the required number of equations to determine the unknowns. The first non-zero term gives the error term.

For \( m = 1 \) and \( r = 1 \) in (4.15), we obtain

\[
h f'(x_k) = a_{-1} f(x_{k-1}) + a_0 f(x_k) + a_1 f(x_{k+1})
= (a_{-1} + a_0 + a_1) f(x_k) + (-a_{-1} + a_1) h f'(x_k) + \frac{1}{2} (a_{-1} + a_1) h^2 f''(x_k)
+ \frac{1}{6} (-a_{-1} + a_1) h^3 f'''(x_k) + ...
\]

Comparing the coefficients of \( f(x_k) \), \( h f'(x_k) \) and \( h^2 / 2 \) \( f''(x_k) \) on both sides, we get

\[
a_{-1} + a_0 + a_1 = 0, \quad -a_{-1} + a_1 = 1, \quad a_{-1} + a_1 = 0
\]

whose solution is \( a_0 = 0, a_{-1} = -a_1 = -1 / 2 \). We obtain the formula

\[
h f_k' = \frac{1}{2} (f_{k+1} - f_{k-1}), \quad \text{or} \quad f_k' = \frac{1}{2h} (f_{k+1} - f_{k-1}).
\]
The error term in approximating \( f'(x_k) \) is given by \(- h^2 / 6 \) \( f'''(\xi), x_{k-1} < \xi < x_{k+1} \).

For \( m = 1 \) and \( r = 2 \) in (4.15), we obtain
\[
h^2 f'''(x_k) = a_{-1} f(x_{k-1}) + a_0 f(x_k) + a_1 f(x_{k+1})
= (a_{-1} + a_0 + a_1) f(x_k) + (a_{-1} + a_1) h f'(x_k)
+ \frac{1}{2} (a_{-1} + a_1) h^2 f''(x_k) + \frac{1}{6} (a_{-1} + a_1) h^3 f'''(x_k)
+ \frac{1}{24} (a_{-1} + a_1) h^4 f^{iv}(x_k) + \ldots.
\]

Comparing the coefficients of \( f(x_k), h f'(x_k) \) and \( h^2 f''(x_k) \) on both sides, we get
\[
a_{-1} + a_0 + a_1 = 0, \quad -a_{-1} + a_1 = 0, \quad a_{-1} + a_1 = 2
\]
whose solution is \( a_{-1} = a_1 = 1, a_0 = -2 \). We obtain the formula
\[
h^2 f'' = f_{k-1} - 2f_k + f_{k+1}, \quad \text{or} \quad f''_h = \frac{1}{h^2} (f_{k-1} - 2f_k + f_{k+1}).
\] (4.19)

The error term in approximating \( f''(x_k) \) is given by \(- h^2 / 12 \) \( f^{(4)}(\xi), x_{k-1} < \xi < x_{k+1} \).

Formulas (4.18) and (4.19) are of second order.

Similarly, for \( m = 2 \) in (4.15) we obtain the fourth order methods
\[
f'(x_k) = (f_{k-2} - 8f_{k-1} + 8f_{k+1} - f_{k+2}) / (12h) \quad \text{(4.20)}
\]
\[
f''(x_k) = (f_{k-2} + 16f_{k-1} - 30f_k + 16f_{k+1} - f_{k+2}) / (12h^2) \quad \text{(4.21)}
\]
with the error terms \( h^4 / 30 \) \( f^{v}(\xi) \) and \( h^4 / 90 \) \( f^{vi}(\xi) \) respectively and \( x_{k-2} < \xi < x_{k+2} \).

### 4.3 Extrapolation Methods

To obtain accurate results, we need to use higher order methods which require a large number of function evaluations and may cause growth of roundoff errors. However, it is generally possible to obtain higher order solutions by combining the computed values obtained by using a certain lower order method with different step sizes.

If \( g(x) \) denotes the quantity \( f^{(r)}(x_k) \) and \( g(h) \) and \( g(qh) \) denote its approximate value obtained by using a certain method of order \( p \) with step sizes \( h \) and \( qh \) respectively, we have
\[
g(h) = g(x) + ch^p + O(h^{p+1}),
\] (4.22)
\[
g(qh) = g(x) + c q^p h^p + O(h^{p+1}).
\] (4.23)

Eliminating \( c \) from (4.22) and (4.23) we get
\[
g(x) = \frac{q^p g(h) - g(qh)}{q^p - 1} + O(h^{p+1})
\] (4.24)
which defines a method of order \( p + 1 \). This procedure is called extrapolation or Richardson’s extrapolation.

If the error term of the method can be written as a power series in \( h \), then by repeating the extrapolation procedure a number of times, we can obtain methods of higher orders. We often take the step sizes as \( h, h / 2, h / 2^2, \ldots \). If the error term of the method is of the form
\[
E(x_k) = c_1 h + c_2 h^2 + \ldots
\] (4.25)
then, we have
\[
g(h) = g(x) + c_1 h + c_2 h^2 + \ldots
\] (4.26)

Writing (4.26) for \( h, h / 2, h / 2^2, \ldots \) and eliminating \( c_i \)'s from the resulting equations, we obtain the extrapolation scheme.
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\[ g^{(p)}(h) = \frac{2^p g^{(p-1)}(h/2) - g^{(p-1)}(h)}{2^p - 1}, \quad p = 1, 2, ... \quad (4.27) \]

where \( g^{(0)}(h) = g(h) \).

The method (4.27) has order \( p + 1 \).

The extrapolation table is given below.

**Table 4.1. Extrapolation table for (4.25).**

<table>
<thead>
<tr>
<th>Step</th>
<th>Order</th>
<th>First</th>
<th>Second</th>
<th>Third</th>
<th>Fourth</th>
</tr>
</thead>
<tbody>
<tr>
<td>h</td>
<td></td>
<td>g(h)</td>
<td>g(h/2)</td>
<td>g(^{(1)})(h)</td>
<td>g(^{(2)})(h)</td>
</tr>
<tr>
<td>h/2</td>
<td></td>
<td>g(h/2)</td>
<td>g(h/2(^2))</td>
<td>g(^{(1)})(h/2)</td>
<td>g(^{(2)})(h/2)</td>
</tr>
<tr>
<td>h/(2^2)</td>
<td></td>
<td>g(h/2(^3))</td>
<td>g(h/2(^2))</td>
<td>g(^{(1)})(h/2(^2))</td>
<td>g(^{(2)})(h/2)</td>
</tr>
<tr>
<td>h/(2^3)</td>
<td></td>
<td>g(h/2(^3))</td>
<td>g(h/2(^3))</td>
<td>g(^{(1)})(h/2(^3))</td>
<td></td>
</tr>
</tbody>
</table>

Similarly, if the error term of the method is of the form

\[ E(x_k) = g(x) + c_1 h^2 + c_2 h^4 + ... \quad (4.28) \]

then, we have

\[ g(h) = g(x) + c_1 h^2 + c_2 h^4 + ... \quad (4.29) \]

The extrapolation scheme is now given by

\[ g^{(p)}(h) = \frac{4^p g^{(p-1)}(h/2) - g^{(p-1)}(h)}{4^p - 1}, \quad p = 1, 2, ... \quad (4.30) \]

which is of order \( 2p + 2 \).

The extrapolation table is given below.

**Table 4.2. Extrapolation table for (4.28).**

<table>
<thead>
<tr>
<th>Step</th>
<th>Order</th>
<th>Second</th>
<th>Fourth</th>
<th>Sixth</th>
<th>Eighth</th>
</tr>
</thead>
<tbody>
<tr>
<td>h</td>
<td></td>
<td>g(h)</td>
<td>g(h/2)</td>
<td>g(^{(1)})(h)</td>
<td>g(^{(2)})(h)</td>
</tr>
<tr>
<td>h/2</td>
<td></td>
<td>g(h/2)</td>
<td>g(h/2(^2))</td>
<td>g(^{(1)})(h/2)</td>
<td>g(^{(2)})(h/2)</td>
</tr>
<tr>
<td>h/(2^2)</td>
<td></td>
<td>g(h/2(^3))</td>
<td>g(h/2(^2))</td>
<td>g(^{(1)})(h/2(^2))</td>
<td>g(^{(2)})(h/2)</td>
</tr>
<tr>
<td>h/(2^3)</td>
<td></td>
<td>g(h/2(^3))</td>
<td>g(h/2(^3))</td>
<td>g(^{(1)})(h/2(^3))</td>
<td></td>
</tr>
</tbody>
</table>

The extrapolation procedure can be stopped when

\[ | g^{(k)}(h) - g^{(k-1)}(h/2) | < \varepsilon \]

where \( \varepsilon \) is the prescribed error tolerance.

### 4.4 PARTIAL DIFFERENTIATION

One way to obtain numerical partial differentiation methods is to consider only one variable at a time and treat the other variables as constants. We obtain

\[
\left( \frac{\partial f}{\partial x} \right)_{(x,y)} = \begin{cases} 
(f_{i+1,j} - f_{i,j})/h + O(h), \\
(f_{i,j} - f_{i-1,j})/h + O(h), \\
(f_{i+1,j} - f_{i-1,j})/2h + O(h^2),
\end{cases}
\quad (4.31)
\]
\[
\left( \frac{\partial f}{\partial y} \right)_{(x_i, y_i)} = \begin{cases} (f_{i,j+1} - f_{i,j})/h + O(k), \\ (f_{i,j} - f_{i,j-1})/k + O(h), \\ (f_{i,j+1} - f_{i,j-1})/(2k) + O(k^2), \end{cases}
\]

where \( h \) and \( k \) are the step sizes in \( x \) and \( y \) directions respectively.

Similarly, we obtain
\[
\left( \frac{\partial^2 f}{\partial x^2} \right)_{(x_i, y_j)} = (f_{i-1,j} - 2f_{i,j} + f_{i+1,j}) / h^2 + O(h^2),
\]
\[
\left( \frac{\partial^2 f}{\partial y^2} \right)_{(x_i, y_j)} = (f_{i,j+1} - 2f_{i,j} + f_{i,j-1}) / k^2 + O(k^2),
\]
\[
\left( \frac{\partial^2 f}{\partial x \partial y} \right)_{(x_i, y_j)} = (f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}) / (4hk) + O(h^2 + k^2).
\]

4.5 OPTIMUM CHOICE OF STEP LENGTH

In numerical differentiation methods, error of approximation or the truncation error is of the form \( ch^p \) which tends to zero as \( h \to 0 \). However, the method which approximates \( f'(x) \) contains \( h^p \) in the denominator. As \( h \) is successively decreased to small values, the truncation error decreases, but the roundoff error in the method may increase as we are dividing by a smaller number. It may happen that after a certain critical value of \( h \), the roundoff error may become more dominant than the truncation error and the numerical results obtained may start worsening as \( h \) is further reduced. When \( f(x) \) is given in tabular form, these values may not themselves be exact. These values contain roundoff errors, that is \( f(x_i) = f_i + \epsilon_i \), where \( f(x_i) \) is the exact value and \( f_i \) is the tabulated value. To see the effect of this roundoff error in a numerical differentiation method, we consider the method
\[
f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2} f''(\xi), \quad x_0 < \xi < x_1.
\]

If the roundoff errors in \( f(x_0) \) and \( f(x_1) \) are \( \epsilon_0 \) and \( \epsilon_1 \) respectively, then we have
\[
f'(x_0) = f_1 - f_0 + \frac{\epsilon_1 - \epsilon_0}{h} - \frac{h}{2} f''(\xi)
\]

or
\[
f'(x_0) = f_1 - f_0 + \text{RE} + \text{TE}
\]

where RE and TE denote the roundoff error and the truncation error respectively. If we take
\[
\epsilon = \max \{|\epsilon_1|, |\epsilon_2|\}, \quad \text{and} \quad M_2 = \max_{x_0 < \xi < x_1} |f''(\xi)|
\]

then, we get
\[
|\text{RE}| \leq \frac{2\epsilon}{h}, \quad \text{and} \quad |\text{TE}| \leq \frac{h}{2} M_2.
\]

We may call that value of \( h \) as an optimal value for which one of the following criteria is satisfied:

(i) \[ |\text{RE}| = |\text{TE}| \] \[4.37 (i)\]
(ii) \[ |\text{RE}| + |\text{TE}| = \text{minimum}. \] \[4.37 (ii)\]
If we use the criterion \( 4.37(i) \), then we have

\[
\frac{2\varepsilon}{h} = \frac{h}{2} M_2
\]

which gives

\[
h_{\text{opt}} = 2\sqrt{\varepsilon M_2}, \quad \text{and} \quad |\text{RE}| = |\text{TE}| = \sqrt{\varepsilon M_2}.
\]

If we use the criterion \( 4.37(ii) \), then we have

\[
\frac{2\varepsilon}{h} + \frac{h}{2} M_2 = \text{minimum}
\]

which gives

\[
-\frac{2\varepsilon}{h^2} + \frac{1}{2} M_2 = 0, \quad \text{or} \quad h_{\text{opt}} = 2\sqrt{\varepsilon M_2}.
\]

The minimum total error is \( 2(\varepsilon M_2)^{1/2} \).

This means that if the roundoff error is of the order \( 10^{-k} \) (say) and \( M_2 = 0(1) \), then the accuracy given by the method may be approximately of the order \( 10^{-k/2} \). Since, in any numerical differentiation method, the local truncation error is always proportional to some power of \( h \), whereas the roundoff error is inversely proportional to some power of \( h \), the same technique can be used to determine an optimal value of \( h \), for any numerical method which approximates \( f^{(r)}(x_k) \), \( r \geq 1 \).

### 4.6 NUMERICAL INTEGRATION

We approximate the integral

\[
I = \int_a^b w(x) f(x) \, dx
\]

by a finite linear combination of the values of \( f(x) \) in the form

\[
I = \int_a^b w(x) f(x) \, dx = \sum_{k=0}^{n} \lambda_k f(x_k)
\]

where \( x_k, k = 0(1)n \) are called the abscissas or nodes which are distributed within the limits of integration \( [a, b] \) and \( \lambda_k, k = 0(1)n \) are called the weights of the integration method or the quadrature rule \( (4.39) \). \( w(x) > 0 \) is called the weight function. The error of integration is given by

\[
R_n = \int_a^b w(x) f(x) \, dx - \sum_{k=0}^{n} \lambda_k f(x_k).
\]

An integration method of the form \( (4.39) \) is said to be of order \( p \), if it produces exact results \( (R_n = 0) \), when \( f(x) \) is a polynomial of degree \( \leq p \).

Since in \( (4.39) \), we have \( 2n + 2 \) unknowns \( (n + 1 \) nodes \( x_k \)'s and \( n + 1 \) weights \( \lambda_k \)'s\), the method can be made exact for polynomials of degree \( \leq 2n +1 \). Thus, the method of the form \( (4.39) \) can be of maximum order \( 2n +1 \). If some of the nodes are known in advance, the order will be reduced.

For a method of order \( m \), we have

\[
\int_a^b w(x) x^i \, dx - \sum_{k=0}^{n} \lambda_k x_k^i = 0, \quad i = 0, 1, \ldots, m
\]

which determine the weights \( \lambda_k \)'s and the abscissas \( x_k \)'s. The error of integration is obtained from
\[ R_n = \frac{C}{(m+1)!} f^{(m+1)}(\xi), \quad a < \xi < b, \]  
\[ C = \int_a^b w(x)x^{m+1} \, dx - \sum_{k=0}^{n} \lambda_k x_k^{m+1}. \]  

4.7 NEWTON-COTES INTEGRATION METHODS

In this case, \( w(x) = 1 \) and the nodes \( x_k \)'s are uniformly distributed in \([a, b]\) with \( x_0 = a, x_n = b \) and the spacing \( h = (b-a) / n \). Since the nodes \( x_k \)'s, \( x_k = x_0 + kh, k = 0, ..., n \), are known, we have only to determine the weights \( \lambda_k \)'s, \( k = 0, ..., n \). These methods are known as Newton-Cotes integration methods and have the order \( n \). When both the end points of the interval of integration are used as nodes in the methods, the methods are called closed type methods, otherwise, they are called open type methods.

**Closed type methods**

For \( n = 1 \) in (4.39), we obtain the trapezoidal rule
\[ \int_a^b f(x) \, dx = \frac{h}{2} [f(a) + f(b)] \]  
where \( h = b - a \). The error term is given as
\[ R_1 = -\frac{h^3}{12} f''(\xi), \quad a < \xi < b. \]  

For \( n = 2 \) in (4.39), we obtain the Simpson's rule
\[ \int_a^b f(x) \, dx = \frac{h}{3} [f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)] \]  
where \( h = (b-a)/2 \). The error term is given by
\[ R_2 = \frac{C}{31} f'''(\xi), \quad a < \xi < b. \]  

We find that in this case
\[ C = \int_a^b x^3 \, dx - \frac{(b-a)}{6} \left[ a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3 \right] = 0 \]  
and hence the method is exact for polynomials of degree 3 also. The error term is now given by
\[ R_2 = \frac{C}{41} f'''(\xi), \quad a < \xi < b. \]  

We find that
\[ C = \int_a^b x^4 \, dx - \frac{(b-a)}{6} \left[ a^4 + 4\left(\frac{a+b}{2}\right)^4 + b^4 \right] = -\frac{(b-a)^5}{120}. \]  

Hence, the error of approximation is given by
\[ R_2 = -\frac{(b-a)^5}{2880} f'''(\xi) = -\frac{h^5}{90} f'''(\xi), \quad a < \xi < b. \]  

Since \( h = (b-a) / 2 \).

For \( n = 3 \) in (4.39), we obtain the Simpson's 3 / 8 rule
Differentiation and Integration

\[ \int_a^b f(x) \, dx = \frac{3h}{8} \left[ f(a) + 3f(a + h) + 3f(a + 2h) + f(b) \right] \quad (4.48) \]

where \( h = (b - a) / 3 \). The error term is given by

\[ R_3 = -\frac{3}{80} h^5 f^{iv}(\xi), \quad a < \xi < b, \quad (4.49) \]

and hence the method \((4.49)\) is also a third order method.

The weights \( \lambda_k \)'s of the Newton-Cotes rules for \( n \leq 5 \) are given in Table 4.3. For large \( n \), some of the weights become negative. This may cause loss of significant digits due to mutual cancellation.

### Table 4.3. Weights of Newton-Cotes Integration Rule \((4.39)\)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \lambda_0 )</th>
<th>( \lambda_1 )</th>
<th>( \lambda_2 )</th>
<th>( \lambda_3 )</th>
<th>( \lambda_4 )</th>
<th>( \lambda_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1/2</td>
<td>1/3</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1/3</td>
<td>4/3</td>
<td>1/3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>3/8</td>
<td>9/8</td>
<td>9/8</td>
<td>3/8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>14/45</td>
<td>64/45</td>
<td>24/45</td>
<td>64/45</td>
<td>14/45</td>
<td></td>
</tr>
</tbody>
</table>

**Open type methods**

We approximate the integral \((4.38)\) as

\[ I = \int_a^b f(x) \, dx = \sum_{k=1}^{n-1} \lambda_k f(x_k), \quad (4.50) \]

where the end points \( x_0 = a \) and \( x_n = b \) are excluded.

