Chapter 5
Numerical Integration

Numerical integration is the study of how the numerical value of an integral can be found. Methods of function approximation discussed in Chapter ??, i.e., function approximation via the global interpolation polynomial or spline interpolation, provides a basis for numerical integration techniques. Let the definite integral under consideration be

\[ I\{f\} = \int_{a}^{b} f(x)dx \]

where \([a, b]\) is a finite closed interval. In this chapter, we primarily consider approximations to \(I\{f\}\) that are of the form

\[ I_{n+1}\{f\} = \sum_{j=0}^{n} a_{j}f(x_{j}) \]

where the quadrature nodes are given by,

\[ a \leq x_{0} < x_{1} < x_{2} < \ldots < x_{n} \leq b \]

and the real coefficients \(a_{j}\) are known as the quadrature coefficients. The nodes \(x_{j}\) are preassigned and often equally spaced.

Numerical approximation of definite integrals is desirable in two cases:

1. a closed form of \(I\{f\}\) is not easily obtained, or
2. the available closed form of \(I\{f\}\) is too complicated for efficient numerical evaluation, as the following example clearly illustrates:

\[
\int_{0}^{x} \frac{dt}{1+t^{4}} = \frac{1}{4\sqrt{2}} \log \left( \frac{x^{2} + x\sqrt{2} + 1}{x^{2} - x\sqrt{2} + 1} \right) + \\
\frac{1}{2\sqrt{2}} \left( \tan^{-1} \frac{x}{\sqrt{2}-x} + \tan^{-1} \frac{x}{\sqrt{2}+x} \right).
\]

In interpolatory quadrature, the only type we will be studying in this chapter in addition to Romberg and adaptive quadrature, we approximate the function \(f(x)\) by the interpolating polynomial (Lagrange form)

\[ P_{n}(x) = \sum_{j=0}^{n} f(x_{j})L_{j}(x) \]

where

\[ L_{j}(x) = \frac{(x-x_{0})}{(x_{j}-x_{0})} \cdots \frac{(x-x_{j-1})}{(x_{j}-x_{j-1})} \cdot \frac{(x-x_{j+1})}{(x_{j}-x_{j+1})} \cdots \frac{(x-x_{n})}{(x_{j}-x_{n})}. \]
Hence,

\[ I_{n+1}\{f\} = \int_a^b P_n(x)dx = \sum_{j=0}^{n} f(x_j) \int_a^b L_j(x)dx = \sum_{j=0}^{n} a_j f(x_j) \]

in which

\[ a_j = \int_a^b L_j(x)dx, \quad j = 0, 1, \ldots, n. \]

Note that the quadrature coefficients \( a_j \) are completely determined by the end points \( a \) and \( b \) and the interpolation nodes \( x_j, j = 0, 1, \ldots, n \). Correspondingly, the quadrature error or truncation error is given by

\[ E_{n+1}\{f\} = I\{f\} - I_{n+1}\{f\} = \int_a^b [f(x) - P_n(x)]dx = \int_a^b e_n(x)dx \]

in which \( e_n(x) \) is the interpolation error

\[ e_n(x) = (x - x_0)(x - x_1)\cdots(x - x_n) \frac{f^{(n+1)}(x^*)}{(n+1)!} \]

where \( x^* \equiv x^*(x) \in (x_0, x_1, \ldots, x_n, x) \). If \( f(x) \) is a polynomial of degree at most \( n \), then \( f^{(n+1)}(x) = 0 \) and hence \( E_{n+1}\{f\} = 0 \). We will use this observation to obtain some basic interpolatory quadrature rules.

### 5.1 Method of Exact Matching

This can also be called Method of Undetermined Coefficients.

#### 5.1.1 The Trapezoidal Rule

The trapezoidal rule uses the function value at two points \( x_0 \) and \( x_1 \) to compute the integral of the function in the interval \([x_0, x_1]\). For \( x_0 = 0 \) and \( x_1 = h \), the integral

\[ I\{f\} = \int_0^h f(x)dx \]

is approximated by the trapezoidal rule

\[ I_2\{f\} = a_0 f_0 + a_1 f_1 \]

where the quadrature coefficients \( a_0 \) and \( a_1 \) need to be determined. Observe that the trapezoidal rule is exact for polynomials of degree zero and one, i.e., for a constant and a straight line. Therefore, it is exact for the following functions:

1. \( f(x) = 1 \)
2. \( f(x) = x \)

From (1) we see that

\[ \int_0^h 1 \cdot dx = a_0 + a_1 = h, \]

and from (2) we have

\[ \int_0^h xdx = a_1 h = \frac{h^2}{2}. \]

