then the quadrature formulae are of the "closed type", otherwise they are the "open type".

11.2 THE TRAPEZOIDAL RULE WITH ERROR TERM

One of the simplest ways to estimate an integral $I = \int_a^b f(x)dx$ is to employ linear interpolation, i.e., to approximate the curve $y = f(x)$ by a straight line $y = P_1(x)$ passing through the points $(a, f(a))$ and $(b, f(b))$ and then to compute the area under the line (see Fig. 11.1).

Let $x_0 = a$, $x_1 = b$, and $h = b - a$. To approximate

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx,$$

we use the formula (11.4) for $n = 1$

$$\int_{x_0}^{x_1} P_1(x)dx = \int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right] dx$$

$$= \frac{-f(x_0)}{h} \int_{x_0}^{x_1} (x - x_1)dx + \frac{f(x_1)}{h} \int_{x_0}^{x_1} (x - x_0)dx.$$

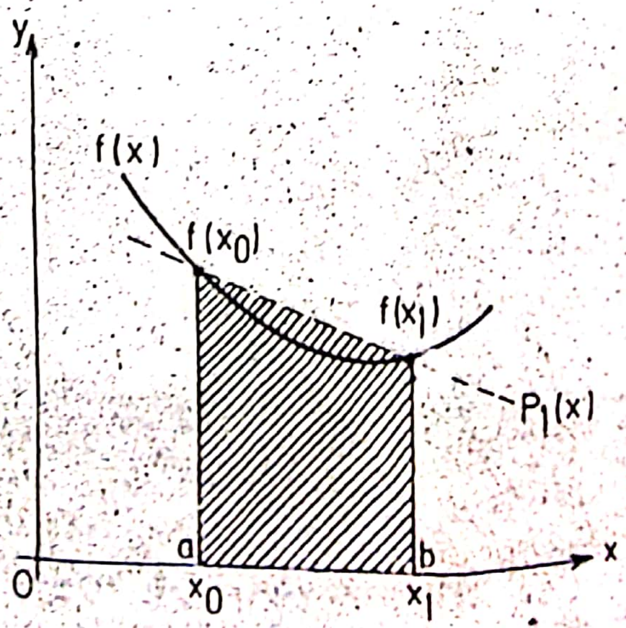

Fig. 11.1 The Trapezoidal Rule

Using the change of variable $x = x_0 + th$, we obtain

$$\int_{x_0}^{x_1} p_1(x)dx = -hf(x_0)\int_0^1 (t-1)dt + hf(x_1)\int_0^1 tdt = \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$

The quadrature formula

$$\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}\left[f(x_0) + f(x_1)\right] \qquad (11.5)$$

is called the **trapezoidal rule** or **trapezoidal formula.**

Let us calculate the error term involved in the quadrature formula (11.5).

Since $(x-x_0)(x-x_1)$ is always negative on (x_0,x_1), Theorem 11.2 implies that, for $f\in C^2[x_0,x_1]$, there is a $\xi\in[x_0,x_1]$ such that

$$E_2(f) = \frac{f''(\xi)}{2!}\int_{x_0}^{x_1} (x - x_0)(x - x_1)dx.$$

After using the change of variable $x = x_0 + ht$ and integrating, we have

$$E_2(f) = -\frac{h^3}{12} f''(\xi).$$

Thus the **trapezoidal rule with error term** is

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^3}{12} f''(\xi). \qquad (11.6)$$

The trapezoidal rule is exact if $f(x)$ is linear, since in this situation the second and higher order derivatives are zero.

EXAMPLE 11.1: Evaluate $I = \int_0^1 (x + 1)dx$

using the trapezoidal rule.

SOLUTION: $I = \int_0^1 (x + 1)dx = 3/2$.

By the trapezoidal rule

$$\int_0^1 (x + 1)dx = \frac{(1-0)}{2}\left[f(0) + f(1)\right] = \frac{1}{2}(1 + 2) = \frac{3}{2}.$$

Hence trapezoidal rule is exact when $f(x)$ is linear.