For \( n = 2 \), we obtain the **mid-point rule**

\[ \int_a^b f(x) \, dx = 2h f(a + b) \quad (4.51) \]

where \( h = (b - a) / 2 \). The error term is given by

\[ R_2 = \frac{h^3}{3} f'''(\xi). \]

Similarly, for different values of \( n \) and \( h = (b - a) / n \), we obtain

- **\( n = 3 \)** : 
  \[ I = \frac{3h}{2} \left[ f(a + h) + f(a + 2h) \right]. \]
  \[ R_3 = \frac{3}{4} h^3 f'''(\xi). \quad (4.52) \]

- **\( n = 4 \)** : 
  \[ I = \frac{4h}{3} \left[ 2f(a + h) - f(a + 2h) + 2f(a + 3h) \right]. \]
  \[ R_4 = \frac{14}{45} h^5 f^{iv}(\xi). \quad (5.53) \]

- **\( n = 5 \)** : 
  \[ I = \frac{5h}{24} \left[ 11f(a + h) + f(a + 2h) + f(a + 3h) + 11f(a + 4h) \right]. \]
  \[ R_5 = \frac{95}{144} h^5 f^{iv}(\xi), \quad (4.54) \]

where \( a < \xi < b \).
4.8 GAUSSIAN INTEGRATION METHODS

When both the nodes and the weights in the integration method (4.39) are to be determined, then the methods are called Gaussian integration methods.

If the abscissas $x_k$'s in (4.39) are selected as zeros of an orthogonal polynomial, orthogonal with respect to the weight function $w(x)$ on the interval $[a, b]$, then the method (4.39) has order $2n + 1$ and all the weights $\lambda_k > 0$.

The proof is given below.

Let $f(x)$ be a polynomial of degree less than or equal to $2n + 1$. Let $q_n(x)$ be the Lagrange interpolating polynomial of degree $\leq n$, interpolating the data $(x_i, f_i)$, $i = 0, 1, ..., n$.

$$q_n(x) = \sum_{k=0}^{n} l_k(x) f(x_k)$$

with

$$l_k(x) = \frac{\pi(x)}{(x - x_k)\pi'(x_k)}.$$

The polynomial $[f(x) - q_n(x)]$ has zeros at $x_0, x_1, ..., x_n$. Hence, it can be written as

$$f(x) - q_n(x) = p_{n+1}(x) r_n(x)$$

where $r_n(x)$ is a polynomial of degree at most $n$ and $p_{n+1}(x_i) = 0, i = 0, 1, 2, ..., n$. Integrating this equation, we get

$$\int_a^b w(x) [f(x) - q_n(x)] \, dx = \int_a^b w(x) p_{n+1}(x) r_n(x) \, dx$$

or

$$\int_a^b w(x)f(x) \, dx = \int_a^b w(x)q_n(x) \, dx + \int_a^b w(x)p_{n+1}(x) r_n(x) \, dx.$$ 

The second integral on the right hand side is zero, if $p_{n+1}(x)$ is an orthogonal polynomial, orthogonal with respect to the weight function $w(x)$, to all polynomials of degree less than or equal to $n$.

We then have

$$\int_a^b w(x)f(x) \, dx = \int_a^b w(x)q_n(x) \, dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

where

$$\lambda_k = \int_a^b w(x) l_k(x) \, dx.$$ 

This proves that the formula (4.39) has precision $2n + 1$.

Observe that $l_j^2(x)$ is a polynomial of degree less than or equal to $2n$.

Choosing $f(x) = l_j^2(x)$, we obtain

$$\int_a^b w(x) l_j^2(x) \, dx = \sum_{k=0}^{n} \lambda_k l_j^2(x_k).$$

Since $l_j(x_k) = \delta_{jk}$, we get

$$\lambda_j = \int_a^b w(x) l_j^2(x) \, dx > 0.$$ 

Since any finite interval $[a, b]$ can be transformed to $[-1, 1]$, using the transformation

$$x = \frac{(b - a)}{2} t + \frac{(b + a)}{2}$$

we consider the integral in the form
\[ \int_{-1}^{1} w(x)f(x)dx = \sum_{k=0}^{n} \lambda_k f(x_k). \]  \hspace{1cm} (4.55)

**Gauss-Legendre Integration Methods**

We consider the integration rule
\[ \int_{-1}^{1} f(x)dx = \sum_{k=0}^{n} \lambda_k f(x_k). \]  \hspace{1cm} (4.56)

The nodes \( x_k \)'s are the zeros of the Legendre polynomials
\[ P_{n+1}(x) = \frac{1}{2^{n+1}(n+1)!} \frac{d^{n+1}}{dx^{n+1}} [(x^2 - 1)^{n+1}] . \]  \hspace{1cm} (4.57)

The first few Legendre polynomials are given by
\[ P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = (3x^2 - 1)/2, \quad P_3(x) = (5x^3 - 3x)/2, \quad P_4(x) = (35x^4 - 30x^2 + 3)/8. \]

The Legendre polynomials are orthogonal on \([-1, 1]\) with respect to the weight function \( w(x) = 1 \). The methods (4.56) are of order \( 2n + 1 \) and are called *Gauss-Legendre integration methods*.

For \( n = 1 \), we obtain the method
\[ \int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \]  \hspace{1cm} (4.58)
with the error term \((1 / 135) f^{(4)}(\xi), -1 < \xi < 1\).

For \( n = 2 \), we obtain the method
\[ \int_{-1}^{1} f(x)dx = \frac{1}{9} [5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})] \]  \hspace{1cm} (4.59)
with the error term \((1 / 15750) f^{(6)}(\xi), -1 < \xi < 1\).

The nodes and the corresponding weights of the method (4.56) for \( n \leq 5 \) are listed in Table 4.4.

**Table 4.4. Nodes and Weights for the Gauss-Legendre Integration Methods (4.56)**

<table>
<thead>
<tr>
<th>( n )</th>
<th>( x_k )</th>
<th>( \lambda_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>± 0.5773502692</td>
<td>1.0000000000</td>
</tr>
<tr>
<td>2</td>
<td>0.0000000000 , ± 0.7745966692</td>
<td>0.8888888889 , 0.5555555556</td>
</tr>
<tr>
<td>3</td>
<td>± 0.3399810436 , ± 0.8611363116</td>
<td>0.6521451549 , 0.3478548451</td>
</tr>
<tr>
<td>4</td>
<td>0.0000000000 , ± 0.5384693101 , ± 0.9061798459</td>
<td>0.5688888889 , 0.4786286705 , 0.2369268851</td>
</tr>
<tr>
<td>5</td>
<td>± 0.2386191861 , ± 0.6612093865 , ± 0.9324695142</td>
<td>0.4679139346 , 0.3607615730 , 0.1713244924</td>
</tr>
</tbody>
</table>
Lobatto Integration Methods

In this case, \( w(x) = 1 \) and the two end points – 1 and 1 are always taken as nodes. The remaining \( n - 1 \) nodes and the \( n + 1 \) weights are to be determined. The integration methods of the form

\[
\int_{-1}^{1} f(x)dx = \lambda_0 f(-1) + \sum_{k=1}^{n-1} \lambda_k f(x_k) + \lambda_n f(1)
\]

are called the \textit{Lobatto integration methods} and are of order \( 2n - 1 \).

For \( n = 2 \), we obtain the method

\[
\int_{-1}^{1} f(x)dx = \frac{1}{3} [f(-1) + 4f(0) + f(1)]
\]

with the error term \(( -1 / 90 ) f^{(4)}(\xi), -1 < \xi < 1 \).

The nodes and the corresponding weights for the method (4.60) for \( n \leq 5 \) are given in Table 4.5.

\textbf{Table 4.5. Nodes and Weights for Lobatto Integration Method (4.60)}

<table>
<thead>
<tr>
<th>( n )</th>
<th>nodes ( x_k )</th>
<th>weights ( \lambda_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>( \pm 1.0000000 )</td>
<td>0.33333333</td>
</tr>
<tr>
<td></td>
<td>0.0000000</td>
<td>1.33333333</td>
</tr>
<tr>
<td>3</td>
<td>( \pm 1.0000000 )</td>
<td>0.16666667</td>
</tr>
<tr>
<td></td>
<td>( \pm 0.44721360 )</td>
<td>0.83333333</td>
</tr>
<tr>
<td>4</td>
<td>( \pm 1.0000000 )</td>
<td>0.10000000</td>
</tr>
<tr>
<td></td>
<td>( \pm 0.65465367 )</td>
<td>0.54444444</td>
</tr>
<tr>
<td></td>
<td>0.0000000</td>
<td>0.71111111</td>
</tr>
<tr>
<td>5</td>
<td>( \pm 1.0000000 )</td>
<td>0.06666667</td>
</tr>
<tr>
<td></td>
<td>( \pm 0.76505532 )</td>
<td>0.37847496</td>
</tr>
<tr>
<td></td>
<td>( \pm 0.28523152 )</td>
<td>0.55485837</td>
</tr>
</tbody>
</table>

Radau Integration Methods

In this case, \( w(x) = 1 \) and the lower limit – 1 is fixed as a node. The remaining \( n \) nodes and \( n + 1 \) weights are to be determined. The integration methods of the form

\[
\int_{-1}^{1} f(x)dx = \lambda_0 f(-1) + \sum_{k=1}^{n} \lambda_k f(x_k)
\]

are called \textit{Radau integration methods} and are of order \( 2n \).

For \( n = 1 \), we obtain the method

\[
\int_{-1}^{1} f(x)dx = \frac{1}{2} f(-1) + \frac{3}{2} f\left(\frac{1}{3}\right)
\]

with the error term \((2 / 27) f^{(4)}(\xi), -1 < \xi < 1 \).

For \( n = 2 \), we obtain the method

\[
\int_{-1}^{1} f(x)dx = \frac{2}{9} f(-1) + \frac{16 + \sqrt{6}}{18} f\left(\frac{1-\sqrt{6}}{5}\right) + \frac{16 - \sqrt{6}}{18} f\left(\frac{1+\sqrt{6}}{5}\right)
\]

with the error term \((1 / 1125) f^{(5)}(\xi), -1 < \xi < 1 \).
The nodes and the corresponding weights for the method (4.62) are given in Table 4.6.

Table 4.6. Nodes and Weights for Radau Integration Method (4.62)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$x_k$</th>
<th>$\lambda_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.0000000</td>
<td>0.5000000</td>
</tr>
<tr>
<td></td>
<td>0.3333333</td>
<td>1.5000000</td>
</tr>
<tr>
<td>2</td>
<td>-1.0000000</td>
<td>0.2222222</td>
</tr>
<tr>
<td></td>
<td>-0.2898979</td>
<td>1.0249717</td>
</tr>
<tr>
<td></td>
<td>0.6898979</td>
<td>0.7528061</td>
</tr>
<tr>
<td>3</td>
<td>-1.0000000</td>
<td>0.1250000</td>
</tr>
<tr>
<td></td>
<td>-0.5753189</td>
<td>0.6576886</td>
</tr>
<tr>
<td></td>
<td>0.1810663</td>
<td>0.7763870</td>
</tr>
<tr>
<td></td>
<td>0.8228241</td>
<td>0.4409244</td>
</tr>
<tr>
<td>4</td>
<td>-1.0000000</td>
<td>0.0800000</td>
</tr>
<tr>
<td></td>
<td>-0.7204803</td>
<td>0.4462078</td>
</tr>
<tr>
<td></td>
<td>0.1671809</td>
<td>0.6236530</td>
</tr>
<tr>
<td></td>
<td>0.4463140</td>
<td>0.5627120</td>
</tr>
<tr>
<td></td>
<td>0.8857916</td>
<td>0.2874271</td>
</tr>
<tr>
<td>5</td>
<td>-1.0000000</td>
<td>0.0555556</td>
</tr>
<tr>
<td></td>
<td>-0.8029298</td>
<td>0.3196408</td>
</tr>
<tr>
<td></td>
<td>-0.3909286</td>
<td>0.4853872</td>
</tr>
<tr>
<td></td>
<td>0.1240504</td>
<td>0.5209268</td>
</tr>
<tr>
<td></td>
<td>0.6039732</td>
<td>0.4169013</td>
</tr>
<tr>
<td></td>
<td>0.9203803</td>
<td>0.2015884</td>
</tr>
</tbody>
</table>

**Gauss-Chebyshev Integration Methods**

We consider the integral

$$
\int_{-1}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} = \sum_{k=0}^{n} \lambda_k f(x_k)
$$

where $w(x) = 1/\sqrt{1-x^2}$ is the weight function. The nodes $x_k$’s are the zeros of the Chebyshev polynomial

$$
T_{n+1}(x) = \cos ((n + 1) \cos^{-1} x).
$$

(4.66)

The first few Chebyshev polynomials are given by

$T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$,

$T_3(x) = 4x^3 - 3x$, $T_4(x) = 8x^4 - 8x^2 + 1$.

The Chebyshev polynomials are orthogonal on $[-1, 1]$ with respect to the weight function $w(x) = 1/\sqrt{1-x^2}$. The methods of the form (4.65) are called *Gauss-Chebyshev integration methods* and are of order $2n + 1$. 

We obtain from (4.66)

\[ x_k = \cos \left( \frac{(2k+1)\pi}{2n+1} \right), \quad k = 0, 1, \ldots, n. \]  

(4.67)

The weights \( \lambda_k \)'s in (4.65) are equal and are given by

\[ \lambda_k = \frac{\pi}{n+1}, \quad k = 0, 1, \ldots, n. \]  

(4.68)

For \( n = 1 \), we obtain the method

\[ \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} \, dx = \frac{\pi}{2} \left[ f \left( -\frac{1}{\sqrt{2}} \right) + f \left( \frac{1}{\sqrt{2}} \right) \right] \]  

(4.69)

with the error term \( (\pi / 192) f^{(4)}(\xi), \quad -1 < \xi < 1 \).

For \( n = 2 \), we obtain the method

\[ \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx = \frac{\pi}{3} \left[ f \left( -\frac{\sqrt{3}}{2} \right) + f(0) + f \left( \frac{\sqrt{3}}{2} \right) \right] \]  

(4.70)

with the error term \( (\pi / 23040) f^{(6)}(\xi), \quad -1 < \xi < 1 \).

\textbf{Gauss-Laguerre Integration Methods}

We consider the integral

\[ \int_{0}^{\infty} e^{-x} f(x) \, dx = \sum_{k=0}^{n} \lambda_k f(x_k) \]  

(4.71)

where \( w(x) = e^{-x} \) is the weight function. The nodes \( x_k \)'s are the zeros of the Laguerre polynomial

\[ L_{n+1}(x) = (-1)^{n+1} e^x \frac{d^{n+1}}{dx^{n+1}} [e^{-x} x^{n+1}] \]  

(4.72)

The first few Laguerre polynomials are given by

\[ L_0(x) = 1, \quad L_1(x) = x - 1, \quad L_2(x) = x^2 - 4x + 2, \]

\[ L_3(x) = x^3 - 9x^2 + 18x - 6. \]

The Laguerre polynomials are orthogonal on \([0, \infty)\) with respect to the weight function \( e^{-x} \). The methods of the form (4.71) are called \textit{Gauss-Laguerre integration method} and are of order \( 2n + 1 \).

For \( n = 1 \), we obtain the method

\[ \int_{0}^{\infty} e^{-x} f(x) \, dx = \frac{2 + \sqrt{2}}{4} f(2 - \sqrt{2}) + \frac{2 - \sqrt{2}}{4} f(2 + \sqrt{2}) \]  

(4.73)

with the error term \( (1 / 6) f^{(4)}(\xi), \quad -1 < \xi < 1 \).

The nodes and the weights of the method (4.71) for \( n \leq 5 \) are given in Table 4.7.
Table 4.7. Nodes and Weights for Gauss-Laguerre Integration Method (4.71)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$x_k$</th>
<th>$\lambda_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5857864376</td>
<td>0.8535533906</td>
</tr>
<tr>
<td></td>
<td>3.4142135624</td>
<td>0.1464466094</td>
</tr>
<tr>
<td>2</td>
<td>0.4157745568</td>
<td>0.7110930099</td>
</tr>
<tr>
<td></td>
<td>2.2942803603</td>
<td>0.2785177336</td>
</tr>
<tr>
<td></td>
<td>6.2899450829</td>
<td>0.0103892565</td>
</tr>
<tr>
<td>3</td>
<td>0.3225476896</td>
<td>0.6031541043</td>
</tr>
<tr>
<td></td>
<td>1.74576111012</td>
<td>0.3574186924</td>
</tr>
<tr>
<td></td>
<td>4.5366202969</td>
<td>0.0388879085</td>
</tr>
<tr>
<td></td>
<td>9.3950709123</td>
<td>0.0005392947</td>
</tr>
<tr>
<td>4</td>
<td>0.2635603197</td>
<td>0.5217556106</td>
</tr>
<tr>
<td></td>
<td>1.4134030591</td>
<td>0.3986681111</td>
</tr>
<tr>
<td></td>
<td>3.5964257710</td>
<td>0.0759424497</td>
</tr>
<tr>
<td></td>
<td>7.0858100059</td>
<td>0.0036117587</td>
</tr>
<tr>
<td></td>
<td>12.6408008443</td>
<td>0.000233700</td>
</tr>
<tr>
<td>5</td>
<td>0.2228466042</td>
<td>0.4589646740</td>
</tr>
<tr>
<td></td>
<td>1.1889321017</td>
<td>0.4170008308</td>
</tr>
<tr>
<td></td>
<td>2.9927363261</td>
<td>0.1133733821</td>
</tr>
<tr>
<td></td>
<td>5.7751435691</td>
<td>0.0103991975</td>
</tr>
<tr>
<td></td>
<td>9.8374674184</td>
<td>0.0002610172</td>
</tr>
<tr>
<td></td>
<td>15.9828739806</td>
<td>0.000008955</td>
</tr>
</tbody>
</table>

Gauss-Hermite Integration Methods

We consider the integral

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

(4.74)

where $w(x) = e^{-x^2}$ is the weight function. The nodes $x_k$'s are the roots of the Hermite polynomial

$$H_{n+1}(x) = (-1)^{n+1} e^{-x^2} \frac{d^{n+1}}{dx^{n+1}} (e^{-x^2}).$$

(4.75)

The first few Hermite polynomials are given by

- $H_0(x) = 1$, $H_1(x) = 2x$, $H_2(x) = 2(2x^2 - 1)$,
- $H_3(x) = 4(2x^3 - 3x)$.

The Hermite polynomials are orthogonal on $(-\infty, \infty)$ with respect to the weight function $w(x) = e^{-x^2}$. Methods of the form (4.74) are called Gauss-Hermite integration methods and are of order $2n + 1$.