Using these equations, we get the values of the coefficients, \( a_0 = a_1 = h/2 \), and the trapezoidal rule can be written as

\[ I_2\{f\} = \frac{h}{2}(f_0 + f_1), \]

where \( h = x_1 - x_0 \). Observe that this is also the area of the shaded trapezoid in Fig. ???. Consequently,

\[ I\{f\} = \int_{x_0}^{x_1} f(x)dx = I_2\{f\} + E_2\{f\} = \frac{h}{2}[f_0 + f_1] + E_2\{f\}, \]

where \( E_2\{f\} \) is the error in trapezoidal rule.
Composite Trapezoidal Rule. From the basic trapezoidal rule we can construct a quadrature rule to compute an integral over the interval $[a, b]$ by dividing the interval into $N$ equal subintervals and using the basic trapezoidal rule for each subinterval. Suppose the interval is divided into $N$ subintervals of equal length using the nodes $x_0, x_1, \ldots, x_N$, where $x_i = a + ih$, for $i = 0, \ldots, N$, and $h = \frac{b-a}{N}$ is the size of each subinterval. Assuming $f(x_i) = f_i$, the composite trapezoidal rule is given as

$$\int_a^b f(x)dx = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \cdots + 2f_{N-1} + f_N] + E_T,$$

where $E_T$ is the error in the composite trapezoidal rule.

5.1.2 Simpson’s Rule

Simpson’s rule uses 3 interpolation nodes and a quadratic interpolating polynomial. The general form is

$$I_3\{f\} = a_{-1}f_{-1} + a_0f_0 + a_1f_1$$
Since the Simpson’s rule is exact for polynomials of degree zero, one, and two, it is exact for the following functions.

1. \( f(x) = 1 \),
2. \( f(x) = x \), and
3. \( f(x) = x^2 \).

Thus, from (1) we have
\[
\int_{-h}^{h} x \, dx = a_{-1} + a_0 + a_1 = 2h,
\]
from (2), we get
\[
\int_{-h}^{h} x^2 \, dx = h a_{-1} + h a_1 = 0,
\]
and from (3) we obtain
\[
\int_{-h}^{h} x^3 \, dx = h^2 a_{-1} + h^2 a_1 = \frac{2}{3} h^3.
\]
These equations yield the quadrature coefficients
\[
a_{-1} = a_1 = \frac{1}{3} h, \quad a_0 = \frac{4}{3} h.
\]
Hence, the Simpson’s rule is given as
\[
I_3\{f\} = \frac{h}{3} [f_{-1} + 4f_0 + f_1],
\]
and
\[
I\{f\} = \int_{x_0}^{x_2} f(x) \, dx = I_3\{f\} + E_3\{f\} = \frac{h}{3} [f_{-1} + 4f_0 + f_1] + E_3\{f\},
\]
where \( h = x_2 - x_1 = x_1 - x_0 \), and \( E_3\{f\} \) is the error in Simpson’s rule.
Composite Simpson’s Rule. Now, let us derive the composite Simpson’s rule for computing integral over the interval \([a, b]\). Suppose we have \(N\) equal subintervals of width \(2h\), i.e., \(b - a = 2hN\). We also define \(2N + 1\) equally spaced points \(x_j = a + jh\), for \(j = 0, \ldots, 2N\) in interval \([a, b]\). The \(i\)th subinterval has the endpoints \(x_{2i-2}\) and \(x_{2i}\), and the midpoint \(x_{2i-1}\), for \(i = 1, \ldots, N\). Applying the basic Simpson’s rule over each subinterval, we obtain the composite rule

\[
\int_a^b f(x)dx = \left[ \frac{h}{3} (f_0 + 4f_1 + f_2) + \frac{h}{3} (f_2 + 4f_3 + f_4) + \cdots \right.
\]

\[
+ \frac{h}{3} (f_{2N-2} + 4f_{2N-1} + f_{2N}) \right] + E_S
\]

\[
= \frac{h}{3} \left[ f_0 + 4 \sum_{i=1}^{N} f_{2i-1} + 2 \sum_{i=1}^{N-1} f_{2i} + f_{2N} \right] + E_S,
\]

where \(E_S\) is the error in the composite Simpson’s rule.

5.2 The Truncation Error

5.2.1 The Trapezoidal Rule

Recall that

\[
I\{f\} = \int_0^h f(x)dx = \frac{h}{2}[f_0 + f_1] + E_2\{f\}
\]

Let us compute the error in the trapezoidal rule for the polynomials of degree 0, 1, and 2, i.e., for \(f(x) = 1, x, x^2\).