EXAMPLE 11.2: Evaluate $I = \int_0^1 3x^2dx$

using the trapezoidal rule. Compare with the correct value of the integral.

SOLUTION: $I = \int_0^1 3x^2dx = 1.$

By the trapezoidal rule, we have

$$\int_0^1 3x^2dx \approx \frac{(1-0)}{2}\left[f(0) + f(1)\right] = \frac{1}{2}(0 + 3) = 1.5.$$

Thus

Actual error $= 1 - 1.5 = -0.5.$

The following theorem is stated (without proof) for the quadrature formulae with equally spaced points for the improvement of error.

THEOREM 11.3: Let $x_0 = a$, $x_n = b$, and $h = \frac{b-a}{n}$. There exists a point $\xi \in [a,b]$ such that

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!}\int_0^n t(t-1)\ldots(t-n)dt \qquad (11.7)$$

if n is odd and $f \in C^{n+1}[a,b]$, and

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!}\int_0^n t^2(t-1)\ldots(t-n)dt \qquad (11.8)$$

if n is even and $f \in C^{n+2}[a,b]$.

In Theorem 11.3, note that, when n is an even integer, the degree of precision is (n+1) although the interpolation polynomial is of degree at most n. When n is odd, the degree of precision is only n. Consequently, if n is even and more points are to be added to increase precision, no accuracy is gained by adding only one point and points should be added in multiples of two.

11.3 SIMPSON'S 1/3 RULE WITH ERROR TERM

The trapezoidal rule tries to simplify integration by approximating the function to be integrated by a straight line or a series of straight line segments. In Simpson's rule we try to approximate by a series of parabolic segments, hoping that the parabola will more closely match a given curve f(x), than would the straight line in the trapezoidal rule. To estimate $I = \int_a^b f(x)$, the curve $y=f(x)$, is approximated by a parabola $y = P_2(x)$ passing through three points $(x_0,f(x_0))$, $(x_1,f(x_1))$, $(x_2,f(x_2))$ and then the area under the parabolic segments is computed (see Fig.11.2).

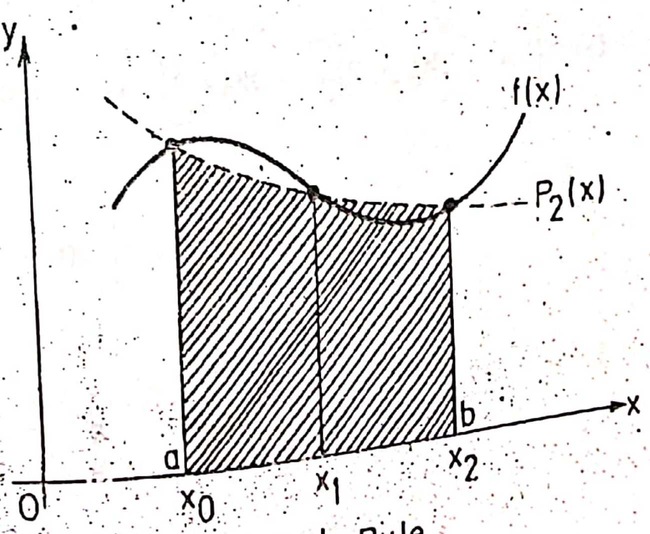

Fig.11.2 Simpson's Rule

Let $x_0 = a$, $h = \frac{b-a}{2}$ so that $x_1 = x_0 + h$, $x_2 = x_0 + 2h = b$.

Then

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx.$$

Applying formula (11.4), we obtain for $n = 2$;

$$\int_{x_0}^{x_2} P_2(x)dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)\right] dx$$

$$= \frac{f(x_0)}{2h^2} \int_{x_0}^{x_2} (x-x_1)(x-x_2)dx - \frac{f(x_1)}{h^2} \int_{x_0}^{x_2} (x-x_0)(x-x_2)dx + \frac{f(x_2)}{2h^2} \int_{x_0}^{x_2} (x-x_0)(x-x_1)dx.$$

Substituting $x = x_0 + th$; then $dx = h\,dt$, we get

$$\int_{x_0}^{x_2} P_2(x)dx = \frac{h}{2} f(x_0)\int_0^2 (t-1)(t-2)dt - hf(x_1)\int_0^2 t(t-2)dt + \frac{h}{2} f(x_2)\int_0^2 t(t-1)dt$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

This quadrature formula

$$\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] \tag{11.9}$$

is called Simpson's 1/3 rule.