For $n = 1$, we obtain the method

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \frac{\sqrt{\pi}}{2} \left[ f\left(-\frac{1}{\sqrt{2}}\right) + f\left(\frac{1}{\sqrt{2}}\right) \right]$$

(4.76)

with the error term $(\sqrt{\pi}/48) f^{(4)}(\xi)$, $-\infty < \xi < \infty$. 
For \( n = 2 \), we obtain the method
\[
\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \frac{\sqrt{\pi}}{6} \left[ f\left(-\frac{\sqrt{6}}{2}\right) + 4f(0) + f\left(\frac{\sqrt{6}}{2}\right) \right]
\]
(4.77)
with the error term \((\sqrt{\pi}/960)f^{(6)}(\xi), \ -\infty < \xi < \infty\).

The nodes and the weights for the integration method (4.74) for \( n \leq 5 \) are listed in Table 4.8.

<table>
<thead>
<tr>
<th>( n )</th>
<th>nodes ( x_k )</th>
<th>weights ( \lambda_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0000000000</td>
<td>1.7724538509</td>
</tr>
<tr>
<td>1</td>
<td>\pm 0.7071067812</td>
<td>0.8862269255</td>
</tr>
<tr>
<td>2</td>
<td>0.0000000000</td>
<td>1.1816359006</td>
</tr>
<tr>
<td></td>
<td>\pm 1.2247448714</td>
<td>0.2954089752</td>
</tr>
<tr>
<td>3</td>
<td>\pm 0.5246476233</td>
<td>0.8049140900</td>
</tr>
<tr>
<td></td>
<td>\pm 1.6506801239</td>
<td>0.0813128354</td>
</tr>
<tr>
<td>4</td>
<td>0.0000000000</td>
<td>0.9453087205</td>
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<tr>
<td></td>
<td>\pm 0.9585724646</td>
<td>0.3936193232</td>
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<tr>
<td></td>
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<td>0.0199532421</td>
</tr>
<tr>
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<td>0.7264295952</td>
</tr>
<tr>
<td></td>
<td>\pm 1.3358490740</td>
<td>0.1570673203</td>
</tr>
<tr>
<td></td>
<td>\pm 2.3506049737</td>
<td>0.0045300099</td>
</tr>
</tbody>
</table>

### 4.9 COMPOSITE INTEGRATION METHODS

To avoid the use of higher order methods and still obtain accurate results, we use the composite integration methods. We divide the interval \([a, b]\) or \([-1, 1]\) into a number of subintervals and evaluate the integral in each subinterval by a particular method.

**Composite Trapezoidal Rule**

We divide the interval \([a, b]\) into \( N \) subintervals \([x_{i-1}, x_i]\), \( i = 1, 2, ..., N \), each of length \( h = (b - a) / N \), \( x_0 = a \), \( x_N = b \) and \( x_i = x_0 + ih \), \( i = 1, 2, ..., N - 1 \). We write
\[
\int_{a}^{b} f(x) dx = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + ... + \int_{x_{N-1}}^{x_N} f(x) dx.
\]
(4.78)

Evaluating each of the integrals on the right hand side of (4.78) by the trapezoidal rule (4.44), we obtain the composite rule
\[
\int_{a}^{b} f(x) dx = \frac{h}{2} \left[ f_0 + 2(f_1 + f_2 + ... + f_{N-1}) + f_N \right]
\]
(4.79)
where \( f_i = f(x_i) \).

The error in the integration method (4.79) becomes
\[
R_1 = -\frac{h^3}{12} \left[ f''(\xi_1) + f''(\xi_2) + ... + f''(\xi_N) \right], \quad x_{i-1} < \xi_i < x_i.
\]
(4.80)

Denoting
\[
f''(\eta) = \max_{a \leq x \leq b} \left| f''(x) \right|, \quad a < \eta < b
\]
Differentiation and Integration

we obtain from (4.80)

\[ | R_1 | \leq \frac{Nh^3}{12} f''(\eta) = \frac{(b-a)^3}{12N^2} f''(\eta) = \frac{(b-a)}{12} h^2 f''(\eta). \]  

(4.81)

**Composite Simpson's Rule**

We divide the interval \([a, b]\) into \(2N\) subintervals each of length \(h = (b-a)/(2N)\). We have \(2N+1\) abscissas \(x_0, x_1, ..., x_{2N}\) with \(x_0 = a, x_i = x_0 + ih, i = 1, 2, ..., 2N-1\).

We write

\[ \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + ... + \int_{x_{2N-2}}^{x_{2N}} f(x)dx. \]  

(4.82)

Evaluating each of the integrals on the right hand side of (4.82) by the Simpson’s rule (4.46), we obtain the composite rule

\[ \int_a^b f(x)dx = \frac{h}{3} [f_0 + 4(f_1 + f_3 + ... + f_{2N-1}) + 2(f_2 + f_4 + ... + f_{2N-2}) + f_{2N}]. \]  

(4.83)

The error in the integration method (4.83) becomes

\[ R_2 = -\frac{h^5}{90} [f^{iv}(\xi_1) + f^{iv}(\xi_2) + ... + f^{iv}(\xi_N)], x_{2i-2} < \xi_i < x_{2i} \]  

(4.84)

Denoting \(f^{iv}(\eta) = \max_{a \leq x \leq b} |f^{iv}(x)|, a < \eta < b\)

we obtain from (4.84)

\[ | R_2 | \leq \frac{Nh^5}{90} f^{iv}(\eta) = \frac{(b-a)^5}{2880N^4} f^{iv}(\eta) = \frac{(b-a)}{180} h^4 f^{iv}(\eta). \]  

(4.85)

**4.10 ROMBERG INTEGRATION**

Extrapolation procedure of section 4.3, applied to the integration methods is called Romberg integration. The errors in the composite trapezoidal rule (4.79) and the composite Simpson’s rule (4.83) can be obtained as

\[ I = I_T + c_1h^2 + c_2h^4 + c_3h^6 + ... \]  

(4.86)

\[ I = I_S + d_1h^4 + d_2h^6 + d_3h^8 + ... \]  

(4.87)

respectively, where \(c_i\)'s and \(d_i\)'s are constants independent of \(h\).

Extrapolation procedure for the trapezoidal rule becomes

\[ I_T^{(m)}(h) = \frac{4^m I_T^{(m-1)}(h/2) - I_T^{(m-1)}(h)}{4^m - 1}, m = 1, 2, ... \]  

(4.88)

where \(I_T^{(0)}(h) = I_T(h)\).

The method (4.88) has order \(2m + 2\).

Extrapolation procedure for the Simpson’s rule becomes

\[ I_S^{(m)}(h) = \frac{4^{m+1} I_S^{(m-1)}(h/2) - I_S^{(m-1)}(h)}{4^{m+1} - 1}, m = 1, 2, ... \]  

(4.89)

where \(I_S^{(0)}(h) = I_S(h)\).

The method (4.89) has order \(2m + 4\).
4.11 DOUBLE INTEGRATION

The problem of double integration is to evaluate the integral of the form

\[
I = \int_{a}^{b} \int_{c}^{d} f(x, y) \, dx \, dy.
\]  

(4.90)

This integral can be evaluated numerically by two successive integrations in \(x\) and any \(y\) directions respectively, taking into account one variable at a time.

**Trapezoidal rule**

If we evaluate the inner integral in (4.90) by the trapezoidal rule, we get

\[
I_T = \frac{d - c}{2} \int_{a}^{b} [f(x, c) + f(x, d)] \, dx.
\]  

(4.91)

Using the trapezoidal rule again in (4.91) we get

\[
I_T = \frac{(b - a)(d - c)}{4} [f(a, c) + f(b, c) + f(a, d) + f(b, d)].
\]  

(4.92)

The composite trapezoidal rule for evaluating (4.90) can be written as

\[
I_T = \frac{hk}{4} \left[ (f_{00} + f_{0M} + 2(f_{01} + f_{0M}) + \cdots + f_{0,M-1}) \right]
\]

\[
+ 2 \sum_{i=1}^{N-1} (f_{i0} + f_{iM} + 2(f_{i1} + f_{i2} + \cdots + f_{i,M-1}))
\]

\[
+ (f_{N0} + f_{NM} + 2(f_{N1} + f_{N2} + \cdots + f_{N,M-1}))
\]  

(4.93)

where \(h\) and \(k\) are the spacings in \(x\) and \(y\) directions respectively and

\[
h = \frac{(b - a)}{N}, \; k = \frac{(d - c)}{M},
\]

\[
x_i = x_0 + ih, \; i = 1, 2, ..., N - 1,
\]

\[
y_j = y_0 + jk, \; j = 1, 2, ..., M - 1,
\]

\[
x_0 = a, \; x_N = b, \; y_0 = c, \; y_M = d.
\]

The computational molecule of the method (4.93) for \(M = N = 1\) and \(M = N = 2\) can be written as

**Simpson’s rule**

If we evaluate the inner integral in (4.90) by Simpson’s rule then we get

\[
I_S = \frac{k}{3} \int_{a}^{b} [f(x, c) + 4f(x, c + k) + f(x, d)] \, dx
\]  

(4.94)

where \(k = \frac{(d - c)}{2}\).
Using Simpson’s rule again in (4.94), we get
\[
I_S = \frac{hk}{9} \left[ f(a, c) + f(a, d) + f(b, c) + f(b, d) \\
+ 4[f(a + h, c) + f(a + h, d) + f(b, c + k) \\
+ f(a, c + k)] + 16f(a + h, c + k) \right] \tag{4.95}
\]
where \( h = (b - a) / 2 \).

The composite Simpson’s rule for evaluating (4.90) can be written as
\[
I_S = \frac{hk}{9} \left[ f_{00} + 4 \sum_{i=1}^{N} f_{2i-1,0} + 2 \sum_{i=1}^{N-1} f_{2i,0} + f_{2N,0} \right] \\
+ 4 \sum_{j=1}^{M} \left( f_{0,2j-1} + 4 \sum_{i=1}^{N} f_{2i-1,2j-1} + 2 \sum_{i=1}^{N-1} f_{2i,2j-1} + f_{2N,2j-1} \right) \\
+ 2 \sum_{j=1}^{M-1} \left( f_{0,2j} + 4 \sum_{i=1}^{N} f_{2i-1,2j} + 2 \sum_{i=1}^{N-1} f_{2i,2j} + f_{2N,2j} \right) \\
+ \left( f_{0,2M} + 4 \sum_{i=1}^{N} f_{2i-1,2M} + 2 \sum_{i=1}^{N-1} f_{2i,2M} + f_{2N,2M} \right) \tag{4.96}
\]
where \( h \) and \( k \) are the spacings in \( x \) and \( y \) directions respectively and
\[
h = (b - a) / (2N), \quad k = (d - c) / (2M),
\]
\[
x_i = x_0 + ih, \quad i = 1, 2, \ldots, 2N - 1,
\]
\[
y_j = y_0 + jk, \quad j = 1, 2, \ldots, 2M - 1,
\]
\[
x_0 = a, \quad x_{2N} = b, \quad y_0 = c, \quad y_{2M} = d.
\]
The computational module for \( M = N = 1 \) and \( M = N = 2 \) can be written as

<table>
<thead>
<tr>
<th>Simpson’s rule</th>
<th>Composite Simpson’s rule</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Simpson's rule diagram" /></td>
<td><img src="image2.png" alt="Composite Simpson's rule diagram" /></td>
</tr>
</tbody>
</table>

### 4.12 PROBLEMS AND SOLUTIONS

**Numerical differentiation**

4.1 A differentiation rule of the form
\[
f'(x_0) = \alpha_0 f_0 + \alpha_1 f_1 + \alpha_2 f_2,
\]
where \( x_i = x_0 + ih \) is given. Find the values of \( \alpha_0, \alpha_1 \) and \( \alpha_2 \) so that the rule is exact for \( f \in P_2 \). Find the error term.
Solution
The error in the differentiation rule is written as
\[ TE = f'(x_0) - \alpha_0 f(x_0) - \alpha_1 f(x_1) - \alpha_2 f(x_2). \]
Expanding each term on the right side in Taylor's series about the point \( x_0 \), we obtain
\[ TE = - (\alpha_0 + \alpha_1 + \alpha_2) f(x_0) + (1 - h(\alpha_1 + 2\alpha_2)) f'(x_0) \]
\[ - \frac{h^2}{2} (\alpha_1 + 4\alpha_2) f''(x_0) - \frac{h^3}{6} (\alpha_1 + 8\alpha_2) f'''(x_0) - ... \]
We choose \( \alpha_0, \alpha_1 \) and \( \alpha_2 \) such that
\[ \alpha_0 + \alpha_1 + \alpha_2 = 0, \]
\[ \alpha_1 + 2\alpha_2 = 1 / h, \]
\[ \alpha_1 + 4\alpha_2 = 0. \]
The solution of this system is
\[ \alpha_0 = - \frac{3}{2h}, \alpha_1 = \frac{4}{2h}, \alpha_2 = - \frac{1}{2h}. \]
Hence, we obtain the differentiation rule
\[ f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} \]
with the error term
\[ TE = \frac{h^3}{6} (\alpha_1 + 8\alpha_2) f'''(\xi) = - \frac{h^2}{3} f'''(\xi), x_0 < \xi < x_2. \]
The error term is zero if \( f(x) \in P_2 \). Hence, the method is exact for all polynomials of degree \( \leq 2 \).

4.2. Using the following data find \( f'(6.0) \), error = \( O(h) \), and \( f''(6.3) \), error = \( O(h^2) \)

<table>
<thead>
<tr>
<th>( x )</th>
<th>6.0</th>
<th>6.1</th>
<th>6.2</th>
<th>6.3</th>
<th>6.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f(x) )</td>
<td>0.1750</td>
<td>-0.1998</td>
<td>-0.2223</td>
<td>-0.2422</td>
<td>-0.2596</td>
</tr>
</tbody>
</table>

Solution
Method of \( O(h) \) for \( f'(x_0) \) is given by
\[ f'(x_0) = \frac{1}{h} [f(x_0 + h) - f(x_0)] \]
With \( x_0 = 6.0 \) and \( h = 0.1 \), we get
\[ f'(6.0) = \frac{1}{0.1} [f(6.1) - f(6.0)] = \frac{1}{0.1} [-0.1998 - 0.1750] = -3.748. \]
Method of \( O(h^2) \) for \( f''(x_0) \) is given by
\[ f''(x_0) = \frac{1}{h^2} [f(x_0 - h) - 2f(x_0) + f(x_0 + h)] \]
With \( x_0 = 6.3 \) and \( h = 0.1 \), we get
\[ f''(6.3) = \frac{1}{(0.1)^2} [f(6.2) - 2f(6.3) + f(6.4)] = 0.25. \]
4.3 Assume that \( f(x) \) has a minimum in the interval \( x_{n-1} \leq x \leq x_{n+1} \) where \( x_k = x_0 + kh \). Show that the interpolation of \( f(x) \) by a polynomial of second degree yields the approximation

\[
f_n = \frac{1}{8} \left( \frac{(f_{n+1} - f_{n-1})^2}{f_{n+1} - 2f_n + f_{n-1}} \right), f_k = f(x_k)
\]

for this minimum value of \( f(x) \). (Stockholm Univ., Sweden, BIT 4 (1964), 197)

**Solution**

The interpolation polynomial through the points \( (x_{n-1}, f_{n-1}), (x_n, f_n) \) and \( (x_{n+1}, f_{n+1}) \) is given as

\[
f(x) = f(x_{n-1}) + \frac{1}{h} (x - x_{n-1}) \Delta f_{n-1} + \frac{1}{2h^2} (x - x_{n-1}) (x - x_n) \Delta^2 f_{n-1}
\]

Since \( f(x) \) has a minimum, set \( f'(x) = 0 \).

Therefore

\[
f'(x) = \frac{1}{h} \Delta f_{n-1} + \frac{1}{2h^2} (2x - x_{n-1} - x_n) \Delta^2 f_{n-1} = 0
\]

which gives

\[
x_{\text{min}} = \frac{1}{2} (x_n + x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}}.
\]

Hence, the minimum value of \( f(x) \) is

\[
f(x_{\text{min}}) = f_{n-1} + \frac{1}{h} \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right] \Delta f_{n-1}
\]

\[
+ \frac{1}{2h^2} \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right] \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right] \Delta^2 f_{n-1}
\]

Since \( x_n - x_{n-1} = h \), we obtain

\[
f_{\text{min}} = f_{n-1} + \frac{1}{2} \Delta f_{n-1} - \frac{(\Delta f_{n-1})^2}{2 \Delta^2 f_{n-1}} - \frac{1}{8} \Delta^2 f_{n-1}
\]

\[
= f_n - \Delta f_{n-1} + \frac{1}{8 \Delta^2 f_{n-1}} [4 \Delta^2 f_{n-1} \Delta^2 f_{n-1} - 4(\Delta^2 f_{n-1})^2 - (\Delta^2 f_{n-1})^2]
\]

\[
= f_n - \frac{1}{8 \Delta^2 f_{n-1}} [(4 \Delta^2 f_{n-1} + \Delta^2 f_{n-1}) \Delta^2 f_{n-1} + 4(\Delta^2 f_{n-1})^2]
\]

Using

\[
\Delta f_{n-1} = f_n - f_{n-1}, \quad \Delta^2 f_{n-1} = f_{n+1} - 2f_n + f_{n-1},
\]

and simplifying, we obtain

\[
f_{\text{min}} = f_n - \frac{f^2_{n+1} - 2f_n + f_{n-1}}{8(f_{n+1} - 2f_n + f_{n-1})} = f_n - \frac{1}{8} \left( \frac{(f_{n+1} - f_{n-1})^2}{f_{n+1} - 2f_n + f_{n-1}} \right).
\]

4.4 Define

\[
S(h) = \frac{-y(x + 2h) + 4y(x + h) - 3y(x)}{2h}
\]

(a) Show that

\[
y'(x) - S(h) = c_1 h^2 + c_2 h^3 + c_3 h^4 + ...
\]

and state \( c_1 \).
Numerical Methods : Problems and Solutions

(b) Calculate \( y'(0.398) \) as accurately as possible using the table below and with the aid of the approximation \( S(h) \). Give the error estimate (the values in the table are correctly rounded).

\[
\begin{array}{cccccc}
  x & 0.398 & 0.399 & 0.400 & 0.401 & 0.402 \\
  f(x) & 0.408591 & 0.409671 & 0.410752 & 0.411834 & 0.412915 \\
\end{array}
\]


Solution

(a) Expanding each term in the formula

\[
S(h) = \frac{1}{2h} \left[ -y(x + 2h) + 4y(x + h) - 3y(x) \right]
\]

in Taylor series about the point \( x \), we get

\[
S(h) = y'(x) - \frac{h^2}{3} y''(x) - \frac{h^3}{4} y'''(x) - \frac{7h^4}{60} y''(x) - ...
\]

Thus we obtain

\[
y'(x) - S(h) = c_1 h^2 + c_2 h^3 + c_3 h^4 + ...
\]

where \( c_1 = y''(x) / 3 \).