\[
E_2\{1\} = \int_0^h 1 \cdot dx - \frac{h}{2}[1 + 1] = 0,
\]

\[
E_2\{x\} = \int_0^h xdx - \frac{h}{2}[0 + h] = 0,
\]

\[
E_2\{x^2\} = \int_0^h x^2dx - \frac{h}{2}[0 + h^2] = -\frac{1}{6}h^3 \neq 0.
\]
Since the error is zero for polynomials of degree 1 or less, the trapezoidal rule is said to have degree of precision $= 1$. By Taylor’s formula,

\[
f(x) = f_0 + x f_0' + \frac{x^2}{2!} f_0'' + \frac{x^3}{3!} f_0''' + \cdots
\]

\[
= \text{(straight line)} + \frac{x^2}{2!} f_0'' + \frac{x^3}{3!} f_0''' + \cdots
\]

Therefore, we have the following expression for error

\[
E_2(f(x)) = E_2\{f_0 + x f_0'\} + E_2\left\{\frac{x^2}{2} f_0'' + \frac{x^3}{6} f_0''' + \cdots\right\}
\]

Since the error for a straight line is zero, the first term on the right hand side is zero, i.e., $E_2\{f_0 + x f_0'\} = 0$. Thus,

\[
E_2(f(x)) = 0 + \frac{1}{2} h^2 f_0'' E_2\{x^2\} + \frac{1}{6} h^3 f_0''' E_2\{x^3\} + \cdots
\]

\[
= -\frac{h^3}{12} f_0'' + O(h^4)
\]

The above expression of the truncation error in the trapezoidal rule is known as an asymptotic error estimate. Over here, the term $O(h^4)$ has the following meaning: a function $q(h) = O(h^\alpha)$ as $h \to 0$, (read as $q(h)$ is of the order $h^\alpha$), means that there exist constants $h_0$ and $K$ such that

\[
|q(h)| \leq K h^\alpha, \quad 0 < h \leq h_0.
\]

### 5.2.2 Simpson’s Rule

Recall that

\[
I(f) = \int_{-h}^{h} f(x) \, dx = \frac{h}{3} [f_{-1} + 4f_0 + f_1] + E_3(f)
\]

Let us compute the error for polynomials of degree 3 or less.
We expected Simpson’s rule to be exact for polynomials of degree 2 or less. It turns out that Simpson’s rule is also exact for cubics. For \( f(x) = x^4 \),

\[
E_3\{x^4\} = \int_{-h}^{h} x^4 dx - \frac{h}{3} [h^4 + 0 + h^4] = -\frac{4}{15} h^5 \neq 0.
\]

Therefore, Simpson’s rule has a degree precision = 3. Using Taylor’s formula,

\[
f(x) = f_0 + x f'_0 + \frac{x^2}{2!} f''_0 + \frac{x^3}{3!} f'''_0 + \frac{x^4}{4!} f^{(iv)}_0 + \cdots
\]

\[
= \text{(degree 3 polynomial)} + \frac{x^4}{24} f^{(iv)}_0 + \frac{x^5}{120} f^{v}_0 + \cdots
\]

We have shown above that Simpson’s rule is exact for cubics. Thus,

\[
E_3\{f\} = 0 + \frac{1}{24} f^{(iv)}_0 E_3\{x^4\} + \frac{1}{120} f^{v}_0 E_3\{x^5\} + \cdots
\]

and the asymptotic error estimate is

\[
E_3\{f\} = -\frac{h^5}{90} f^{(iv)}_0 + O(h^7).
\]

We should mention here that one can obtain strict error estimates for the above two quadrature rules, rather than just asymptotic estimates. A complete discussion of this question, however, is outside the scope of this book. We only state the result as follows.
**Theorem 5.1** If an interpolatory quadrature formula has a degree of precision \( m \), then its truncation error is given by

\[
E_{n+1}\{f\} = \frac{f^{(m+1)}(z)}{(m+1)!} E_{n+1}\{x^{m+1}\}
\]

where \( a < z < b \).

Thus, for the trapezoidal rule \( m = 1 \), and

\[
E_2\{f\} = \frac{f''(z)}{2!} E_2\{x^2\} = -\frac{h^3}{12} f''(z), \quad x_0 < z < x_1.
\]

While for Simpson’s rule, \( m = 3 \) and

\[
E_3\{f\} = \frac{f^{(iv)}(z)}{4!} E_3\{x^4\} = -\frac{h^5}{90} f^{(iv)}(z), \quad x_0 < z < x_2.
\]

The truncation error for the composite trapezoidal rule is given by

\[
E_T = -\frac{h^3 N}{12} f''(z^*) = -\frac{(b-a)h^2}{12} f''(z^*), \quad b - a = Nh,
\]

where \( x_0 < z^* < x_n \). Similarly, the error for the composite Simpson’s rule is given by

\[
E_S = -\frac{h^5 N}{90} f^{(iv)}(y^*) = -\frac{(b-a)h^4}{180} f^{(iv)}(y^*), \quad b - a = 2Nh
\]

where \( a < y^* < b \).