If $f \in C^{(4)}[x_0, x_2]$, the Theorem 11.3 (Eq.11.2) implies that there exists a point $\xi \in [x_0, x_2]$ such that

$$E_3(f) = \frac{h^5 f^{(4)}(\xi)}{4!}\int_0^2 t^2(t-1)(t-2)dt$$

$$= -\frac{h^5 f^{(4)}(\xi)}{90}.$$

Thus, Simpson's 1/3 rule with error term is

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] - \frac{h^5 f^{(4)}(\xi)}{90} \tag{11.10}$$

11.4 SIMPSON'S 3/8 RULE WITH ERROR TERM

Let $x_0 = a$, $h = \frac{b-a}{3}$ so that $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, $x_3 = x_0 + 3h = b$.

We have

$$\int_a^b f(x)dx = \int_{x_0}^{x_3} f(x)dx.$$

For $n = 3$, we get from the formula (11.4)

$$\int_{x_0}^{x_3} P_3(x)dx = \int_{x_0}^{x_3}\left[\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f(x_0) + \right.$$

$$\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f(x_1) +$$

$$\left.\frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)}f(x_2) + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)}f(x_3)\right]dx$$

$$\int_{x_0}^{x_3} P_3(x)dx = -\frac{f(x_0)}{6h^3}\int_{x_0}^{x_3}(x - x_1)(x - x_2)(x - x_3)dx +$$

$$\frac{f(x_1)}{2h^3}\int_{x_0}^{x_3}(x - x_0)(x - x_2)(x - x_3)dx -$$

$$\frac{f(x_2)}{2h^3}\int_{x_0}^{x_3}(x - x_0)(x - x_1)(x - x_3)dx +$$

$$\frac{f(x_3)}{6h^3}\int_{x_0}^{x_3}(x - x_0)(x - x_1)(x - x_2)dx.$$

Using the change of variable $x = x_0 + ht$, we get

$$\int_{x_0}^{x_3} P_3(x)dx = \frac{-hf(x_0)}{6}\int_0^3 (t-1)(t-2)(t-3)dt + \frac{hf(x_1)}{2}\int_0^3 t(t-2)(t-3)dt$$

$$-\frac{hf(x_2)}{2}\int_0^3 t(t-1)(t-3)dt + \frac{hf(x_3)}{6}\int_0^3 t(t-1)(t-2)dt$$

$$= \frac{hf(x_0)}{6}\frac{9}{4} + \frac{hf(x_1)}{2}\frac{9}{4} - \frac{hf(x_2)}{2}\left(\frac{-9}{4}\right) + \frac{hf(x_3)}{6}\frac{9}{4}$$

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

The integration formula

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3}{8} h\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \qquad (11.11)$$

is called **Simpson's 3/8 rule.**

The Theorem 11.3 (Eq. 11.7) implies that, for $f\epsilon C^4[x_0,x_3]$, there exists a point $\xi\epsilon[x_0,x_3]$ such that

$$E_4(f) = \frac{h^5 f^{(4)}(\xi)}{4!} \int_0^3 t(t-1)(t-2)(t-3)dt$$

$$= \frac{h^5 f^{(4)}(\xi)}{24} \int_0^3 (t^4 - 6t^3 + 11t^2 - 6t)dt$$

$$= -\frac{3}{80} h^5 f^{(4)}(\xi).$$

Thus

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] - \frac{3}{80}h^5 f^{(4)}(\xi) \qquad (11.12)$$

is called **Simpson's 3/8 rule with error term.**

The rules (11.9) and (11.11) are exact for all polynomials of degree three or less as their error terms involve 4th derivative of f(x) which vanish identically.