(b) Using the given formula with \( x_0 = 0.398 \) and \( h = 0.001 \), we obtain

\[
y'(0.398) = \frac{1}{2(0.001)} \left[ -y(0.400) + 4y(0.399) - 3y(0.398) \right]
\]

\[
= 1.0795.
\]

The error in the approximation is given by

\[
\text{Error} = c_1 h^2 = \frac{h^2}{3} y''(x_0) = \frac{h^2}{3} \left( \frac{1}{h^3} \Delta^3 y_0 \right)
\]

\[
= \frac{1}{3h} (y_3 - 3y_2 + 3y_1 - y_0)
\]

\[
= \frac{1}{3h} [y(0.401) - 3y(0.400) + 3y(0.399) - y(0.398)] = 0.
\]

Hence, the error of approximation is given by the next term, which is

\[
\text{Error} = c_2 h^3 = \frac{1}{4} h^3 y'''(x_0) = \frac{1}{4} \left( \frac{1}{h^4} \Delta^4 f_0 \right)
\]

\[
= \frac{1}{4h} (y_4 - 4y_3 + 6y_2 - 4y_1 + y_0)
\]

\[
= \frac{1}{4h} [y(0.402) - 4y(0.401) + 6y(0.400) - 4y(0.399) + y(0.398)]
\]

\[
= -0.0005.
\]

4.5 Determine \( \alpha, \beta, \gamma \) and \( \delta \) such that the relation

\[
y'(\frac{a+b}{2}) = \alpha y(a) + \beta y(b) + \gamma y''(a) + \delta y'''(b)
\]

is exact for polynomials of as high degree as possible. Give an asymptotically valid expression for the truncation error as \( |b - a| \to 0 \).
Solution

We write the error term in the form

\[ TE = y' \left( \frac{a + b}{2} \right) - \alpha y(a) - \beta y(b) - \gamma y''(a) - \delta y''(b). \]

Letting \((a + b) / 2 = s, (b - a) / 2 = h / 2 = t\), in the formula, we get

\[ TE = y'(s) - \alpha y(s - t) - \beta y(s + t) - \gamma y''(s - t) - \delta y''(s + t). \]

Expanding each term on the right hand side in Taylor series about \(s\), we obtain

\[ TE = y'(s) - \alpha y(s - t) - \beta y(s + t) - \gamma y''(s - t) - \delta y''(s + t). \]

We choose \(\alpha, \beta, \gamma\) and \(\delta\) such that

\[ \alpha + \beta = 0, \]
\[ -\alpha + \beta = 1 / t = 2 / h, \]
\[ \frac{h^2}{8} (\alpha + \beta) + \frac{h^3}{48} (\delta + \gamma) = 0, \]
\[ \frac{h^3}{48} (-\alpha + \beta) + \frac{h}{2} (\delta - \gamma) = 0. \]

The solution of this system is

\[ \alpha = -1 / h, \beta = 1 / h, \gamma = h / 24 \text{ and } \delta = -h / 24. \]

Since,

\[ \frac{t^4}{24} (\beta + \alpha) + \frac{t^2}{2} (\delta + \gamma) = \left[ \frac{h^4}{384} (\alpha + \beta) + \frac{h^2}{8} (\delta + \gamma) \right] = 0, \]

we obtain the error term as

\[ TE = - \left[ \frac{h^5}{3840} (\beta - \alpha) + \frac{h^3}{48} (\delta - \gamma) \right] y''(\xi), \]
\[ = -h^4 \left( \frac{1}{1920} - \frac{1}{576} \right) y''(\xi) = \frac{7}{5760} h^4 y''(\xi), a < \xi < b. \]

4.6 Find the coefficients \(a_\delta\)'s in the expansion

\[ D = \sum_{\delta=1}^{\infty} a_\delta \mu \delta^s \]

\((h = 1, D = \text{differentiation operator}, \mu = \text{mean value operator} \text{ and } \delta = \text{central difference operator}) \quad (\text{Arhus Univ., Denmark, BIT 7 (1967), 81})
Solution

Since \( \mu = [1 + \frac{1}{4} \delta^2]^{1/2} \), we get

\[
hD = 2 \sinh^{-1} \left( \frac{\delta}{2} \right) = \frac{2\mu}{\mu} \sinh^{-1} \left( \frac{\delta}{2} \right) = \frac{2\mu}{[1 + (\delta^2/4)]^{1/2}} \sinh^{-1} \left( \frac{\delta}{2} \right)
\]

\[
= 2\mu \left[ 1 + \frac{\delta^2}{4} \right]^{1/2} \sinh^{-1} \left( \frac{\delta}{2} \right)
\]

\[
= \mu \left[ 1 - \frac{1}{2} \frac{\delta^2}{4} + \frac{3}{8} \left( \frac{\delta^2}{4} \right)^2 - \ldots \right] \left[ \delta - \frac{1^2}{2^2(3!)} \delta^3 + \ldots \right]
\]

\[
= \mu \left[ \delta - \frac{1^2}{3!} \delta^3 + \frac{(2!)^2}{5!} \delta^5 - \ldots \right]
\]

(4.97)

The given expression is

\[
D = a_1 \mu \delta + a_2 \mu \delta^2 + a_3 \mu \delta^3 + \ldots \quad \text{(4.98)}
\]

Taking \( h = 1 \) and comparing the right hand sides in (4.97) and (4.98), we get

\[
a_{2n} = 0, \quad a_{2n+1} = \frac{(-1)^n (n!)^2}{(2n + 1)!}.
\]

4.7 (a) Determine the exponents \( k_i \) in the difference formula

\[
f''(x_0) = \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} + \sum_{i=1}^{\infty} a_i h^{k_i}
\]

assuming that \( f(x) \) has convergent Taylor expansion in a sufficiently large interval around \( x_0 \).

(b) Compute \( f''(0.6) \) from the following table using the formula in (a) with \( h = 0.4, 0.2 \) and 0.1 and perform repeated Richardson extrapolation.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>1.420072</td>
</tr>
<tr>
<td>0.4</td>
<td>1.881243</td>
</tr>
<tr>
<td>0.5</td>
<td>2.128147</td>
</tr>
<tr>
<td>0.6</td>
<td>2.386761</td>
</tr>
<tr>
<td>0.7</td>
<td>2.657971</td>
</tr>
<tr>
<td>0.8</td>
<td>2.942897</td>
</tr>
<tr>
<td>1.0</td>
<td>3.559753</td>
</tr>
</tbody>
</table>

(Lund Univ., Sweden, BIT 13 (1973), 123)

Solution

(a) Expanding each term in Taylor series about \( x_0 \) in the given formula, we obtain

\[ k_i = 2i, \quad i = 1, 2, \ldots \]

(b) Using the given formula, we get

\[
h = 0.4: \quad f''(0.6) = \frac{f(1.0) - 2f(0.6) + f(0.2)}{(0.4)^2} = 1.289394.
\]
Differentiation and Integration

\[ h = 0.2 : \quad f''(0.6) = \frac{f(0.8) - 2f(0.6) + f(0.4)}{(0.2)^2} = 1.265450. \]

\[ h = 0.1 : \quad f''(0.6) = \frac{f(0.7) - 2f(0.6) + f(0.5)}{(0.1)^2} = 1.259600. \]

Applying the Richardson extrapolation

\[ f_{i,h}'' = \frac{4^i f_{i-1,h}'' - f_{i-1,2h}''}{4^i - 1}, \]

where \( i \) denotes the \( i \)th iterate, we obtain the following extrapolation table.

**Extrapolation Table**

<table>
<thead>
<tr>
<th>( h )</th>
<th>( O(h^2) )</th>
<th>( O(h^4) )</th>
<th>( O(h^6) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>1.289394</td>
<td>1.257469</td>
<td>1.257662</td>
</tr>
<tr>
<td>0.2</td>
<td>1.265450</td>
<td>1.257650</td>
<td>1.257662</td>
</tr>
<tr>
<td>0.1</td>
<td>1.259600</td>
<td>1.257650</td>
<td>1.257662</td>
</tr>
</tbody>
</table>

4.8 (a) Prove that one can use repeated Richardson extrapolation for the formula

\[ f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \]

What are the coefficients in the extrapolation scheme?

(b) Apply this to the table given below, and estimate the error in the computed \( f''(0.3) \).

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>17.60519</td>
</tr>
<tr>
<td>0.2</td>
<td>17.68164</td>
</tr>
<tr>
<td>0.3</td>
<td>17.75128</td>
</tr>
<tr>
<td>0.4</td>
<td>17.81342</td>
</tr>
<tr>
<td>0.5</td>
<td>17.86742</td>
</tr>
</tbody>
</table>

(Stockholm Univ., Sweden, BIT 9(1969), 400)

 Solution

(a) Expanding each term in the given formula in Taylor series, we get

\[ \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + c_1 h^2 + c_2 h^4 + ... \]

If we assume that the step lengths form a geometric sequence with common ratio \( 1/2 \), we obtain the extrapolation scheme

\[ f_{i,h}'' = \frac{4^i f_{i-1,h}'' - f_{i-1,2h}''}{4^i - 1}, \quad i = 1, 2, ... \]

where \( i \) denotes the \( i \)th iterate.
(b) Using the given formula, we obtain for \( x = 0.3 \)

\[
\begin{align*}
  h = 0.2 : \quad f''(0.3) &= \frac{f(0.5) - 2f(0.3) + f(0.1)}{(0.2)^2} = -0.74875. \quad (4.99) \\
  h = 0.1 : \quad f''(0.3) &= \frac{f(0.4) - 2f(0.3) + f(0.2)}{(0.1)^2} = -0.75. \quad (4.100)
\end{align*}
\]

Using extrapolation, we obtain

\[
  f''(0.3) = -0.750417. \quad (4.101)
\]

If the roundoff error in the entries in the given table is \( \leq 5 \times 10^{-6} \), then we have

- Roundoff error in (4.99) is \( \leq \frac{4 \times 5 \times 10^{-6}}{(0.2)^2} = 0.0005 \),
- Roundoff error in (4.100) is \( \leq \frac{4 \times 5 \times 10^{-6}}{(0.1)^2} = 0.002 \),
- Roundoff error in (4.101) is \( \leq \frac{4(0.002) + 0.0005}{3} = 0.0028 \),

and the truncation error in the original formula is

\[
  \text{TE} = \frac{h^2}{12} f^{iv}(0.3) = \frac{1}{12h^2} 8^4 f(0.3)
\]

\[
  = \frac{1}{12h^2} [f(0.5) - 4f(0.4) + 6f(0.3) - 4f(0.2) + f(0.1)] = 0.000417.
\]

4.9 By use of repeated Richardson extrapolation find \( f'(1) \) from the following values:

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>0.707178</td>
</tr>
<tr>
<td>0.8</td>
<td>0.859892</td>
</tr>
<tr>
<td>0.9</td>
<td>0.925863</td>
</tr>
<tr>
<td>1.0</td>
<td>0.984007</td>
</tr>
<tr>
<td>1.1</td>
<td>1.033743</td>
</tr>
<tr>
<td>1.2</td>
<td>1.074575</td>
</tr>
<tr>
<td>1.4</td>
<td>1.127986</td>
</tr>
</tbody>
</table>

Apply the approximate formula

\[
  f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h}
\]

with \( h = 0.4, 0.2, 0.1 \).

(Royal Inst. Tech., Stockholm, Sweden, BIT 6 (1966), 270)

**Solution**

Applying the Richardson’s extrapolation formula

\[
  f_{i+1, h} = \frac{4^i f_{i-1, h} - f_{i-1, 2h}}{4^i - 1}, \quad i = 1, 2, ...
\]

where \( i \) denotes the \( i \)th iterate, we obtain
Differentiation and Integration

The formula
\[ D_h = (2h)^{-1} (3f(a) - 4f(a-h) + f(a-2h)) \]
is suitable to approximation of \( f'(a) \) where \( x \) is the last \( x \)-value in the table.

(a) State the truncation error \( D_h - f'(a) \) as a power series in \( h \).

(b) Calculate \( f'(2.0) \) as accurately as possible from the table.

### Solution

(a) Expanding each term in Taylor series about \( a \) in the given formula, we obtain
\[ D_h - f'(a) = -\frac{h^2}{3} f'''(a) + \frac{h^3}{4} f^{(4)}(a) - \frac{7h^4}{60} f^{(5)}(a) + \ldots \]
Hence, the error in \( D_h - f'(a) \) of the form \( c_1 h^2 + c_2 h^3 + \ldots \)

(b) The extrapolation scheme for the given method can be obtained as
\[ f'_{i,h} = \frac{2^{i} f'_{i-1,h} - f'_{i-2,h}}{2^{i} - 1}, \quad i = 1, 2, \ldots \]
where \( i \) denotes the \( i \)th iterate. Using the values given in the table, we obtain
\[ h = 0.4 : \quad f'(2.0) = \frac{1}{2(0.4)} [3f(2.0) - 4f(1.6) + f(1.2)] = 0.436618. \]
\[ h = 0.2 : \quad f'(2.0) = \frac{1}{2(0.2)} [3f(2.0) - 4f(1.8) + f(1.6)] = 0.453145. \]
\[ h = 0.1 : \quad f'(2.0) = \frac{1}{2(0.1)} [3f(2.0) - 4f(1.9) + f(1.8)] = 0.457735. \]
\[ h = 0.05 : \quad f'(2.0) = \frac{1}{2(0.05)} [3f(2.0) - 4f(1.95) + f(1.9)] = 0.458970. \]
Using the extrapolation scheme, we obtain the following extrapolation table.

<table>
<thead>
<tr>
<th>Extrapolation Table</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h )</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>0.4</td>
</tr>
<tr>
<td>0.2</td>
</tr>
<tr>
<td>0.1</td>
</tr>
<tr>
<td>0.05</td>
</tr>
</tbody>
</table>

Hence, \( f'(2.0) = 0.4594 \) with the error \( 2.0 \times 10^{-6} \).
4.11 For the method

\[ f'(x_0) = \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h} + \frac{h^2}{3} f''(\xi), \quad x_0 < \xi < x_2 \]

determine the optimal value of \( h \), using the criteria

(i) \( |\text{RE}| = |\text{TE}| \),

(ii) \( |\text{RE}| + |\text{TE}| = \text{minimum} \).

Using this method and the value of \( h \) obtained from the criterion \( |\text{RE}| = |\text{TE}| \), determine an approximate value of \( f'(2.0) \) from the following tabulated values of \( f(x) = \log_{e} x \)

<table>
<thead>
<tr>
<th>( x )</th>
<th>2.0</th>
<th>2.01</th>
<th>2.02</th>
<th>2.06</th>
<th>2.12</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f(x) )</td>
<td>0.69315</td>
<td>0.69813</td>
<td>0.70310</td>
<td>0.72271</td>
<td>0.75142</td>
</tr>
</tbody>
</table>

given that the maximum roundoff error in the function evaluations is \( 5 \times 10^{-6} \).

**Solution**

If \( \varepsilon_0, \varepsilon_1 \) and \( \varepsilon_2 \) are the roundoff errors in the given function evaluations \( f_0, f_1 \) and \( f_2 \) respectively, then we have

\[ f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} + \frac{h^2}{3} f''(\xi) \]

Using \( \varepsilon = \max (|\varepsilon_0|, |\varepsilon_1|, |\varepsilon_2|) \),

and

\[ M_3 = \max_{x_0 \leq x \leq x_2} |f'''(x)|, \]

we obtain

\[ |\text{RE}| \leq \frac{8\varepsilon}{2h}, \quad |\text{TE}| \leq \frac{h^2M_3}{3}. \]

If we use \( |\text{RE}| = |\text{TE}| \), we get

\[ \frac{8\varepsilon}{2h} = \frac{h^2M_3}{3} \]

which gives

\[ h^3 = \frac{12\varepsilon}{M_3}, \quad \text{or} \quad h_{\text{opt}} = \left( \frac{12\varepsilon}{M_3} \right)^{1/3} \]

and

\[ |\text{RE}| = |\text{TE}| = \frac{4\varepsilon^{2/3}M_3^{1/3}}{(12)^{1/3}}. \]

If we use \( |\text{RE}| + |\text{TE}| = \text{minimum} \), we get

\[ \frac{4\varepsilon}{h} + \frac{M_3h^2}{3} = \text{minimum} \]

which gives

\[ \frac{-4\varepsilon}{h^2} + \frac{2M_3}{3} = 0, \quad \text{or} \quad h_{\text{opt}} = \left( \frac{6\varepsilon}{M_3} \right)^{1/3}. \]

Minimum total error = \( 6^{2/3} \varepsilon^{2/3} M_3^{1/3} \).
When, \( f(x) = \log_e(x) \), we have

\[
M_3 = \max_{2.0 \leq x \leq 2.1} |f'''(x)| = \max_{2.0 \leq x \leq 2.1} \left| \frac{2}{x^3} \right| = \frac{1}{4}.
\]

Using the criterion, \(|RE| = |TE|\) and \(\varepsilon = 5 \times 10^{-6}\), we get

\[
h_{\text{opt}} = (4 \times 12 \times 5 \times 10^{-6})^{1/3} \approx 0.06.
\]

For \(h = 0.06\), we get

\[
f'(2.0) = -3(0.69315) + 4(0.72271) - 0.75142 \approx 0.49975.
\]

If we take \(h = 0.01\), we get

\[
f'(2.0) = -3(0.69315) + 4(0.69813) - 0.70310 = 0.49850.
\]

The exact value of \(f'(2.0) = 0.5\).

This verifies that for \(h < h_{\text{opt}}\), the results deteriorate.

**Newton-Cotes Methods**

4.12 (a) Compute by using Taylor development

\[
\int_{0.1}^{0.2} \frac{x^2}{\cos x} dx
\]

with an error \(< 10^{-6}\).

(b) If we use the trapezoidal formula instead, which step length (of the form \(10^{-k}\), \(2 \times 10^{-k}\) or \(5 \times 10^{-k}\)) would be largest giving the accuracy above? How many decimals would be required in function values?


**Solution**

(a) \[
\int_{0.1}^{0.2} \frac{x^2}{\cos x} dx = \int_{0.1}^{0.2} x^2 \left(1 - \frac{x^2}{2} + \frac{x^4}{24} - ...\right)^{-1} dx
\]

\[
= \int_{0.1}^{0.2} x^2 \left(1 + \frac{x^2}{2} + \frac{5x^4}{24} + ...\right) dx = \left[ \frac{x^3}{3} + \frac{x^5}{10} + \frac{5x^7}{168} + ...ight]_{0.1}^{0.2}
\]

\[
= 0.00233333 + 0.000031 + 0.000000378 + ... = 0.002365.
\]

(b) The error term in the composite trapezoidal rule is given by

\[
|TE| \leq \frac{h^2}{12} (b - a) \max_{0.1 \leq x \leq 0.2} |f''(x)|
\]

\[
= \frac{h^2}{120} \max_{0.1 \leq x \leq 0.2} |f''(x)|.
\]

We have

\[
f(x) = x^2 \sec x,
\]

\[
f'(x) = 2x \sec x + x^2 \sec x \tan x,
\]

\[
f''(x) = 2 \sec x + 4x \sec x \tan x + x^2 \sec x (\tan^2 x + \sec^2 x).
\]

Since \(f''(x)\) is an increasing function, we get

\[
\max_{0.1 \leq x \leq 0.2} |f''(x)| = f''(0.2) = 2.2503.
\]
We choose $h$ such that
\[
\frac{h^2}{120} = (2.2503) \leq 10^{-6}, \text{ or } h < 0.0073.
\]
Therefore, choose $h = 5 \times 10^{-3} = 0.005$.