### 5.3 Spline Quadrature

Consider the definite integral

\[
I\{f\} = \int_a^b f(x)dx.
\]

If we approximate \( f(x) \) via spline interpolation, such as the cubic interpolatory spline \( s(x) \) discussed in Chapter 5, where

\[
a = x_1 < x_2 < \cdots < x_n = b, \quad h_i = x_{i+1} - x_i,
\]

then we obtain an interesting approximation of \( I\{f\} \) that is given by

\[
I_{sp}\{f\} = \sum_{i=1}^{n-1} \int_{x_i}^{x_i+h_i} s_i(x)dx,
\]

where \( s_i(x) \) is the cubic spline function for the \( i \)th subinterval \([x_i, x_{i+1}]\), and is given by

\[
s_i(x) = \frac{\sigma_i}{h_i} (x_{i+1} - x)^3 + \frac{\sigma_{i+1}}{h_i} (x - x_i)^3 + \left( \frac{f_{i+1}}{h_i} - \sigma_{i+1} h_i \right) (x - x_i)
\]

\[
+ \left( \frac{f_i}{h_i} - \sigma_i h_i \right) (x_{i+1} - x)
\]

(see Chapter 5). Let us define

\[
w = \frac{1}{h_i} (x - x_i), \quad \bar{w} = 1 - w = \frac{1}{h_i} (x_{i+1} - x)
\]
Thus,

\[ s_i(x) = s_i(w) = h_i^2 \sigma_i \bar{w}^3 + h_i^3 \sigma_{i+1} w^3 + w[f_{i+1} - \sigma_{i+1} h_i^2] + \bar{w}[f_i - \sigma_i h_i^2] \]

\[ = \bar{w} f_i + w f_{i+1} + h_i^2 [\sigma_{i+1}(w^3 - w) + \sigma_i (\bar{w}^3 - \bar{w})], \]

and

\[ \int_{x_i}^{x_{i+1}} s_i(x) dx = h_i \int_0^1 s_i(w) dw. \]

Moreover, observing that

\[ \int_0^1 w dw = \int_0^1 \bar{w} d\bar{w} = \frac{1}{2}, \]

and

\[ \int_0^1 (w^3 - w) dw = \int_0^1 (\bar{w}^3 - \bar{w}) d\bar{w} = -\frac{1}{4}, \]

we obtain

\[ \int_{x_i}^{x_{i+1}} s_i(x) dx = \frac{h_i}{2} [f_i + f_{i+1}] - \frac{h_i^3}{4} [\sigma_i + \sigma_{i+1}]. \]

Note that this equation can be regarded as the trapezoidal rule plus a correction term. This correction term is given by

\[ \tau_i = -\frac{h_i^3}{24} [s''(x_i) + s''(x_{i+1})], \]

which indicates that if \( f''(x) \) is not too badly behaved, then

\[ \tau_i \simeq -\frac{h_i^3}{12} f''(\theta) \simeq E_2 \{f\}, \quad x_i < \theta < x_{i+1}. \]

In other words if \( f''(x) \) is well behaved, we have

\[ \int_{x_i}^{x_{i+1}} s_i(x) dx \simeq \frac{h_i}{2} [f_i + f_{i+1}] + E_2 \{f\} \]

which can be remarkably close to the integral

\[ \int_{x_i}^{x_{i+1}} f(x) dx. \]

### 5.4 Richardson’s Extrapolation

In many calculations what one would really like to know is the limiting value of a certain quantity \( F(h) \) as \( F \to 0 \). Needless to say, the work required for computing \( F(h) \) increases sharply as \( h \) approaches zero. Furthermore, the effects of rounding errors set a practical limit on how small \( h \) can be chosen. Usually, one has some knowledge of how the truncation error \( [F(0) - F(h)] \) behaves as \( h \to 0 \). Let

\[ F(h) = F(0) + \alpha_1 h^p + O(h^r) \]

where \( r > p \), and \( \alpha_1 \) is an unknown. Compute \( F \) for two step lengths: \( h \) and \( qh \), \( (q > 1) \)

\[ F(h) = F(0) + \alpha_1 h^p + O(h^r) \]

\[ F(qh) = F(0) + \alpha_1 (qh)^p + O(h^r). \]

Multiplying the first equation by \( q^p \), the second by \(-1\), and adding, we get

\[ a^p F(h) - F(qh) = [q^p - 1] F(0) + O(h^r), \]
or

\[ F(0) = \left[ F(h) + \frac{F(h) - F(qh)}{q^p - 1} \right] + O(h^r). \]

This simple technique known as Richardson’s extrapolation improves the asymptotic error bound from \( O(h^p) \) to \( O(h^r) \).