EXAMPLE 11.3: Use the trapezoidal and Simpson's rules to estimate the integral

$$\int_1^3 f(x)dx = \int_1^3 (x^3 - 2x^2 + 7x - 5)dx.$$

SOLUTION:

$$\int_1^3 f(x)dx = \int_1^3 (x^3 - 2x^2 + 7x - 5)dx.$$

$$= \left[\frac{x^4}{4} - \frac{2x^3}{3} + \frac{7x^2}{2} - 5x\right]_1^3 = 20\frac{2}{3}.$$

For the trapezoidal rule (11.6), $x_0 = 1$, $x_1 = 3$ so that $h = 3 - 1 = 2$,

$$\int_1^3 f(x)dx = \frac{h}{2}\left[f(1) + f(3)\right] - \frac{h^3}{12}f''(\xi)$$

$$= \frac{2}{2}[1 + 25] - \frac{2}{3}f''(\xi) = 26 - \frac{2}{3}f''(\xi).$$

Since $f''(x) = 6x - 4$, the error is given by

$$\frac{-2}{3}f''(\xi) = -\frac{2}{3}(6\xi - 4), \ \xi\in[1,3]$$

which has an extreme value $-9\frac{1}{3}$ for $\xi = 3$.

The actual error $= 20\frac{2}{3} - 26 = -5\frac{1}{3}$, which is smaller than the bound as expected, but still quite large.

For Simpson's $\frac{1}{3}$ rule (11.10), $x_0 = 1$; $h = \frac{3-1}{2} = 1$, $x_1 = 2$, $x_2 = 3$,

$$\int_1^3 f(x)dx = \frac{h}{3}\left[f(1) + 4f(2) + f(3)\right] - \frac{h^5}{90}f^{(4)}(\xi)$$

$$= \frac{1}{3}[1 + 4\times 9 + 25] - \frac{1}{90}f^{(4)}(\xi) = 20\frac{2}{3} - \frac{1}{90}f^{(4)}(\xi).$$

Since the fourth derivative of $f(x)$ vanishes for all x, the error term vanishes and the result is exact.

For Simpson's $\frac{3}{8}$ rule, $x_0 = 1$, $h = \frac{3-1}{3} = \frac{2}{3}$, $x_1 = \frac{5}{3}$, $x_2 = \frac{7}{3}$, $x_3 = 3$,

$$\int_1^3 f(x)dx = \frac{3}{8}h\left[f(1) + 3f(\tfrac{5}{3}) + 3f(\tfrac{7}{3}) + f(3)\right] - \frac{3}{80}h^5 f^{(4)}(\xi)$$

$$= \frac{3}{8}\times\frac{2}{3}\left[1 + 3\times\frac{155}{27} + 3\times\frac{355}{27} + 25\right] - \frac{3}{80}(\tfrac{2}{3})^5 f^{(4)}(\xi)$$

$$= \frac{1}{4}\left[\frac{9 + 155 + 355 + 225}{9}\right] - \frac{3}{80}(\tfrac{2}{3})^5 f^{(4)}(\xi)$$

$$= \frac{1}{4}(\frac{744}{9}) - \frac{3}{80}(\tfrac{2}{3})^5 f^{(4)}(\xi) = 20\frac{2}{3} - \frac{3}{80}(\tfrac{2}{3})^5 f^{(4)}(\xi).$$

The result is exact again as the 4th derivative of f(x) vanishes identically.

11.5 ERROR ESTIMATION

Before proceeding further we will consider an easy way to estimate the error involved in the quadrature formulae.

The trapezoid rule (11.5), for example, is exact if f(x) is linear. If this is not the case, however, there will be an error which is about $\frac{-h^3}{12} f''(\xi)$. The value of ξ at which $f''(\xi)$ should be evaluated is not known, except that it lies within the range of integration. This expression can thus only be used to determine an upper bound for the error and then only if we have an exact or approximate expression for f(x). We do learn, however, that the error is approximately proportional to h^3.