If the maximum roundoff error in computing $f_i$, $i = 0, 1, ..., n$ is $\epsilon$, then the roundoff error in the trapezoidal rule is bounded by
\[
| RE | \leq \frac{h}{2} \left[ 1 + \sum_{i=1}^{n-1} 2 + 1 \right] \epsilon = nh\epsilon = (b - a)\epsilon = 0.1\epsilon.
\]

To meet the given error criterion, 5 decimal accuracy will be required in the function values.

4.13 Compute
\[
I_p = \int_0^1 \frac{x^p dx}{x^3 + 10}
\]
for $p = 0, 1$ using trapezoidal and Simpson’s rules with the number of points 3, 5 and 9. Improve the results using Romberg integration.

Solution
For 3, 5 and 9 points, we have $h = 1/2, 1/4$ and $1/8$ respectively. Using the trapezoidal and Simpson’s rules and Romberg integration we get the following

<table>
<thead>
<tr>
<th>$h$</th>
<th>$O(h^2)$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>0.09710999</td>
<td>0.09763534</td>
<td>0.09763357</td>
</tr>
<tr>
<td>1/4</td>
<td>0.09750400</td>
<td>0.09763368</td>
<td></td>
</tr>
<tr>
<td>1/8</td>
<td>0.09760126</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$h$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
<th>$O(h^8)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>0.09766180</td>
<td>0.09763537</td>
<td></td>
</tr>
<tr>
<td>1/4</td>
<td>0.09763533</td>
<td>0.0976357</td>
<td></td>
</tr>
<tr>
<td>1/8</td>
<td>0.09763368</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$p = 0$:

<table>
<thead>
<tr>
<th>$h$</th>
<th>$O(h^2)$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>0.04741863</td>
<td>0.04811455</td>
<td></td>
</tr>
<tr>
<td>1/4</td>
<td>0.04794057</td>
<td>0.04811645</td>
<td></td>
</tr>
<tr>
<td>1/8</td>
<td>0.04807248</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$p = 1$:

<table>
<thead>
<tr>
<th>$h$</th>
<th>$O(h^2)$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>0.04741863</td>
<td>0.04811455</td>
<td></td>
</tr>
<tr>
<td>1/4</td>
<td>0.04794057</td>
<td>0.04811645</td>
<td></td>
</tr>
<tr>
<td>1/8</td>
<td>0.04807248</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ p = 0, 1 \]
Differentiation and Integration

4.14 The arc length \( L \) of an ellipse with half axes \( a \) and \( b \) is given by the formula \( L = 4aE(m) \) where \( m = (a^2 - b^2) / a^2 \) and

\[
E(m) = \int_{0}^{\pi/2} (1 - m \sin^2 \phi)^{1/2} \, d\phi.
\]

The function \( E(m) \) is an elliptic integral, some values of which are displayed in the table:

<table>
<thead>
<tr>
<th>( m )</th>
<th>0</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E(m) )</td>
<td>1.57080</td>
<td>1.53076</td>
<td>1.48904</td>
<td>1.44536</td>
<td>1.39939</td>
<td>1.35064</td>
</tr>
</tbody>
</table>

We want to calculate \( L \) when \( a = 5 \) and \( b = 4 \).

(a) Calculate \( L \) using quadratic interpolation in the table.

(b) Calculate \( L \) applying Romberg’s method to \( E(m) \), so that a Romberg value is got with an error less than \( 5 \times 10^{-5} \). (Trondheim Univ., Sweden, BIT 24(1984), 258)

Solution

(a) For \( a = 5 \) and \( b = 4 \), we have \( m = 9 / 25 = 0.36 \).

Taking the points as \( x_0 = 0.3, x_1 = 0.4, x_2 = 0.5 \) we have the following difference table.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
<th>( \Delta f )</th>
<th>( \Delta^2 f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>1.44536</td>
<td>– 0.04597</td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>1.39939</td>
<td>– 0.04875</td>
<td>– 0.00278</td>
</tr>
<tr>
<td>0.5</td>
<td>1.35064</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The Newton forward difference interpolation gives

\[
P_2(x) = 1.44536 + (x - 0.3) \left( - \frac{0.04597}{0.1} \right) + (x - 0.3)(x - 0.4) \left( - \frac{0.00278}{2(0.01)} \right).
\]

We obtain \( E(0.36) = P_2(0.36) = 1.418112 \).

Hence,

\[
L = 4aE(m) = 20E(0.36) = 28.36224.
\]

(b) Using the trapezoidal rule to evaluate

\[
E(m) = \int_{0}^{\pi/2} (1 - m \sin^2 \phi)^{1/2} \, d\phi, \ m = 0.36
\]

and applying Romberg integration, we get
Hence, using the trapezoidal rule with $h = \pi / 4$, $h = \pi / 8$ and with one extrapolation, we obtain $E(m)$ correct to four decimal places as

$$E(m) = 1.4181, m = 0.36.$$ 

Hence,

$$L = 28.362.$$ 

4.15 Calculate $\int_0^{1/2} \frac{x}{\sin x} \, dx$.

(a) Use Romberg integration with step size $h = 1 / 16$.
(b) Use 4 terms of the Taylor expansion of the integrand.

(Uppsala Univ., Sweden, BIT 26(1986), 135)

**Solution**

(a) Using trapezoidal rule we have with

$$h = \frac{1}{2} : \quad I = \frac{h}{2} [f(a) + f(b)] = \frac{1}{4} \left[1 + \frac{1/2}{\sin 1/2}\right] = 0.510729$$

where we have used the fact that $\lim_{x \to 0} (x / \sin x) = 1$.

$$h = \frac{1}{4} : \quad I = \frac{1}{8} \left[1 + 2 \left(\frac{1/4}{\sin 1/4}\right) + \left(\frac{1/2}{\sin 1/2}\right)\right] = 0.507988.$$ 

$$h = \frac{1}{8} : \quad I = \frac{1}{16} \left[1 + 2 \left(\frac{1/8}{\sin 1/8} + \frac{2/8}{\sin 2/8} + \frac{3/8}{\sin 3/8}\right) + \left(\frac{1/2}{\sin 1/2}\right)\right] = 0.507298.$$ 

$$h = \frac{1}{16} : \quad I = \frac{1}{32} \left[1 + 2 \left(\frac{1/16}{\sin 1/16} + \frac{2/16}{\sin 2/16} + \frac{3/16}{\sin 3/16} + \frac{4/16}{\sin 4/16}\right.ight.$$ 

$$+ \frac{5/16}{\sin 5/16} + \frac{6/16}{\sin 6/16} + \frac{7/16}{\sin 7/16} + \frac{1/2}{\sin 1/2}\left)\right]$$

$$= 0.507126.$$ 

Using extrapolation, we obtain the following Romberg table:

**Romberg Table**

<table>
<thead>
<tr>
<th>$h$</th>
<th>$O(h^2)$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
<th>$O(h^8)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/2$</td>
<td>0.510729</td>
<td>0.507074</td>
<td>0.507068</td>
<td>0.507069</td>
</tr>
<tr>
<td>$1/4$</td>
<td>0.507988</td>
<td>0.507068</td>
<td>0.507068</td>
<td>0.507069</td>
</tr>
<tr>
<td>$1/8$</td>
<td>0.507298</td>
<td>0.507069</td>
<td>0.507069</td>
<td>0.507069</td>
</tr>
<tr>
<td>$1/16$</td>
<td>0.507126</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
(b) We write

\[ I = \int_0^{\frac{1}{2}} x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040} + \ldots \, dx \]

\[ = \int_0^{\frac{1}{2}} \left[ 1 - \left( \frac{x^2}{6} - \frac{x^4}{120} + \frac{x^6}{5040} - \ldots \right) \right]^{-1} \, dx \]

\[ = \int_0^{\frac{1}{2}} \left[ \frac{1 + \frac{x^2}{6} + \frac{7}{360} x^4 + \frac{31}{15120} x^6 + \ldots}{360} \right] \, dx \]

\[ = \left[ x + \frac{x^3}{18} + \frac{7x^5}{1800} + \frac{31x^7}{105840} + \ldots \right]_0^{\frac{1}{2}} = 0.507068. \]

4.16 Compute the integral \( \int_0^1 y \, dx \) where \( y \) is defined through \( x = ye^y \), with an error < \( 10^{-4} \).

(Uppsala Univ., Sweden, BIT 7(1967), 170)

**Solution**

We shall use the trapezoidal rule with Romberg integration to evaluate the integral. The solution of \( ye^y - x = 0 \) for various values of \( x \), using Newton-Raphson method is given in the following table.

<table>
<thead>
<tr>
<th>( x )</th>
<th>( y )</th>
<th>( x )</th>
<th>( y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.500</td>
<td>0.351734</td>
</tr>
<tr>
<td>0.125</td>
<td>0.111780</td>
<td>0.625</td>
<td>0.413381</td>
</tr>
<tr>
<td>0.250</td>
<td>0.203888</td>
<td>0.750</td>
<td>0.469150</td>
</tr>
<tr>
<td>0.375</td>
<td>0.282665</td>
<td>0.875</td>
<td>0.520135</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.000</td>
<td>0.567143</td>
</tr>
</tbody>
</table>

Romberg integration gives

<table>
<thead>
<tr>
<th>( h )</th>
<th>( O(h^2) )</th>
<th>( O(h^4) )</th>
<th>( O(h^6) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>method</td>
<td>method</td>
<td>method</td>
</tr>
<tr>
<td>0.5</td>
<td>0.317653</td>
<td>0.330230</td>
<td>0.330363</td>
</tr>
<tr>
<td>0.25</td>
<td>0.327086</td>
<td>0.330355</td>
<td></td>
</tr>
<tr>
<td>0.125</td>
<td>0.329538</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The error of integration is \( 0.330363 - 0.330355 = 0.000008 \).
The result correct to five decimals is 0.33036.

4.17 The area \( A \) inside the closed curve \( y^2 + x^2 = \cos x \) is given by

\[ A = 4 \int_0^\alpha (\cos x - x^2)^{1/2} \, dx \]

where \( \alpha \) is the positive root of the equation \( \cos x = x^2 \).
(a) Compute \( \alpha \) to three correct decimals.

(b) Use Romberg's method to compute the area \( A \) with an absolute error less than 0.05.

( Linköping Univ., Sweden, BIT 28(1988), 904)

**Solution**

(a) Using Newton-Raphson method to find the root of equation

\[ f(x) = \cos x - x^2 = 0 \]

we obtain the iteration scheme

\[ x_{k+1} = x_k + \frac{\cos x_k - x_k^2}{\sin x_k + 2x_k}, \quad k = 0, 1, ... \]

Starting with \( x_0 = 0.5 \), we get

\[ x_1 = 0.5 + \frac{0.627583}{1.479426} = 0.924207. \]
\[ x_2 = 0.924207 + \frac{-0.251691}{2.646557} = 0.829106. \]
\[ x_3 = 0.829106 + \frac{-0.011882}{2.395540} = 0.824146. \]
\[ x_4 = 0.824146 + \frac{-0.000033}{2.382260} = 0.824132. \]

Hence, the value of \( \alpha \) correct to three decimals is 0.824.

The given integral becomes

\[ A = 4 \int_0^{0.824} (\cos x - x^2)^{1/2} \, dx. \]

(b) Using the trapezoidal rule with \( h = 0.824, 0.412 \) and 0.206 respectively, we obtain the approximation

\[ A = \frac{4(0.824)}{2} \left[ 1 + 0.017753 \right] = 1.677257 \]
\[ A = \frac{4(0.412)}{2} \left[ 1 + 2(0.864047) + 0.017753 \right] = 2.262578. \]
\[ A = \frac{4(0.206)}{2} \left[ 1 + 2(0.967688 + 0.864047 + 0.658115) + 0.017753 \right] = 2.470951. \]

Using Romberg integration, we obtain

<table>
<thead>
<tr>
<th>( h )</th>
<th>( O(h^2) )</th>
<th>( O(h^4) )</th>
<th>( O(h^6) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.824</td>
<td>1.677257</td>
<td>2.457685</td>
<td>2.545924</td>
</tr>
<tr>
<td>0.412</td>
<td>2.262578</td>
<td>2.540409</td>
<td></td>
</tr>
<tr>
<td>0.206</td>
<td>2.470951</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Hence, the area with an error less than 0.05 is 2.55.
Differentiation and Integration

4.18 (a) The natural logarithm function of a positive \( x \) is defined by

\[
\ln x = - \int_x^1 \frac{dt}{t}.
\]

We want to calculate \( \ln (0.75) \) by estimating the integral by the trapezoidal rule \( T(h) \).

Give the maximal step size \( h \) to get the truncation error bound \( 0.5(10^{-3}) \). Calculate \( T(h) \) with \( h = 0.125 \) and \( h = 0.0625 \). Extrapolate to get a better value.

(b) Let \( f_n(x) \) be the Taylor series of \( \ln x \) at \( x = 3/4 \), truncated to \( n + 1 \) terms. Which is the smallest \( n \) satisfying

\[
| f_n(x) - \ln x | \leq 0.5(10^{-3}) \quad \text{for all } x \in [0.5, 1].
\]

(Trondheim Univ., Sweden, BIT 24(1984), 130)

Solution

(a) The error in the composite trapezoidal rule is given as

\[
| R | \leq \frac{(b-a)h^2}{12} \max_{0.75 \leq x \leq 1} | f''(x) | = \frac{h^2}{48} f''(\xi),
\]

where \( f''(\xi) = \max_{0.75 \leq x \leq 1} | f''(x) | \).

Since \( f(t) = -\frac{1}{t} \), we have \( f'(t) = \frac{1}{t^2}, f''(t) = -\frac{2}{t^3} \)

and therefore \( \max_{0.75 \leq x \leq 1} | f''(t) | = \max_{0.75 \leq x \leq 1} \left| \frac{2}{t^3} \right| = 4.740741. \)

Hence, we find \( h \) such that

\[
\frac{h^2}{48} (4.740741) < 0.0005
\]

which gives \( h < 0.0712 \). Using the trapezoidal rule, we obtain

\[
h = 0.125 : t_0 = 0.75, t_1 = 0.875, t_2 = 1.0,
\]

\[
I = -0.125 \left[ \frac{1}{t_0} + \frac{2}{t_1} + \frac{1}{t_2} \right] = -0.288690.
\]

\[
h = 0.0625 : t_0 = 0.75, t_1 = 0.8125, t_2 = 0.875, t_3 = 0.9375, t_4 = 1.0,
\]

\[
I = -0.0625 \left[ \frac{1}{t_0} + 2\left( \frac{1}{t_1} + \frac{1}{t_2} + \frac{1}{t_3} \right) + \frac{1}{t_4} \right] = -0.287935.
\]

Using extrapolation, we obtain the extrapolated value as

\[
I = -0.287683.
\]

(b) Expanding \( \ln x \) in Taylor series about the point \( x = 3/4 \), we get

\[
\ln x = \ln(3/4) + \left( x - \frac{3}{4} \right) \left( \frac{4}{3} \right)
\]

\[
- \left( x - \frac{3}{4} \right)^2 \cdot \frac{1}{2} \left( \frac{4}{3} \right)^2 + \ldots + \left( x - \frac{3}{4} \right)^n \frac{(n-1)!(-1)^{n-1}}{n!} \left( \frac{4}{3} \right)^n + R_n
\]

with the error term

\[
R_n = \frac{(x - 3/4)^{n+1}}{(n+1)!} \frac{n!(-1)^n}{\xi^{n+1}}, \quad 0.5 < \xi < 1.
\]

We have

\[
| R_n | \leq \frac{1}{(n+1)} \max_{0.5 \leq x \leq 1} \left| \left( x - \frac{3}{4} \right)^{n+1} \right| \max_{0.5 \leq x \leq 1} \left| \frac{1}{x^{n+1}} \right| = \frac{1}{(n+1)2^{n+1}}.
\]
We find the smallest $n$ such that
\[
\frac{1}{(n + 1)2^{n+1}} \leq 0.0005
\]
which gives $n = 7$.

**4.19** Determine the coefficients $a$, $b$ and $c$ in the quadrature formula
\[
\int_{x_0}^{x_1} y(x)dx = h(ay_0 + by_1 + cy_2) + R
\]
where $x_i = x_0 + ih$, $y(x_i) = y_i$. Prove that the error term $R$ has the form
\[
R = ky^{(n)}(\xi), \quad x_0 \leq \xi \leq x_2
\]
and determine $k$ and $n$. (Bergen Univ., Sweden, BIT 4(1964), 261)

**Solution**

Making the method exact for $y(x) = 1$, $x$ and $x^2$ we obtain the equations
\[
\begin{align*}
  x_1 - x_0 &= h(a + b + c), \\
  \frac{1}{2}(x_1^2 - x_0^2) &= h(ax_0 + bx_1 + cx_2), \\
  \frac{1}{3}(x_1^3 - x_0^3) &= h(ax_0^2 + bx_1^2 + cx_2^2).
\end{align*}
\]
Simplifying the above equations, we get
\[
\begin{align*}
  a + b + c &= 1, \\
  b + 2c &= 1/2, \\
  b + 4c &= 1/3.
\end{align*}
\]
which give $a = 5/12$, $b = 2/3$ and $c = -1/12$.

The error term $R$ is given by
\[
R = \frac{C}{3!} y^{(n)}(\xi), \quad x_0 < \xi < x_2
\]
where
\[
C = \int_{x_0}^{x_1} x^3 dx - h[a x_0^3 + b x_1^3 + c x_2^3] = \frac{h^4}{4}.
\]

Hence, we have the remainder as
\[
R = \frac{h^4}{24} y^{(n)}(\xi).
\]

Therefore, $k = h^4/24$ and $n = 3$.

**4.20** Obtain a generalized trapezoidal rule of the form
\[
\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) + ph^2(f_0' - f_1').
\]
Find the constant $p$ and the error term. Deduce the composite rule for integrating
\[
\int_{a}^{b} f(x)dx, \quad a = x_0 < x_1 < x_2 \ldots < x_N = b.
\]

**Solution**

The method is exact for $f(x) = 1$ and $x$. Making the method exact for $f(x) = x^2$, we get
\[
\frac{1}{3}(x_1^3 - x_0^3) = \frac{h}{2}(x_0^2 + x_1^2) + 2ph^2(x_0 - x_1).
\]
Since, \( x_1 = x_0 + h \), we obtain on simplification \( p = 1 / 12 \).