The repeated application of Richardson’s extrapolation to numerical integration is known as Romberg Integration. As an illustration, consider the composite trapezoidal rule on \( N \) panels, each of width \( h \),

\[ T(h) = \frac{h}{2} \left[ f_0 + 2 \sum_{j=1}^{N-1} f_j + f_N \right]. \]

In Appendix ??, we show that

\[ I\{f\} \equiv I = T(h) + \alpha_1 h^2 + \alpha_2 h^4 + \alpha_3 h^6 + \cdots \]

Using panels of half the width, we get

\[ I = T \left( \frac{h}{2} \right) + \alpha_1 \left( \frac{h^2}{4} \right) + \alpha_2 \left( \frac{h^4}{16} \right) + \alpha_3 \left( \frac{h^6}{64} \right) + \cdots \]

Multiplying this equation by \(-1/4\) and adding to the previous equation, we obtain

\[ \frac{3}{4} I = \left[ T \left( \frac{h}{2} \right) - \frac{1}{4} T(h) \right] - \frac{3}{16} \alpha_2 h^4 - \cdots \]

or

\[ I = \frac{1}{3} \left[ 4T \left( \frac{h}{2} \right) - T(h) \right] - \frac{1}{4} \alpha_2 h^4 + O(h^6) \]

(5.1)

\[ = \left[ T \left( \frac{h}{2} \right) + \frac{1}{3} \left( T \left( \frac{h}{2} \right) - T(h) \right) \right] + O(h^4) \]

(5.2)

Suppose \( b - a = Nh \), and let us denote the composite formula with \( N \) panels by \( T_N \), and the formula with \( 2N \) panels by \( T_{2N} \). Thus,

\[ T_N = T(h), \quad T_{2N} = T \left( \frac{h}{2} \right). \]

The formula using Richardson’s extrapolation is given by

\[ T_{2N}^{(1)} = \frac{1}{3} (4T_{2N} - T_N) = T_{2N} + \frac{1}{3} (T_{2N} - T_N). \]

Now, equation ?? can be written as

\[ I = T_{2N}^{(1)} - \frac{1}{4} \alpha_2 h^4 + O(h^6). \]

(5.3)

Similarly

\[ I = T_{4N}^{(1)} - \frac{1}{4} \alpha_2 \left( \frac{h}{2} \right)^4 + O(h^6), \]

(5.4)

in which

\[ T_{4N}^{(1)} = \frac{1}{3} (4T_{4N} - T_{2N}) = T_{4N} + \frac{1}{3} (T_{4N} - T_{2N}). \]

Eliminating \( \alpha_2 \) from equations (??) and (??), we have

\[ I = \frac{1}{15} \left[ 16T_{4N}^{(1)} - T_{2N}^{(1)} \right] + O(h^6) \]

\[ = \left[ T_{4N}^{(1)} + \frac{1}{15} (T_{4N}^{(1)} - T_{2N}^{(1)}) \right] + O(h^6) \]

\[ = T_{4N}^{(2)} + O(h^6). \]
If we systematically halve the interval, taking \( h, \frac{h}{2}, \frac{h}{4}, \ldots \), etc., we can construct the table of which a section is shown below.

\[
\begin{array}{c|c}
T_N & T_{2N} \\
T_{2N} & T_{4N} \\
T_{4N} & T_{8N} \\
T_{8N} & T_{16N} \\
\end{array}
\]

Error: \( O(h^2) \), \( O(h^4) \), \( O(h^6) \), \( O(h^8) \)

In general, \( I = T^{(j)} + O(h^r) \) in which \( r = 2(j + 1) \), and

\[
T_{2i}^{(j)} = \frac{4^j T_{2i}^{(j-1)} - T_i^{(j-1)}}{4^j - 1} = T_{2i}^{(j-1)} + \frac{T_i^{(j-1)} - T_i^{(j-1)}}{4^j - 1}.
\]

**Example 5.1** Compute \( \int_0^{0.8} \frac{\sin x}{x} \, dx \) using Romberg’s integration.

**Solution**

\[
\begin{array}{c|c|c|c}
h & T_1 & T_2 & T_4 \\
\hline
0.8 & .758680 & .772120 & \frac{.772120}{.772096} = .772095 \\
0.4 & .768760 & .772096, & \frac{.772096}{.772095} = .772095 \\
0.2 & .771262, & \frac{.771262}{.772095} = .772095, & \frac{.772095}{.771887} = .772095 \\
0.1 & .771887, & \frac{.771887}{.772095} = .772095, & \frac{.772095}{.772095} = .772095 \\
\end{array}
\]

\( \square \)

### 5.5 Adaptive Quadrature

An adaptive quadrature algorithm uses one or two basic quadrature rules, namely, the trapezoidal rule and Simpson’s rule, and determines the subinterval sizes so that the computed result meets some prescribed accuracy requirement. In this way, an attempt is made to provide a result with the prescribed accuracy at the lowest cost possible. By cost we mean computer time, which in turn is directly proportional to the number of function evaluations necessary to obtain the result. The user of an adaptive quadrature routine specifies the interval \([a, b]\), provides a subroutine which computes the function \( f(x) \) for any \( x \in [a, b] \), and chooses a tolerance \( \epsilon \). The adaptive routine attempts to compute a quantity \( Q \) such that

\[
|Q - \int_a^b f(x) \, dx| \leq \epsilon.
\]
Example 5.2 Consider the problem of approximation $I = \int_{a}^{b} f(x)dx$ using an adaptive Simpson’s rule with a prescribed tolerance $\epsilon$.