If we confine ourselves to an examination of quadrature formulae with equally spaced points, the accuracy of the quadrature formula, in this case, is mainly characterized by the order of the error term.

$$E_{n+1}(f) = O(h^m) \tag{11.13}$$

where

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

is the spacing (n is the number of divisions) and m is a natural number. For example, for the trapezoidal rule (Sec. 11.2) we have

$$E_2(f) = -\frac{h^3}{12} f''(\xi) = -\frac{b - a}{12} h^2 f''(\xi)$$

and so m = 2 giving the relation

$$E_2(f) = O(h^2).$$

That is, the trapezoidal rule is a 2nd order approximation process. For Simpson's rule (Sec. 11.3) we have

$$E_3(f) = -\frac{b - a}{180} h^4 f^{(4)}(\xi)$$

and hence $m = 4$. Thus $E_3(f) = O(h^4)$,

that is, the Simpson's rule is a fourth order process.

EXAMPLE 11.4: Find the upper bound for error term in the trapezoidal rule for the integral

$$I = \int_1^2 \left(\frac{e^{-x}}{x}\right) dx.$$

SOLUTION: We have

$$E_2(f) = -\frac{h^3}{12} f''(\xi).$$

Also

$$f(x) = \frac{e^{-x}}{x}, \quad f'(x) = -\left(\frac{1}{x} + \frac{1}{x^2}\right)e^{-x}, \quad f''(x) = \left(\frac{1}{x} + \frac{2}{x^2} + \frac{2}{x^3}\right)e^{-x}.$$

The second derivative attains its maximum value on $[1,2]$ at $x = 1$; hence we can take

$$M_2 = \max_{x \in [1,2]} f''(x) = f''(1) = 5e^{-1} \approx 1.84.$$

Thus error bound $= \frac{h^3}{12} M_2 = \frac{1}{12}(1.84) = 0.1533$.

EXERCISE 11.1

1. The integral $\int_0^{\pi} \sin x \, dx$ is evaluated by interpolating the function $f(x) = \sin x$ at the points $x = 0$ and $x = \pi$. Calculate the bound for the error and compare it with the actual error.

2. Use the trapezoidal and Simpson's 1/3 rules to approximate $\int_0^{\pi/2} \sin^2 x \, dx$. Find a maximum bound for the error in each case. Compare your approximations with the actual result.

3. Approximate $\int_0^1 x^{1/3} dx$, using the trapezoidal and Simpson's 1/3 rules. Compare the approximations with the actual value.

4. Approximate $\int_1^2 \ln x \, dx$, using the trapezoidal and Simpson's rules. Compare the approximations with the actual value.

5. Use the table below to find an approximation to

$$\int_{1.1}^{1.5} e^x \, dx, \text{ using:}$$

a) The trapezoidal rule with $x_0 = 1.1$, and $x_1 = 1.5$;

b) Simpson's rule with $x_0 = 1.1$, $x_1 = 1.3$, and $x_2 = 1.5$.

x	1.1	1.3	1.5
e^x	3.0042	3.6693	4.4817

6. Show that the trapezoidal rule yields for n > 1 the exact value of the integrals

$$\int_0^{2\pi} \cos x \, dx, \int_0^{2\pi} \sin x \, dx.$$

7. Consider the computation of $I = \int_a^b f(x)dx$, and suppose that I_1, and I_2 denote the estimates of I obtained using Simpson's 1/3 and 3/8 rules, respectively, with step sizes $h_1 = (b - a)/2$ and $h_2 = (b - a)/3$, respectively.

a) Show that (subject to appropriate assumptions concerning the truncation errors) a better estimate of I is given by

$$I^* \approx \frac{9}{5} I_2 - \frac{4}{5} I_1.$$

b) If $f(x)=x^{-2}$, a=1 and b=3, find the values of I_1, I_2 and I^*. What are the percentage errors in the three values?

8. Approximate the integral $\int_1^2 \frac{1}{x} dx$, using the trapezoidal rule and Simpson's rule.