The error term is given by

\[
\text{Error} = \frac{C}{3!} f'''(\xi), \quad x_0 < \xi < x_1
\]

where

\[
C = \int_{x_0}^{x_1} x^3 dx - \left[ \frac{h}{2} (x_0^3 + x_1^3) + 3ph^2(x_0^2 - x_1^2) \right] = 0.
\]

Therefore, the error term becomes

\[
\text{Error} = \frac{C}{4!} f^{iv}(\xi), \quad x_0 < \xi < x_1
\]

where

\[
C = \int_{x_0}^{x_1} x^4 dx - \left[ \frac{h}{2} (x_0^4 + x_1^4) + 4ph^2(x_0^3 - x_1^3) \right] = \frac{h^5}{30}.
\]

Hence, we have the remainder as

\[
\text{Error} = \frac{h^5}{720} f^{iv}(\xi).
\]

Writing the given integral as

\[
\int_a^b f(x) dx = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \ldots + \int_{x_{N-1}}^{x_N} f(x) dx
\]

where \( x_0 = a, x_N = b \), \( h = (b - a) / N \), and replacing each integral on the right side by the given formula, we obtain the composite rule

\[
\int_a^b f(x) dx = h \sum_{i=0}^{N-1} \left[ f(x_i) + \alpha h f'(x_i) + \beta h^2 f''(x_i) \right] + O(h^p)
\]

with the integer \( p \) as large as possible. (Uppsala Univ., Sweden, BIT 11(1971), 225)

**Solution**

First we determine the formula

\[
\int_{x_0}^{x_1} f(x) dx = h[af_0 + bf_0' + cf_0''],
\]

Making the method exact for \( f(x) = 1, x \) and \( x^2 \), we get \( a = 1, b = h / 2 \) and \( c = h^2 / 6 \).

Hence, we have the formula

\[
\int_{x_0}^{x_1} f(x) dx = h \left[ f_0 + \frac{h}{2} f_0' + \frac{h^2}{6} f_0'' \right]
\]

which has the error term

\[
\text{TE} = \frac{C}{3!} f'''(\xi)
\]

where

\[
C = \int_{x_0}^{x_1} x^3 dx - h \left[ x_0^3 + \frac{3h}{2} x_0^2 + h^2 x_0 \right] = \frac{h^4}{4}.
\]
Using this formula, we obtain the composite rule as
\[
\int_a^b f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \ldots + \int_{x_{n-1}}^{x_n} f(x)\,dx
\]
\[
= h \sum_{i=0}^{n-1} \left( f_i + \frac{h}{2} f_i' + \frac{h^2}{6} f_i'' \right)
\]

The error term of the composite rule is obtained as
\[
| TE | = \frac{h^4}{24} \left| f'''(\xi_1) + f'''(\xi_2) + \ldots + f'''(\xi_n) \right|
\]
\[
\leq \frac{nh^4}{24} f'''(\xi) = \frac{(b-a)h^3}{24} f'''(\xi),
\]
where \( a < \xi < b \) and \( f'''(\xi) = \max | f'''(x) |, \ a < x < b. \)

### 4.22 Determine \( a, b \) and \( c \) such that the formula
\[
\int_0^h f(x)\,dx = h \left\{ af(0) + bf \left( \frac{h}{3} \right) + cf(h) \right\}
\]
is exact for polynomials of as high degree as possible, and determine the order of the truncation error.

**Solution**

Making the method exact for polynomials of degree up to 2, we obtain

- \( f(x) = 1 \):
  \[
  h = h(a + b + c), \quad \text{or} \quad a + b + c = 1.
  \]

- \( f(x) = x \):
  \[
  \frac{h^2}{2} = h\left( \frac{bh}{3} + ch \right), \quad \text{or} \quad \frac{1}{2} b + c = \frac{1}{2}.
  \]

- \( f(x) = x^2 \):
  \[
  \frac{h^3}{3} = h\left( \frac{bh^2}{9} + ch^2 \right), \quad \text{or} \quad \frac{1}{3} b + c = \frac{1}{3}.
  \]

Solving the above equations, we get \( a = 0, b = 3/4 \) and \( c = 1/4 \).

Hence, the required formula is
\[
\int_0^h f(x)\,dx = \frac{h}{4} [3f(h/3) + f(h)].
\]

The truncation error of the formula is given by
\[
TE = \frac{C}{3!} f'''(\xi), \quad 0 < \xi < h
\]

where
\[
C = \int_0^h x^2 \,dx - h \left[ \frac{bh^3}{27} + ch^3 \right] = -\frac{h^4}{36}.
\]

Hence, we have
\[
TE = -\frac{h^4}{216} f'''(\xi) = O(h^4).
\]
Find the values of $a$, $b$ and $c$ such that the truncation error in the formula

\[ \int_{-h}^{h} f(x) \, dx = h[af(-h) + bf(0) + af(h)] + h^2c \left[ f'(-h) - f'(h) \right] \]

is minimized.

Suppose that the composite formula has been used with the step length $h$ and $h/2$, giving $I(h)$ and $I(h/2)$. State the result of using Richardson extrapolation on these values.

(Lund Univ., Sweden, BIT 27(1987), 286)

**Solution**

Note that the abscissas are symmetrically placed. Making the method exact for $f(x) = 1$, $x^2$ and $x^4$, we obtain the system of equations

\[
\begin{align*}
  f(x) = 1 : & 2a + b = 2, \\
  f(x) = x^2 : & 2a - 4c = 2/3, \\
  f(x) = x^4 : & 2a - 8c = 2/5,
\end{align*}
\]

which gives $a = 7/15$, $b = 16/15$, $c = 1/15$.

The required formula is

\[ \int_{-h}^{h} f(x) \, dx = \frac{h}{15} \left[ 7f(-h) + 16f(0) + 7f(h) \right] + \frac{h^2}{15} \left[ f'(-h) - f'(h) \right]. \]

The error term is obtained as

\[ R = C f^{vi}(\xi), \quad -h < \xi < h \]

where

\[ C = \int_{-h}^{h} x^6 \, dx - \frac{h}{15} \left( 14h^6 - \frac{12h^7}{15} \right) = \frac{16}{105} h^7. \]

Hence, we get the error term as

\[ R = \frac{h^7}{4725} f^{vi}(\xi), \quad -h < \xi < h. \]

The composite integrating rule can be written as

\[ \int_{a}^{b} f(x) \, dx = \frac{h}{15} \left[ 7(f_0 + f_{2n}) + 16(f_1 + f_3 + \ldots + f_{2n-1}) + 14(f_2 + f_4 + \ldots + f_{2n-2}) \right] \\
+ \frac{h^2}{15} (f_0' - f_n') + O(h^6). \]

The truncation error in the composite integration rule is obtained as

\[ R = c_1 h^6 + c_2 h^8 + \ldots \]

If $I(h)$ and $I(h/2)$ are the values obtained by using step sizes $h$ and $h/2$ respectively, then the extrapolated value is given

\[ I = \left[ 64 I(h/2) - I(h) \right] / 63. \]

Consider the quadrature rule

\[ \int_{a}^{b} f(x) \, dx = \sum_{i=0}^{n} w_i f(x_i) \]

where $w_i > 0$ and the rule is exact for $f(x) = 1$. If $f(x_i)$ are in error atmost by $(0.5)10^{-k}$, show that the error in the quadrature rule is not greater than $10^{-k}(b - a)/2$. 

4.24
Solution
We have $w_i > 0$. Since the quadrature rule is exact for $f(x) = 1$, we have
\[
\sum_{i=0}^{n} w_i = b - a.
\]
We also have
\[
|\text{Error}| = \left| \sum_{i=0}^{n} w_i [f(x_i) - f^*(x_i)] \right| \leq \sum_{i=0}^{n} w_i |f(x_i) - f^*(x_i)|
\]
\[
\leq (0.5)10^{-k} \sum_{i=0}^{n} w_i = \frac{1}{2} (b - a)10^{-k}.
\]

Gaussian Integration Methods

4.25 Determine the weights and abscissas in the quadrature formula
\[
\int_{-1}^{1} f(x)dx = \sum_{k=1}^{4} A_k f(x_k)
\]
with $x_1 = -1$ and $x_4 = 1$ so that the formula becomes exact for polynomials of highest possible degree. (Gothenburg Univ., Sweden, BIT 7(1967), 338)

Solution
Making the method
\[
\int_{-1}^{1} f(x)dx = A_1 f(-1) + A_2 f(x_2) + A_3 f(x_3) + A_4 f(1)
\]
exact for $f(x) = x^i, i = 0, 1, ..., 5$, we obtain the equations
\[
A_1 + A_2 + A_3 + A_4 = 2, \quad (4.102)
\]
\[
-A_1 + A_2 x_2 + A_3 x_3 + A_4 = 0, \quad (4.103)
\]
\[
A_1 + A_2 x_2^2 + A_3 x_3^2 + A_4 = \frac{2}{3}, \quad (4.104)
\]
\[
-A_1 + A_2 x_2^3 + A_3 x_3^3 + A_4 = 0, \quad (4.105)
\]
\[
A_1 + A_2 x_2^4 + A_3 x_3^4 + A_4 = \frac{2}{5}, \quad (4.106)
\]
\[
-A_1 + A_2 x_2^5 + A_3 x_3^5 + A_4 = 0. \quad (4.107)
\]
Subtracting (4.104) from (4.102), (4.105) from (4.103), (4.106) from (4.104) and (4.107) from (4.105), we get
\[
\frac{4}{3} = A_2 (1 - x_2^2) + A_3 (1 - x_3^2),
\]
\[
0 = A_2 x_2 (1 - x_2^2) + A_3 x_3 (1 - x_3^2),
\]
\[
\frac{4}{15} = A_2 x_2^2 (1 - x_2^2) + A_3 x_3^2 (1 - x_3^2),
\]
\[
0 = A_2 x_2^3 (1 - x_2^2) + A_3 x_3^3 (1 - x_3^2).
\]
Eliminating $A_3$ from the above equations, we get

$$\frac{4}{3}x_3 = A_2(1 - x_2^2)(x_3 - x_2),$$

$$-\frac{4}{15} = A_2x_2(1 - x_2^2)(x_3 - x_2),$$

$$\frac{4}{15}x_3 = A_2x_2^2(1 - x_2^2)(x_3 - x_2),$$

which give $x_2x_3 = -1/5$, $x_2 = -x_3 = 1/\sqrt{5}$ and $A_1 = A_4 = 1/6$, $A_2 = A_3 = 5/6$.

The error term of the method is given by

$$TE = \frac{C}{6!} f^{(6)}(\xi), \quad -1 < \xi < 1$$

where

$$C = \int_{-1}^{1} x^6 - [A_1 + A_2x_2^2 + A_3x_3^2 + A_4] = \frac{2}{7} - \frac{26}{75} = -\frac{32}{525}.$$

Hence, we have $TE = -\frac{2}{23625} f^{(6)}(\xi)$.

4.26 Find the value of the integral

$$I = \int_{2}^{3} \frac{\cos 2x}{1 + \sin x} \, dx$$

using Gauss-Legendre two and three point integration rules.

**Solution**

Substituting $x = (t + 5)/2$ in $I$, we get

$$I = \int_{2}^{3} \frac{\cos 2x}{1 + \sin x} \, dx = \int_{-1}^{1} \frac{\cos(t + 5)}{1 + \sin ((t + 5)/2)} \, dt.$$

Using the Gauss-Legendre two-point formula

$$\int_{-1}^{1} f(x) \, dx = f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right)$$

we obtain $I = \frac{1}{2} [0.56558356 - 0.15856672] = 0.20350842$.

Using the Gauss-Legendre three-point formula

$$\int_{-1}^{1} f(x) \, dx = \frac{1}{9} \left[ 5f\left(-\frac{3}{\sqrt{5}}\right) + 8f(0) + 5f\left(\frac{3}{\sqrt{5}}\right) \right]$$

we obtain $I = \frac{1}{18} [-1.26018516 + 1.41966658 + 3.48936887] = 0.20271391$.

4.27 Determine the coefficients in the formula

$$\int_{2h}^{\infty} x^{-1/2} f(x) \, dx = (2h)^{1/2} [A_0 f(0) + A_1 f(h) + A_2 f(2h)] + R$$

and calculate the remainder $R$, when $f'''(x)$ is constant.

(Gothenburg Univ., Sweden, BIT 4(1964), 61)
Solution
Making the method exact for \( f(x) = 1, x \) and \( x^2 \), we get

\[
f(x) = 1 : \quad 2\sqrt{2h} = \sqrt{2h}(A_0 + A_1 + A_2)
\]

or \( A_0 + A_1 + A_2 = 2. \)

\[
f(x) = x : \quad \frac{4h\sqrt{2h}}{3} = \sqrt{2h}(A_1h + 2A_2h)
\]

or \( A_1 + 2A_2 = \frac{4}{3}. \)

\[
f(x) = x^2 : \quad \frac{8h^2\sqrt{2h}}{5} = \sqrt{2h}(A_1h^2 + 4A_2h^2)
\]

or \( A_1 + 4A_2 = \frac{8}{5}. \)

Solving the above system of equations, we obtain

\( A_0 = 12/15, \quad A_1 = 16/15 \) and \( A_2 = 2/15. \)

The remainder \( R \) is given by

\[
R = \frac{C}{3!} f^{(3)}(\xi), \quad 0 < \xi < 2h
\]

where

\[
C = \int_{0}^{2h} x^{-1/2}(x^3)dx - \sqrt{2h} [A_1h^3 + 8A_2h^3] = \frac{16\sqrt{2}}{105} h^{7/2}.
\]

Hence, we have the remainder as

\[
R = \frac{8\sqrt{2}}{315} h^{7/2} f^{(3)}(\xi).
\]

4.28 In a quadrature formula

\[
\int_{-1}^{1} (a-x)f(x)dx = A_{-1} f(-x_1) + A_0 f(0) + A_1 f(x_1) + R
\]

the coefficients \( A_{-1}, A_0, A_1 \) are functions of the parameter \( a \), \( x_1 \) is a constant and the error \( R \) is of the form \( C f^{(k)}(\xi) \). Determine \( A_{-1}, A_0, A_1 \) and \( x_1 \), so that the error \( R \) will be of highest possible order. Also investigate if the order of the error is influenced by different values of the parameter \( a. \) (Inst. Tech., Lund, Sweden, BIT 9(1969), 87)

Solution
Making the method exact for \( f(x) = 1, x, x^2 \) we get the system of equations

\[
A_{-1} + A_0 + A_1 = 2a,
\]

\[
x_1(-A_{-1} + A_1) = -\frac{2}{3},
\]

\[
x_1^2(A_{-1} + A_1) = \frac{2a}{3},
\]

\[
x_1^3(-A_{-1} + A_1) = -\frac{2}{5},
\]

which has the solution

\[
x_1 = \frac{3}{\sqrt{5}}, \quad A_{-1} = \frac{5}{9} \left[ a + \frac{3}{\sqrt{5}} \right],
\]
Differentiation and Integration

\[ A_0 = \frac{8a}{9}, \ A_1 = \frac{5}{9} \left[ a - \sqrt{\frac{3}{5}} \right] \]

The error term in the method is given by

\[ R = \frac{C}{4^i} f^{iv}(\xi), \ -1 < \xi < 1 \]

where

\[ C = \int_{-1}^{1} (a-x)x^4 dx - \left[ x_1^4 (A_{-1} + A_1) \right] = 0 \]

Therefore, the error term becomes

\[ R = \frac{C}{5^i} f^{iv}(\xi), \ -1 < \xi < 1 \]

where

\[ C = \int_{-1}^{1} (a-x)x^5 dx - x_1^5 (-A_{-1} + A_1) = -\frac{8}{175} \]

Hence, we get

\[ R = -\frac{1}{2625} f^{iv}(\xi). \]

The order of the method is four for arbitrary \( a \). The error term is independent of \( a \).

4.29 Determine \( x_i \) and \( A_i \) in the quadrature formula below so that \( \sigma \), the order of approximation will be as high as possible

\[ \int_{-1}^{1} (2x^2 + 1)f(x)dx = A_1 f(x_1) + A_2 f(x_2) + A_3 f(x_3) + R. \]

What is the value of \( \sigma \)? Answer with 4 significant digits.

(Gothenburg Univ., Sweden, BIT 17 (1977), 369)

**Solution**

Making the method exact for \( f(x) = x^i \), \( i = 0, 1, 2, ..., 5 \) we get the system of equations

\[
\begin{align*}
A_1 + A_2 + A_3 &= \frac{10}{3}, \\
A_1 x_1 + A_2 x_2 + A_3 x_3 &= 0, \\
A_1 x_1^2 + A_2 x_2^2 + A_3 x_3^2 &= \frac{22}{15}, \\
A_1 x_1^3 + A_2 x_2^3 + A_3 x_3^3 &= 0, \\
A_1 x_1^4 + A_2 x_2^4 + A_3 x_3^4 &= \frac{34}{35}, \\
A_1 x_1^5 + A_2 x_2^5 + A_3 x_3^5 &= 0,
\end{align*}
\]

which simplifies to

\[
\begin{align*}
A_1(x_3 - x_1) + A_2(x_3 - x_2) &= \frac{10}{3} x_3, \\
A_1(x_3 - x_1)x_1 + A_2(x_3 - x_2)x_2 &= -\frac{22}{15}, \\
A_1(x_3 - x_1)x_1^2 + A_2(x_3 - x_2)x_2^2 &= \frac{22}{15} x_3, \\
A_1(x_3 - x_1)x_1^3 + A_2(x_3 - x_2)x_2^3 &= -\frac{34}{35}, \\
A_1(x_3 - x_1)x_1^4 + A_2(x_3 - x_2)x_2^4 &= \frac{34}{35} x_3,
\end{align*}
\]
or
\[ A_1(x_3 - x_1)(x_2 - x_1) = \frac{10}{3} x_2 x_3 + \frac{22}{15}, \]
\[ A_1(x_3 - x_1)(x_2 - x_1) = -\frac{22}{15} (x_2 + x_3), \]
\[ A_1(x_3 - x_1)(x_2 - x_1)x_1^2 = \frac{22}{15} x_2 x_3 + \frac{34}{35}, \]
\[ A_1(x_3 - x_1)(x_2 - x_1)x_1^3 = -\frac{34}{35} (x_2 + x_3). \]

Solving this system, we have \( x_1^2 = \frac{51}{77} \) or \( x_1 = \pm 0.8138 \) and \( x_2 x_3 = 0. \)

For \( x_2 = 0 \), we get \( x_3 = -x_1 \)
\[ A_1 = \frac{11}{15 x_1} = 1.1072, \]
\[ A_2 = \frac{10}{3} - 2A_1 = 1.1190, A_3 = 1.1072. \]

For \( x_3 = 0 \), we get the same method.

The error term is obtained as
\[ R = \frac{C}{6!} f^{vi}(\xi), \quad -1 < \xi < 1 \]
where
\[ C = \int_{-1}^{1} (2x^2 + 1) x^6 dx - [A_1 x_1^6 + A_2 x_2^6 + A_3 x_3^6] = 0.0867. \]

The order \( \sigma \) of approximation is 5.