We first approximate $I$ using the basic Simpson’s rule over the interval $[a, b]$, i.e., using one panel, thus

$$P_1 = \frac{H}{6} \left[ f(a) + 4f \left( a + \frac{H}{2} \right) + f(b) \right].$$

Divide $[a, b]$ into two equal subintervals, and apply Simpson’s rule to each. For the left half we get

$$P_{11} = \frac{H}{12} \left[ f(a) + 4f \left( a + \frac{H}{4} \right) + f \left( a + \frac{H}{2} \right) \right],$$

and for the right half we obtain

$$P_{12} = \frac{H}{12} \left[ f \left( a + \frac{H}{2} \right) + 4f \left( a + \frac{3}{4} H \right) + f(b) \right].$$

Note that we need only compute $f \left( a + \frac{H}{4} \right)$ and $f \left( a + \frac{3}{4} H \right)$, since the other values of $f$ are available from the previous level. Now, compute

$$Q = P_{11} + P_{12}$$
and compare with $P_1$. If $|P_1 - Q| \leq \epsilon$ for a prescribed tolerance $\epsilon$, report $Q$ as the desired approximation to $I$. If not, set the right half $[a + \frac{H}{4}, b]$ aside for the moment and proceed in the same way with the left half. In other words, compute

$$
P_{111} = \frac{H}{24} \left[ f(a) + 4f \left( a + \frac{H}{8} \right) + f \left( a + \frac{H}{4} \right) \right],$$

$$
P_{112} = \frac{H}{24} \left[ f \left( a + \frac{H}{4} \right) + 4f \left( a + \frac{3H}{8} \right) + f \left( a + \frac{H}{2} \right) \right].$$

We accept $(P_{111} + P_{112})$ as an approximation to $\int_a^{a + H/2} f(x)dx$ if

$$
|P_{11} - (P_{111} + P_{112})| \leq \frac{\epsilon}{2},
$$

and repeat the process for the right half $[a + \frac{H}{2}, b]$. Thus, we have constructed the following tree

```
Level 1  
P_1 : [a, b]
Level 2  
P_{111} : [a, a + \frac{H}{4}]
         \downarrow P_{11} \downarrow P_{12} \downarrow P_2 : [a + \frac{H}{2}, b]
Level 3  
P_{111} : [a, a + \frac{H}{4}]
         \downarrow P_{112} \downarrow P_{122} \downarrow P_{22} : [a + \frac{H}{2}, a + \frac{3H}{4}]
```

If the above test fails, however, set the right half of $[a, a + \frac{H}{2}]$ aside and repeat the process for the left half $[a, a + \frac{H}{4}]$.

In practice, we have to limit the number of levels used since the number of function evaluations increases rapidly. Hence, when we reach the maximum level permitted the last approximation is accepted and we move to the right.

In general, let us assume that on an interval $[x_i, x_{i+1}]$ the basic Simpson’s rule yields an approximation $S_i$ to the true value $I_i = \int_{x_i}^{x_{i+1}} f(x)dx$. Then

$$
I_i - S_i = -\frac{\left( h_i/2 \right)^5}{90} f^{(iv)}(z_i)
$$

where $x_i < z_i < x_{i+1}$ and $h_i = x_{i+1} - x_i$. Let $S^{(L)}_i$ and $S^{(R)}_i$ be the results of the basic Simpson’s rules on $[x_i, x_i + \frac{h_i}{2}]$ and $[x_i + \frac{h_i}{2}, x_{i+1}]$, respectively. Also, let $Q_i = S^{(L)}_i + S^{(R)}_i$, then

$$
I_i - Q_i = -\frac{1}{24} \left( h_i/2 \right)^5 \frac{f^{(iv)}(y_i)}{90}
$$

where $x_i < y_i < x_{i+1}$. Assuming that $h_i$ is small enough so that $f^{(iv)}(x)$ is essentially constant, i.e., $f^{(iv)}(\eta) \approx f^{(iv)}(y_i) \approx f^{(iv)}(z_i)$, equations (5.5) and (5.6) yield

$$
Q_i - S_i \approx -\frac{\left( h_i/2 \right)^5}{90} f^{(iv)}(\eta) \left[ 1 - \frac{1}{2^i} \right]
$$