4.30 Find a quadrature formula
\[ \int_0^1 \frac{f(x)dx}{\sqrt{x(1-x)}} = \alpha_1 f(0) + \alpha_2 f\left(\frac{1}{2}\right) + \alpha_3 f(1) \]
which is exact for polynomials of highest possible degree. Then use the formula on
\[ \int_0^1 \frac{dx}{\sqrt{x-x^3}} \]
and compare with the exact value. \hspace{1cm} (Oslo Univ., Norway, BIT 7(1967), 170)

**Solution**

Making the method exact for polynomials of degree upto 2, we obtain

for \( f(x) = 1 \) : \( I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = \alpha_1 + \alpha_2 + \alpha_3, \)

for \( f(x) = x \) : \( I_2 = \int_0^1 \frac{x dx}{\sqrt{x(1-x)}} = \frac{1}{2} \alpha_2 + \alpha_3, \)

for \( f(x) = x^2 \) : \( I_3 = \int_0^1 \frac{x^2 dx}{\sqrt{x(1-x)}} = \frac{1}{4} \alpha_2 + \alpha_3, \)
where
\[ I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{dx}{\sqrt{1 - (2x-1)^2}} = \int_1^1 \frac{dt}{\sqrt{1-t^2}} = \sin^{-1} t \bigg|_0^1 = \pi, \]
\[ I_2 = \int_0^1 \frac{x \, dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{x \, dx}{\sqrt{1 - (2x-1)^2}} = \int_1^1 \frac{(t+1)^2}{2\sqrt{1-t^2}} \, dt \]
\[ = \frac{1}{2} \int_{-1}^1 t \, dt + \frac{1}{2} \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \frac{\pi}{2}, \]
\[ I_3 = \int_0^1 \frac{x^2 \, dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{x^2 \, dx}{\sqrt{1 - (2x-1)^2}} = \frac{1}{4} \int_{-1}^1 \frac{(t+1)^2}{\sqrt{1-t^2}} \, dt \]
\[ = \frac{1}{4} \int_{-1}^1 \frac{t^2}{\sqrt{1-t^2}} \, dt + \frac{1}{2} \int_{-1}^1 \frac{t}{\sqrt{1-t^2}} \, dt + \frac{1}{4} \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \frac{3\pi}{8}. \]

Hence, we have the equations
\[ \alpha_1 + \alpha_2 + \alpha_3 = \pi, \]
\[ \frac{1}{2} \alpha_2 + \alpha_3 = \frac{\pi}{2}, \]
\[ \frac{1}{4} \alpha_2 + \alpha_3 = \frac{3\pi}{8}, \]
which gives \( \alpha_1 = \pi / 4, \alpha_2 = \pi / 2, \alpha_3 = \pi / 4 \).

The quadrature formula is given by
\[ \int_0^1 \frac{f(x) \, dx}{\sqrt{x(1-x)}} = \frac{\pi}{4} f(0) + 2f \left( \frac{1}{2} \right) + f(1). \]

We now use this formula to evaluate
\[ I = \int_0^1 \frac{dx}{\sqrt{x-x^2}} = \int_1^0 \frac{dx}{\sqrt{1+x} \, \sqrt{x(1-x)}} = \int_0^1 \frac{f(x) \, dx}{\sqrt{x(1-x)}} \]
where \( f(x) = \sqrt{1+x} \).

We obtain
\[ I = \frac{\pi}{4} \left[ 1 + \frac{2\sqrt{2}}{\sqrt{3}} + \frac{\sqrt{2}}{2} \right] = 2.62331. \]

The exact value is
\[ I = 2.62205755. \]

4.31 There is a two-point quadrature formula of the form
\[ I_2 = w_1 f(x_1) + w_2 f(x_2) \]
where \(-1 < x_1 < x_2 < 1\) and \(w_1 > 0, w_2 > 0\) to calculate the integral \( \int_{-1}^1 f(x) \, dx \).

(a) Find \( w_1, w_2, x_1 \) and \( x_2 \) so that \( I_2 = \int_{-1}^1 f(x) \, dx \) when \( f(x) = 1, x, x^2 \) and \( x^3 \).
(b) To get a quadrature formula \( I_n \) for the integral \( \int_a^b f(x)dx \), let \( x_i = a + ih \), 

\( i = 0, 1, 2, ..., n \), where \( h = (b - a) / n \), and approximate \( \int_{x_{i-1}}^{x_i} f(x)dx \) by a suitable variant of the formula in (a). State \( I_n \).

(Inst. Tech. Lyngby, Denmark, BIT 25(1985), 428)

Solution

(a) Making the method

\[
\int_{-1}^{1} f(x)dx = w_1 f(x_1) + w_2 f(x_2)
\]

exact for \( f(x) = 1, x, x^2 \) and \( x^3 \), we get the system of equations

\[
\begin{align*}
  w_1 + w_2 &= 2, \\
  w_1 x_1 + w_2 x_2 &= 0, \\
  w_1 x_1^2 + w_2 x_2^2 &= 2/3, \\
  w_1 x_1^3 + w_2 x_2^3 &= 0,
\end{align*}
\]

whose solution is \( x_2 = -x_1 = 1 / \sqrt{3} \), \( w_2 = w_1 = 1 \).

Hence

\[
\int_{-1}^{1} f(x)dx = f(-1/\sqrt{3}) + f(1/\sqrt{3})
\]

is the required formula.

(b) We write

\[
I_n = \int_a^b f(x)dx
\]

\[
= \int_{x_{i-1}}^{x_i} f(x)dx + \int_{x_{i-1}}^{x_{i-2}} f(x)dx + ... + \int_{x_1}^{x_2} f(x)dx + ... + \int_{x_{n-1}}^{x_n} f(x)dx
\]

where \( x_0 = a, x_n = b, x_i = x_0 + ih, h = (b - a) / n \).

Using the transformation

\[
x = \frac{1}{2} [(x_i - x_{i-1}) t + (x_i + x_{i-1})] = \frac{h}{2} t + m_i
\]

where \( m_i = (x_i + x_{i-1}) / 2 \), we obtain, on using the formula in (a),

\[
\int_{x_{i-1}}^{x_i} f(x)dx = \frac{h}{2} \left[ f \left( m_i - \frac{h \sqrt{3}}{6} \right) + f \left( m_i + \frac{h \sqrt{3}}{6} \right) \right].
\]

Hence, we get

\[
I_n = \frac{h}{2} \sum_{i=1}^{n} \left[ f \left( m_i - \frac{h \sqrt{3}}{6} \right) + f \left( m_i + \frac{h \sqrt{3}}{6} \right) \right].
\]

4.32 Compute by Gaussian quadrature

\[
I = \int_0^1 \frac{\ln (x + 1)}{\sqrt{x(1-x)}}dx
\]

The error must not exceed \( 5 \times 10^{-5} \). (Uppsala Univ., Sweden, BIT 5(1965), 294)
Solution
Using the transformation, \( x = (t + 1) / 2 \), we get
\[
I = \int_0^1 \frac{\ln (x + 1)}{\sqrt{x(1-x)}} \, dx = \int_{-1}^1 \frac{\ln (t+3/2)}{\sqrt{1-t^2}} \, dt
\]
Using Gauss-Chebyshev integration method
\[
\int_{-1}^1 \frac{f(t)}{\sqrt{1-t^2}} \, dt = \sum_{k=0}^{n} \lambda_k f(t_k)
\]
where
\[
t_k = \cos \left( \frac{(2k+1)\pi}{2n+2} \right), \quad k = 0, \ldots, n,
\]
\[
\lambda_k = \pi / (n+1), \quad k = 0, \ldots, n,
\]
we get for \( f(t) = \ln \left( \frac{t+3}{2} \right) \), and
\[
n = 1 : \quad I = \frac{\pi}{2} \left[ f\left( -\frac{1}{\sqrt{2}} \right) + f\left( \frac{1}{\sqrt{2}} \right) \right] = 1.184022,
\]
\[
n = 2 : \quad I = \frac{\pi}{3} \left[ f\left( -\frac{\sqrt{3}}{2} \right) + f(0) + f\left( \frac{\sqrt{3}}{2} \right) \right] = 1.182688,
\]
\[
n = 3 : \quad I = \frac{\pi}{4} \left[ f\left( \cos \left( \frac{\pi}{8} \right) \right) + f\left( \cos \left( \frac{3\pi}{8} \right) \right) + f\left( -\cos \left( \frac{3\pi}{8} \right) \right) + f\left( -\cos \left( \frac{\pi}{8} \right) \right) \right]
= 1.182662.
\]
Hence, the result correct to five decimal places is \( I = 1.18266 \).

4.33 Calculate
\[
\int_0^1 (\cos 2x)(1-x^2)^{-1/2} \, dx
\]
correct to four decimal places. (Lund Univ., Sweden, BIT 20(1980), 389)
Solution
Since, the integrand is an even function, we write the integral as
\[
I = \int_0^1 \frac{\cos (2x)}{\sqrt{1-x^2}} \, dx = \frac{1}{2} \int_{-1}^1 \frac{\cos (2x)}{\sqrt{1-x^2}} \, dx.
\]
Using the Gauss-Chebyshev integration method, we get for \( f(x) = (\cos (2x)) / 2 \),
(see problem 4.32)
\[
n = 1 : \quad I = 0.244956,
\]
\[
n = 2 : \quad I = 0.355464,
\]
\[
n = 3 : \quad I = 0.351617,
\]
\[
n = 4 : \quad I = \frac{\pi}{5} \left[ f\left( \cos \left( \frac{\pi}{10} \right) \right) + f\left( \cos \left( \frac{3\pi}{10} \right) \right) + f(0) + f\left( -\cos \left( \frac{3\pi}{10} \right) \right) + f\left( -\cos \left( \frac{\pi}{10} \right) \right) \right]
= 0.351688.
\]
Hence, the result correct to four decimal places is \( I = 0.3517 \).
4.34 Compute the value of the integral

\[ \int_{0.5}^{1.5} \frac{2 - 2x + \sin(x - 1) + x^2}{1 + (x - 1)^2} \, dx \]

with an absolute error less than \(10^{-4}\). (Uppsala Univ., Sweden, BIT 27(1987), 130)

**Solution**

Using the trapezoidal rule, we get

\[
\begin{align*}
h = 1.0 : & \quad I = \frac{1}{2} [f(0.5) + f(1.5)] = 1.0. \\
\end{align*}
\]

\[
\begin{align*}
h = 0.5 & \quad I = \frac{1}{4} [f(0.5) + 2f(1) + f(1.5)] = 1.0. \\
\end{align*}
\]

Hence, the solution is \(I = 1.0\).

4.35 Derive a suitable two point and three point quadrature formulas to evaluate

\[ \int_0^{\pi/4} \left( \frac{1}{\sin x} \right)^{1/4} \, dx \]

Obtain the result correct to 3 decimal places. Assume that the given integral exists.

**Solution**

The integrand and its derivatives are all singular at \(x = 0\). The open type formulas or a combination of open and closed type formulas discussed in the text converge very slowly.

We write

\[
\begin{align*}
\int_0^{\pi/2} \left( \frac{1}{\sin x} \right)^{1/4} \, dx &= \int_0^{\pi/2} x^{-1/4} \left( \frac{x}{\sin x} \right)^{1/4} \, dx \\
&= \int_0^{\pi/2} x^{-1/4} f(x) \, dx.
\end{align*}
\]

We shall first construct quadrature rules for evaluating this integral.

We write

\[
\int_0^{\pi/2} x^{-1/4} f(x) \, dx = \sum_{i=0}^n \lambda_i f(x_i).
\]

Making the formula exact for \(f(x) = 1, x, x^2, \ldots\), we obtain the following results for \(n = 1\) and 2

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<th>(n = 1)</th>
<th>(x_i)</th>
<th>(\lambda_i)</th>
</tr>
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<tr>
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<td>0.260479018</td>
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<td>0.133831762</td>
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<tr>
<td></td>
<td>1.380816210</td>
<td>0.430604430</td>
</tr>
</tbody>
</table>

Using these methods with \(f(x) = (x / \sin x)^{1/4}\), we obtain for

\[
\begin{align*}
n = 1 : & \quad I = 1.927616. \\
n = 2 : & \quad I = 1.927898.
\end{align*}
\]

Hence, the result correct to 3 decimals is 1.928.
4.36 Compute
\[ \int_0^{n/2} \frac{\cos x \log_2(\sin x)}{1 + \sin^2 x} \, dx \]
to 2 correct decimal places. (Uppsala Univ., Sweden, BIT 11(1971), 455)

**Solution**
Substituting \( \sin x = e^{-t} \), we get
\[ I = -\int_0^{\infty} e^{-t} \left( \frac{t}{1 + e^{-2t}} \right) \, dt. \]
We can now use the Gauss-Laguerre’s integration methods (4.71) for evaluating the integral with \( f(t) = t / (1 + e^{-2t}) \). We get for
\[
\begin{align*}
n = 1 : & \quad I = -[0.3817 + 0.4995] = -0.8812. \\
n = 2 : & \quad I = -[0.2060 + 0.6326 + 0.0653] = -0.9039. \\
n = 3 : & \quad I = -[0.1276 + 0.6055 + 0.1764 + 0.0051] = -0.9146. \\
n = 4 : & \quad I = -[0.0865 + 0.5320 + 0.2729 + 0.0256 + .0003] = -0.9173. \\
n = 5 : & \quad I = -[0.0624 + 0.4537 + 0.3384 + 0.0601 + 0.0026 + 0.0000] \\
& \quad \quad = -0.9172.
\end{align*}
\]
Hence, the required value of the integral is \( -0.917 \) or \( -0.92 \).

4.37 Compute
\[ \int_0^{0.8} \left( \frac{\sin x}{x} \right) \, dx \]
correct to five decimals. (Umea Univ., Sweden, BIT 20(1980), 261)

**Solution**
We have
\[ I = 0.8 + \int_0^{0.8} \left( \frac{\sin x}{x} \right) \, dx. \]
The integral on the right hand side can be evaluated by the open type formulas. Using the methods (4.50) with \( f(x) = \sin x / x \), we get for
\[
\begin{align*}
n = 2 : & \quad I = 0.8 + 0.8 f(0.4) = 1.578837. \\
n = 3 : & \quad I = 0.8 + \frac{3}{2} \left( \frac{0.8}{3} \right) \left[ f \left( \frac{0.8}{3} \right) + f \left( \frac{1.6}{3} \right) \right] = 1.576581. \\
n = 4 : & \quad I = 0.8 + \frac{0.8}{3} \left[ 2f(0.2) - f(0.4) + 2f(0.6) \right] = 1.572077. \\
n = 5 : & \quad I = 0.8 + \frac{0.8}{24} \times [11f(0.16) + f(0.32) + f(0.48) + 11f(0.64)] = 1.572083.
\end{align*}
\]
Hence, the solution correct to five decimals is 1.57208.

4.38 Integrate by Gaussian quadrature \( n = 3 \)
\[ \int_1^2 \frac{dx}{1 + x^3} \]
Solution
Using the transformation \( x = (t + 3) / 2 \), we get
\[
I = \int_1^2 \frac{dx}{1 + x^3} = \frac{1}{2} \int_{-1}^1 \frac{dt}{1 + [(t + 3)/2]^3}.
\]

Using the Gauss-Legendre four-point formula
\[
\int_{-1}^1 f(x)dx = 0.652145 \left[ f(0.339981) + f(-0.339981) \right] \\
+ 0.347855 \left[ f(0.861136) + f(-0.861136) \right]
\]
we obtain
\[
I = \frac{1}{2} \left[ 0.652145(0.176760 + 0.298268) + 0.347855(0.122020 + 0.449824) \right] = 0.254353.
\]

4.39 Use Gauss-Laguerre or Gauss-Hermite formulas to evaluate

\( (i) \int_0^\infty \frac{e^{-x}}{1 + x} \, dx, \quad (ii) \int_0^\infty \frac{e^{-x}}{\sin x} \, dx, \quad (iii) \int_{-\infty}^\infty \frac{e^{-x^2}}{1 + x^2} \, dx, \quad (iv) \int_{-\infty}^\infty e^{-x^2} \, dx. \)

Use two-point and three-point formulas.

Solution
\( (i, ii) \) Using the Gauss-Laguerre two-point formula
\[
\int_0^\infty e^{-x} f(x) \, dx = 0.853553 f(0.585786) + 0.146447 f(3.414214)
\]
we obtain
\[
I_1 = \int_0^\infty \frac{e^{-x}}{1 + x} \, dx = 0.571429, \quad \text{where } f(x) = \frac{1}{1 + x}.
\]
\[
I_2 = \int_0^\infty e^{-x} \sin x \, dx = 0.432459, \quad \text{where } f(x) = \sin x.
\]

Using the Gauss-Laguerre three-point formula
\[
\int_0^\infty e^{-x} f(x) \, dx = 0.711093 f(0.415775) + 0.278518 f(2.294280) \\
+ 0.010389 f(6.289945)
\]
we obtain
\[
I_1 = \int_0^\infty \frac{e^{-x}}{1 + x} \, dx = 0.588235.
\]
\[
I_2 = \int_0^\infty e^{-x} \sin x \, dx = 0.496030.
\]

\( (iii, iv) \) Using Gauss-Hermite two-point formula
\[
\int_{-\infty}^\infty e^{-x^2} f(x) \, dx = 0.886227 \left[ f(0.707107) + f(-0.707107) \right]
\]
we get
\[
I_3 = \int_{-\infty}^\infty \frac{e^{-x^2}}{1 + x^2} \, dx = 1.181636, \quad \text{where } f(x) = \frac{1}{1 + x^2}.
\]
\[
I_4 = \int_{-\infty}^\infty e^{-x^2} \, dx = 1.772454, \quad \text{where } f(x) = 1.
\]
Using Gauss-Hermite three-point formula
\[
\int_{-\infty}^{\infty} e^{-x^2} f(x) \, dx = 1.181636 f(0) + 0.295409 [f(1.224745) + f(-1.224745)]
\]
we obtain
\[
I_3 = \int_{-\infty}^{\infty} \frac{e^{-x^2}}{1+x^2} \, dx = 1.417963.
\]
\[
I_4 = \int_{-\infty}^{\infty} e^{-x^2} \, dx = 1.772454.
\]

4.40 Obtain an approximate value of

\[
I = \int_{-1}^{1} (1-x^2)^{1/2} \cos x \, dx
\]
using

(a) Gauss-Legendre integration method for \(n = 2, 3\).

(b) Gauss-Chebyshev integration method for \(n = 2, 3\).

Solution

(a) Using Gauss-Legendre three-point formula
\[
\int_{-1}^{1} f(x) \, dx = \frac{1}{9} [5f(-\sqrt{0.6}) + 8f(0) + 5f(\sqrt{0.6})]
\]
we obtain
\[
I = \frac{1}{9} [5\sqrt{0.4} \cos \sqrt{0.6} + 8 + 5\sqrt{0.4} \cos \sqrt{0.6}]
\]
\[
= 1.391131.
\]

Using Gauss-Legendre four-point formula
\[
\int_{-1}^{1} f(x) \, dx = 0.652145 [f(0.339981) + f(-0.339981)]
\]
\[
+ 0.347855 [f(0.861136) + f(-0.861136)]
\]
we obtain
\[
I = 2 \times 0.652145 [\sqrt{1-(0.339981)^2} \cos (0.339981)]
\]
\[
+ 2 \times 0.347855 [\sqrt{1-(0.861136)^2} \cos (0.861136)]
\]
\[
= 1.156387 + 0.230450 = 1.386837.
\]

(b) We write
\[
I = \int_{-1}^{1} \sqrt{1-x^2} \cos x \, dx = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx
\]
where \(f(x) = (1-x^2) \cos x\).

Using Gauss-Chebyshev three-point formula
\[
\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx = \frac{\pi}{3} \left[ f\left(\frac{\sqrt{3}}{2}\right) + f(0) + f\left(-\frac{\sqrt{3}}{2}\right) \right]
\]
we obtain
\[
I = \frac{\pi}{3} \left[ \frac{1}{4} \cos \frac{\sqrt{3}}{2} + \frac{1}{4} \cos \frac{\sqrt{3}}{2} \right] = 1.386416.
\]
Using Gauss-Chebyshev four-point formula
\[
\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx = \frac{\pi}{4} [f(0.923880) + f(0.382683) + f(-0.382683) + f(-0.923880)]
\]
we obtain
\[
I = \frac{\pi}{4} [2(0.088267) + 2(0.791813)] = 1.382426.
\]

4.41 The Radau quadrature formula is given by
\[
\int_{-1}^{1} f(x) \, dx = B_1 f(-1) + \sum_{k=1}^{n} H_k f(x_k) + R
\]
Determine \(x_k, H_k\) and \(R\) for \(n = 1\).

Solution
Making the method
\[
\int_{-1}^{1} f(x) \, dx = B_1 f(-1) + H_1 f(x_1) + R
\]
exact for \(f(x) = 1, x\) and \(x^2\), we obtain the system of equations
\[
B_1 + H_1 = 2,
\]
\[-B_1 + H_1 x_1 = 0,
\]
\[B_1 + H_1 x_1^2 = 2/3,
\]
which has the solution \(x_1 = 1/3, H_1 = 3/2, B_1 = 1/2\).
Hence, we obtain the method
\[
\int_{-1}^{1} f(x) \, dx = \frac{1}{2} f(-1) + \frac{3}{2} f\left(\frac{1}{3}\right).
\]
The error term is given by
\[
R = C \frac{3}{3!} f'''(\xi), \quad -1 < \xi < 1
\]
where
\[
C = \int_{-1}^{1} x^3 \, dx - [-B_1 + H_1 x_1^3] = \frac{4}{9}.
\]
Hence, we have
\[
R = \frac{2}{27} f'''(\xi), -1 < \xi < 1.
\]

4.42 The Lobatto quadrature formula is given by
\[
\int_{-1}^{1} f(x) \, dx = B_1 f(-1) + B_2 f(1) + \sum_{k=1}^{n-1} H_k f(x_k) + R
\]
Determine \(x_k, H_k\) and \(R\) for \(n = 3\).

Solution
Making the method
\[
\int_{-1}^{1} f(x) \, dx = B_1 f(-1) + B_2 f(-1) + H_1 f(x_1) + H_2 f(x_2) + R
\]
exact for \(f(x) = x^i, i = 0, 1, ..., 5\), we obtain the system of equations
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\[ B_1 + B_2 + H_1 + H_2 = 2, \]
\[- B_1 + B_2 + H_1x_1 + H_2x_2 = 0, \]
\[ B_1 + B_2 + H_1x_1^2 + H_2x_2^2 = \frac{2}{3}, \]
\[- B_1 + B_2 + H_1x_1^3 + H_2x_2^3 = 0, \]
\[ B_1 + B_2 + H_1x_1^4 + H_2x_2^4 = \frac{2}{5}, \]
\[- B_1 + B_2 + H_1x_1^5 + H_2x_2^5 = 0, \]
or
\[ H_1(1 - x_1^2) + H_2(1 - x_2^2) = \frac{4}{3}, \]
\[ H_1(1 - x_1^2)x_1 + H_2(1 - x_2^2)x_2 = 0, \]
\[ H_1(1 - x_1^2)x_1^2 + H_2(1 - x_2^2)x_2^2 = \frac{4}{15}, \]
\[ H_1(1 - x_1^2)x_1^3 + H_2(1 - x_2^2)x_2^3 = 0, \]
or
\[ H_1(1 - x_1^2)(x_2 - x_1) = \frac{4}{3}x_2, \]
\[ H_1(1 - x_1^2)(x_2 - x_1)x_1 = -\frac{4}{15}, \]
\[ H_1(1 - x_1^2)(x_2 - x_1)x_1^2 = \frac{4}{15}x_2. \]

Solving the system, we get \( x_1x_2 = -\frac{1}{5} \), and \( x_1 = -x_2 \).

The solution is obtained as
\[ x_1 = \frac{1}{\sqrt{5}}, \quad x_2 = -\frac{1}{\sqrt{5}}, \]
\[ H_1 = H_2 = \frac{5}{6}, \quad B_1 = B_2 = \frac{1}{6}. \]

The method is given by
\[ \int_{-1}^{1} f(x)dx = \frac{1}{6} \left[ f(-1) + f(1) \right] + \frac{5}{6} \left[ f\left( \frac{1}{\sqrt{5}} \right) + f\left( -\frac{1}{\sqrt{5}} \right) \right]. \]

The error term is
\[ R = \frac{C}{6!} f^{(5)}(\xi), \quad -1 < \xi < 1 \]

where
\[ C = \int_{-1}^{1} x^6dx - [B_1 + B_2 + H_1x_1^6 + H_2x_2^6] \]
\[ = \left[ \frac{2}{7} - \frac{1}{3} \frac{1}{75} \right] = \frac{-32}{525}. \]

Hence, we have
\[ R = -\frac{2}{23625} f^{(5)}(\xi), \quad -1 < \xi < 1. \]
4.43 Obtain the approximate value of
\[ I = \int_{-1}^{1} e^{-x^2} \cos x \, dx \]
using
(a) Gauss-Legendre integration method for \( n = 2, 3 \).
(b) Radau integration method for \( n = 2, 3 \).
(c) Lobatto integration method for \( n = 2, 3 \).

Solution
(a) Using Gauss-Legendre 3-point formula
\[ \int_{-1}^{1} f(x) \, dx = \frac{1}{9} \left[ 5f \left( -\frac{\sqrt{3}}{5} \right) + 8f(0) + 5f \left( \frac{\sqrt{3}}{5} \right) \right] \]
we obtain \( I = 1.324708 \).

Using Gauss-Legendre 4-point formula
\[ \int_{-1}^{1} f(x) \, dx = 0.652145 \left[ f(0.339981) + f(-0.339981) \right] + 0.347855 \left[ f(0.861136) + f(-0.861136) \right] \]
we obtain \( I = 1.311354 \).

(b) Using Radau 3-point formula
\[ \int_{-1}^{1} f(x) \, dx = \frac{2}{9} f(-1) + \frac{16 + \sqrt{6}}{18} f \left( \frac{1 - \sqrt{6}}{5} \right) + \frac{16 - \sqrt{6}}{18} f \left( \frac{1 + \sqrt{6}}{5} \right) \]
we obtain \( I = 1.307951 \).

Using Radau 4-point formula
\[ \int_{-1}^{1} f(x) \, dx = 0.125000 f(-1) + 0.657689 f(-0.575319) + 0.776387 f(0.181066) + 0.440924 f(0.822824) \]
we obtain \( I = 1.312610 \).

(c) Using Lobatto 3-point formula
\[ \int_{-1}^{1} f(x) \, dx = \frac{1}{3} \left[ f(-1) + 4f(0) + f(1) \right] \]
we obtain \( I = 1.465844 \).

Using Lobatto 4-point formula
\[ \int_{-1}^{1} f(x) \, dx = 0.166667 \left[ f(-1) + f(1) \right] + 0.833333 \left[ f(0.447214) + f(-0.447214) \right] \]
we obtain \( I = 1.296610 \).

4.44 Evaluate
\[ I = \int_{0}^{\infty} e^{-x} \log_{10}(1 + x) \, dx \]
correct to two decimal places, using the Gauss-Laguerre's integration methods.
Solution
Using the Gauss-Laguerre’s integration methods (4.71) and the abscissas and weights given in Table 4.7, with \( f(x) = \log_{10}(1 + x) \), we get for
\[
\begin{align*}
n = 1 &: \quad I = 0.2654. \\
n = 2 &: \quad I = 0.2605. \\
n = 3 &: \quad I = 0.2594. \\
n = 4 &: \quad I = 0.2592.
\end{align*}
\]
Hence, the result correct to two decimals is 0.26.

4.45 Calculate the weights, abscissas and the remainder term in the Gaussian quadrature formula
\[
\frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{\exp(-t)f(t)}{\sqrt{t}} \, dt = A_1 f(t_1) + A_2 f(t_2) + C f^{(n)}(\xi).
\]
(Royal Inst. Tech., Stockholm, Sweden, BIT 20(1980), 529)

Solution
Making the method
\[
\frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-t} f(t) \, dt = A_1 f(t_1) + A_2 f(t_2)
\]
extact for \( f(t) = 1, t, t^2 \) and \( t^3 \) we obtain
\[
A_1 + A_2 = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{e^{-t}}{\sqrt{t}} \, dt \\
= \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-t^2} \, dT = \frac{2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} = 1.
\]
\[
A_1 t_1 + A_2 t_2 = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \sqrt{t} e^{-t} \, dt \\
= \frac{1}{2\sqrt{\pi}} \int_0^{\infty} \frac{e^{-t}}{\sqrt{t}} \, dt = \frac{1}{2}.
\]
\[
A_1 t_1^2 + A_2 t_2^2 = \frac{1}{\sqrt{\pi}} \int_0^{\infty} t^{3/2} e^{-t} \, dt \\
= \frac{3}{2\sqrt{\pi}} \int_0^{\infty} \sqrt{t} e^{-t} \, dt = \frac{3}{4}.
\]
\[
A_1 t_1^3 + A_2 t_2^3 = \frac{1}{\sqrt{\pi}} \int_0^{\infty} t^{5/2} e^{-t} \, dt \\
= \frac{5}{2\sqrt{\pi}} \int_0^{\infty} t^{3/2} e^{-t} \, dt = \frac{15}{8}.
\]
Simplifying the above system of equations, we get
\[
A_1 (t_2 - t_1) = t_2 - \frac{1}{2},
\]
\[
A_1 (t_2 - t_1) t_1 = \frac{1}{2} t_2 - \frac{3}{4},
\]
\[ A_1(t_2 - t_1) = \frac{3}{4} t_2 - \frac{15}{8}, \]

which give
\[ t_1 = \frac{1}{2} t_2 - \frac{3}{4} = \frac{3}{4} t_2 - \frac{15}{8}. \]

Simplifying, we get
\[ 4t_2^2 - 12t_2 + 3 = 0, \quad \text{or} \quad t_2 = \frac{3 \pm \sqrt{6}}{2}. \]

We also obtain
\[ t_1 = \frac{3 + \sqrt{6}}{2}, \quad A_1 = \frac{3 + \sqrt{6}}{6}, \quad A_2 = \frac{3 - \sqrt{6}}{6}. \]

Hence, the required method is
\[ E = \int_0^\infty E(v)dv = \frac{2\pi h}{c^3} \int_0^\infty \frac{v^3dv}{e^{\frac{hv}{kT}} - 1}. \]

We write
\[ I = \int_0^\infty \frac{x^3dx}{e^x - 1} = \int_0^\infty e^{-x} \left( \frac{x^3}{1 - e^{-x}} \right) dx \]

Applying the Gauss-Laguerre integration methods (4.71) with \( f(x) = \frac{x^3}{1 - e^{-x}} \), we get for
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\[ n = 1 : \quad I = 6.413727, \]
\[ n = 2 : \quad I = 6.481130, \]
\[ n = 3 : \quad I = 6.494531. \]

Hence, the result correct to 3 decimal places is 6.494.

4.47  (a) Estimate \( \int_0^{0.5} \int_0^{0.5} \frac{\sin xy}{1 + xy} \, dx \, dy \) using Simpson’s rule for double integrals with both step sizes equal to 0.25.

(b) Calculate the same integral correct to 5 decimals by series expansion of the integrand.

(Uppsala Univ., Sweden, BIT 26(1986), 399)

Solution

(a) Using Simpson’s rule with \( h = k = 0.25 \), we have three nodal points each, in \( x \) and \( y \) directions. The nodal points are \((0, 0), (0, 1/4), (0, 1/2), (1/4, 0), (1/4, 1/4), (1/4, 1/2), (1/2, 0), (1/2, 1/4)\) and \((1/2, 1/2)\). Using the double Simpson’s rule, we get

\[
I = \frac{1}{144} \left[ f(0,0) + 4f\left(\frac{1}{4},0\right) + f\left(\frac{1}{2},0\right) + 4f\left(0,\frac{1}{4}\right) + 4f\left(\frac{1}{4},\frac{1}{4}\right) + f\left(\frac{1}{2},\frac{1}{4}\right) + f\left(0,\frac{1}{2}\right) + 4f\left(\frac{1}{4},\frac{1}{2}\right) + f\left(\frac{1}{2},\frac{1}{2}\right) \right]
\]

\[ = \frac{1}{144} \left[ 0 + 0 + 0 + 4 \left( 0 + 0.235141 + 0.110822 \right) + 0 + 0.443288 + 0.197923 \right] \]
\[ = 0.014063. \]

(b) Using the series expansions, we get

\[
I = \int_0^{1/2} \int_0^{1/2} (1 + xy)^{-1} \sin xy \, dx \, dy
\]

\[ = \int_0^{1/2} \int_0^{1/2} \left( 1 - xy + x^2y^2 + \ldots \right) \left( xy - \frac{x^3y^3}{6} + \ldots \right) dx \, dy
\]

\[ = \int_0^{1/2} \int_0^{1/2} \left[ xy - x^2y^2 + \frac{5}{6}x^3y^3 - \frac{5}{6}x^4y^4 + \frac{101}{120}x^5y^5 - \frac{101}{120}x^6y^6 + \ldots \right] dx \, dy
\]

\[ = \int_0^{1/2} \left[ \frac{x - x^2}{8} + \frac{5x^3}{24} + \frac{5x^4}{384} + \frac{101x^5}{960} + \frac{101x^6}{60752} + \ldots \right] dx
\]

\[ = \frac{1}{64} - \frac{1}{576} + \frac{5}{24576} - \frac{5}{153600} + \frac{101}{1769472} - \frac{101}{96337920} + \ldots = 0.014064. \]

4.48 Evaluate the double integral

\[
\int_0^1 \left( \int_1^2 \frac{2xy}{(1 + x^2)(1 + y^2)} \, dy \right) \, dx
\]

using

(i) the trapezoidal rule with \( h = k = 0.25 \).

(ii) the Simpson’s rule with \( h = k = 0.25 \).

Compare the results obtained with the exact solution.
Solution

Exact solution is obtained as

\[ I = \int_{0}^{1} \frac{2x}{1 + x^2} \, dx \cdot \int_{1}^{2} \frac{y}{1 + y^2} \, dy = \frac{1}{2} \left[ \ln(1 + x^2) \right]_{0}^{1} \left[ \ln(1 + y^2) \right]_{1}^{2} \]
\[ = \frac{1}{2} \ln(2) \ln(5/2) = 0.317562. \]

With \( h = k = 1/4 \), we have the nodal points

\((x_i, y_j), i = 0, 1, 2, 3, 4, j = 0, 1, 2, 3, 4, \)

where \( x_i = i/4, i = 0, 1, ..., 4; y_j = 1 + (j/4), j = 0, 1, ..., 4. \)

Using the trapezoidal rule, we obtain

\[ I = \sum_{i=0}^{3} \sum_{j=0}^{3} \left[ f(x_i, y_j) + f(x_{i+1}, y_j) + f(x_i, y_{j+1}) + f(x_{i+1}, y_{j+1}) \right] = 0.312330. \]

Using Simpson's rule, we obtain

\[ I = \sum_{i=0}^{3} \sum_{j=0}^{3} \left[ 2f(x_i, y_j) + 4f(x_{i+1}, y_j) + 2f(x_{i+1}, y_{j+1}) + f(x_i, y_{j+1}) + f(x_{i+1}, y_{i+1}) \right] = 0.317716. \]

4.49 Evaluate the double integral

\[ \int_{1}^{5} \left( \int_{1}^{5} \frac{dx}{(x^2 + y^2)^{3/2}} \right) \, dy \]

using the trapezoidal rule with two and four subintervals and extrapolate.
Solution

With \( h = k = 2 \), the nodal points are
\[(1, 1), (3, 1), (5, 1), (1, 3), (3, 3), (5, 3), (1, 5), (3, 5), (5, 5).\]

Using the trapezoidal rule, we get
\[
I = \frac{2 \times 2}{4} \left[ f(1, 1) + 2f(1, 3) + f(1, 5) + 2f(3, 1) + 2f(3, 3) + f(3, 5)
+ f(5, 1) + 2f(5, 3) + f(5, 5) \right]
= 4.1345.
\]

With \( h = k = 1 \), the nodal points are
\[(i, j), \quad i = 1, 2, ..., 5, j = 1, 2, ..., 5.\]

Using the trapezoidal rule, we get
\[
I = \frac{1}{4} \left[ f(1, 1) + 2(f(1, 2) + f(1, 3)) + f(1, 4) + f(1, 5)
+ 2f(2, 1) + 2(f(2, 2) + f(2, 3)) + f(2, 4) + f(2, 5)
+ 2f(3, 1) + 2(f(3, 2) + f(3, 3)) + f(3, 4) + f(3, 5)
+ 2f(4, 1) + 2(f(4, 2) + f(4, 3)) + f(4, 4) + f(4, 5)
+ f(5, 1) + 2(f(5, 2) + f(5, 3) + f(5, 4)) + f(5, 5) \right]
= 3.9975.
\]

Using extrapolation, we obtain the better approximation as
\[
I = \frac{4(3.9975) - 4.1345}{3} = 3.9518.
\]

4.50 A three dimensional Gaussian quadrature formula has the form
\[
\int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(x, y, z) \, dx \, dy \, dz = f(\alpha, \alpha, \alpha) + f(-\alpha, \alpha, \alpha) + f(\alpha, -\alpha, \alpha)
+ f(\alpha, \alpha, -\alpha) + f(-\alpha, -\alpha, \alpha) + f(-\alpha, \alpha, -\alpha)
+ f(-\alpha, -\alpha, -\alpha) + f(\alpha, -\alpha, -\alpha) + R
\]

Determine \( \alpha \) so that \( R = 0 \) for every \( f \) which is a polynomial of degree 3 in 3 variables \( i.e. \)
\[
f = \sum_{i, j, k=0}^{3} a_{ijk} x^i y^j z^k \quad \text{(Lund Univ., Sweden, BIT 15(1975), 111)}
\]

Solution

For \( i = j = k = 0 \), the method is exact.

The integral
\[
\int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} x^i y^j z^k \, dx \, dy \, dz = 0
\]
when \( i \) and / or \( j \) and / or \( k \) is odd. In this case also, the method is exact.

For \( f(x, y, z) = x^2 y^2 z^2 \), we obtain
\[
\frac{8}{27} = 8\alpha^6.
\]

The value of \( \alpha \) is therefore \( \alpha = 1 / \sqrt{3} \).

Note that \( \alpha = -1 / \sqrt{3} \) gives the same expression on the right hand side.