or

$$
I_i \approx Q_i + \frac{1}{2^i - 1} [Q_i - S_i].
$$

Note that (5.7) is one step of Richardson’s extrapolation. In fact, similar to Appendix ??, we can show that

$$
I_i = S_i + \beta_1 h_i^4 + \beta_2 h_i^6 + \cdots
$$

and

$$
I_i = Q_i + \beta_1 \left( \frac{h_i}{2} \right)^4 + \beta_2 \left( \frac{h_i}{2} \right)^6 + \cdots
$$

and

$$
I_i = Q_i + \frac{1}{2^i - 1} [Q_i - S_i] + O(h_i^6).$$
Therefore, the basic task of a typical routine is to bisect each subinterval until the following inequality is satisfied
\[ \frac{|S_i - Q_i|}{2^4 - 1} \leq \frac{h_i}{b - a} \epsilon \]
where \( \epsilon \) is the user specified tolerance. To see this, let
\[
Q = \sum_{i=0}^{N-1} Q_i, \\
I = \sum_{i=0}^{N-1} I_i = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx.
\]
Thus,
\[
\left| Q - \int_a^b f(x)dx \right| = \left| \sum_{i=0}^{N-1} (Q_i - I_i) \right| \\
\leq \sum_{i=0}^{N-1} |Q_i - I_i| \\
\approx \sum_{i=0}^{N-1} \frac{1}{2^4 - 1}|Q_i - S_i| \\
\leq \frac{\epsilon}{b - a} \sum_{i=0}^{N-1} h_i = \epsilon,
\]
which is the desired goal!

In this example we have assumed that the routine is using an absolute error criterion
\[
\left| Q - \int_a^b f(x)dx \right| \leq \epsilon.
\]
It is usually preferable to use the relative error tolerance
\[
\frac{\left| Q - \int_a^b f(x)dx \right|}{\int_a^b |f(x)|dx} \leq \sigma.
\]

Finally, we would like to note that it is not difficult to construct a function \( f(x) \) for which a given adaptive quadrature routine fails. For example, the above adaptive Simpson’s rule fails for the integral
\[
I = \int_a^b f(x)dx, \quad f(x) = x^2(x - 1)^2(x - 2)^2(x - 3)^2(x - 4)^2.
\]
In this case, \( P_1 = 0 \), and both \( P_{11} = 0 \) and \( P_{12} = 0 \) because \( f(x) \) has roots at \( x = 0, 1, 2, 3, \) and \( 4 \). And since \( P_1 = P_{11} + P_{12} = 0 \), the quadrature rule will assume the answer to be accurate!

5.6 Some Difficulties in Numerical Integration

Discontinuous functions. When \( f(x) \) is is a discontinuity at the point \( c \) lying within the interval \([a, b]\), we can split the integral as shown below
\[
\int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx.
\]
Example 5.3 Compute the integral \( I = \int_0^1 f(x)dx \) for the pulse function
\[
f(x) = \begin{cases} 
1 & x \geq 1/3 \\
-1 & x < 1/3
\end{cases}
\]
Without splitting, the adaptive Simpson’s procedure converges slowly:

\[
P_1 = 2/3, \quad P_{11} = -1/3, \quad P_{12} = 1/2, \quad P_1 \neq P_{11} + P_{12},
\]
and

\[
P_{111} = 1/4, \quad P_{112} = 1/6, \quad P_{11} \neq P_{111} + P_{112}, \quad \ldots
\]
and so on. On the other hand, we get immediate convergence by splitting the integral

\[
I = \int_a^{1/3} f(x)dx + \int_{1/3}^1 f(x)dx.
\]

Integration over infinite interval. When the range of integration is infinite, i.e.,

\[ I = \int_a^\infty f(x)dx, \quad a > 0. \]

we can resort to change of variables. Let \( y = \frac{1}{x} \), then

\[ I = \int_0^{1/a} f \left( \frac{1}{y} \right) \frac{dy}{y^2}. \]

**Example 5.4** Compute the infinite integral

\[ I = \int_1^\infty \frac{e^{-x}}{x}dx. \]

Let \( y = \frac{1}{x} \); then \( x = 1 \Rightarrow y = 1 \), and \( x = \infty \Rightarrow y = 0 \). Moreover, \( dx = -\frac{dy}{y^2} \). Hence,

\[ I = \int_0^1 e^{-1/y} \frac{dy}{y} = \int_0^1 g(y)dy, \]

where we can easily evaluate \( g(y) \) for any \( y > 0 \). For \( y = 0 \) we see that

\[ \lim_{y \to 0} \frac{e^{-1/y}}{y} = \lim_{y \to 0} \frac{1}{y(1 + y^{-1} + \frac{1}{2!}y^{-2} + \ldots)} = 0. \]

\[ \square \]

**Singularity.** Singularity at a point \( c \in [a,b] \) is tackled as follows: We split the function into two parts

\[ I = \int_a^b f(x)dx = \int_a^b f_1(x)dx + \int_a^b f_2(x)dx, \]

where \( f_1(x) \) is smooth and can be integrated using an adaptive procedure, and \( f_2(x) \) contains the singularity but can be integrated analytically.

**Example 5.5** Compute the integral

\[ I = \int_0^1 \frac{\cos x}{\sqrt{x}}dx \]

which has a singularity at \( x = 0 \).

Clearly, the function can be split as follows

\[ \frac{\cos x}{\sqrt{x}} = \frac{\cos x - 1}{\sqrt{x}} + \frac{1}{\sqrt{x}} = f_1(x) + f_2(x). \]

Even though \( f_2(x) \) has a singularity at \( x = 0 \), its integral can be obtained analytically,

\[ \int_0^1 f_2(x)dx = \int_0^1 \frac{1}{\sqrt{x}}dx = 2. \]

Integral of \( f_1(x) \) can now be handled by an adaptive quadrature routine provided we observe that

\[ \lim_{x \to 0} \frac{\cos x - 1}{\sqrt{x}} = \lim_{x \to 0} \frac{1}{\sqrt{x}} \left[ -1 + \left( 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots \right) \right] \]

\[ = \lim_{x \to 0} \left[ -\frac{x^{3/2}}{2!} + \frac{x^{7/2}}{4!} - \frac{x^{11/2}}{6!} + \ldots \right] \]

\[ = 0, \]

and in the neighborhood of \( x = 0 \), \( \cos x - 1 \simeq -\frac{x^2}{2} \).

\[ \square \]
5.7 Appendix: Numerical Integration

We wish to show that the truncation error in trapezoidal rule is given by the following

\[ I\{f\} = \int_a^b f(x)dx = T(h) + \alpha_1 h^2 + \alpha_2 h^4 + \alpha_3 h^6 + \cdots \]

where

\[ T(h) = \frac{h}{2} \left[ f_0 + 2 \sum_{i=1}^{N-1} f_i + f_N \right], \quad h = \frac{b-a}{N}. \]
Consider the panel \([x_i, x_{i+1}]\) with the midpoint \(y_i = (x_i + x_{i+1})/2\). Then

\[
f(x) = f(y_i) + (x - y_i)f'(y_i) + \frac{(x - y_i)^2}{2!}f''(y_i) + \frac{(x - y_i)^3}{3!}f'''(y_i) + \cdots
\]

Observing that

\[
\int_{x_i}^{x_{i+1}} (x - y_i)^m dx = \begin{cases} 
  h & m = 0 \\
  0 & m = 1 \\
  \frac{h^2}{2} & m = 2 \\
  \frac{h^3}{3!} & m = 3 \\
  \frac{h^4}{4!} & m = 4
\end{cases}
\]

where \(h = x_{i+1} - x_i\), then

\[
\int_{x_i}^{x_{i+1}} f(x)dx = hf(y_i) + \frac{h^3}{24}f''(y_i) + \frac{h^5}{1920}f^{(iv)}(y_i) + \cdots
\]

(5.8)

However,

\[
f(x_i) = f(y_i) - \frac{h}{2}f'(y_i) + \frac{h^2}{8}f''(y_i) - \frac{h^3}{48}f'''(y_i) + \frac{h^4}{384}f^{(iv)}(y_i) - \cdots
\]

\[
f(x_{i+1}) = f(y_i) + \frac{h}{2}f'(y_i) + \frac{h^2}{8}f''(y_i) + \frac{h^3}{48}f'''(y_i) + \frac{h^4}{384}f^{(iv)}(y_i) + \cdots
\]

Hence,

\[
T_i = \frac{h}{2}[f(x_i) + f(x_{i+1})] = hf(y_i) + \frac{h^3}{8}f''(y_i) + \frac{h^5}{384}f^{(iv)}(y_i) + \cdots
\]

Substituting in (5.7), we obtain

\[
\int_{x_i}^{x_{i+1}} f(x)dx = T_i - \frac{h^3}{12}f''(y_i) - \frac{h^5}{480}f^{(iv)}(y_i) - \cdots
\]

Consequently,

\[
\int_a^b f(x)dx = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} f(x)dx
\]

\[
= T(h) - \frac{h^2}{12}(b - a)f''(\eta_1) - \frac{h^4}{480}(b - a)f^{(iv)}(\eta_2) \cdots
\]

in which \(a < \eta_1, \eta_2 < b\). In other words,

\[
I\{f\} = T(h) + \alpha_1 h^2 + \alpha_2 h^4 + \cdots
\]