Again, using Eq. (7.30), we obtain

$$F_2\left(\frac{h}{2^2}\right) = \frac{4^2 F_1\left(\frac{h}{2^2}\right) - F_1\left(\frac{h}{2}\right)}{4^2 - 1} = 400.00195 \tag{5}$$

The above computation can be summarized in the following table:

h	F	F_1	F_2
0.0128	428.0529		
		399.5327	
0.0064	406.6627		400.00195
		399.9726	
0.0032	401.6452		

Thus, after two steps, it is found that $y'(0.05) = 400.00195$ while the exact value is

$$y'(0.05) = \left(\frac{1}{x^2}\right)_{x=0.05} = \frac{1}{0.0025} = 400$$

7.5 NUMERICAL INTEGRATION

Consider the definite integral

$$I = \int_{x=a}^{b} f(x)\, dx \tag{7.31}$$

where $f(x)$ is known either explicitly or is given as a table of values corresponding to some values of x, whether equispaced or not. Integration of such functions can be carried out using numerical techniques. Of course, we assume that the function to be integrated is smooth and Riemann integrable in the interval of integration. In the following section, we shall develop Newton–Cotes formulae based on interpolation which form the basis for trapezoidal rule and Simpson's rule of numerical integration.

7.6 NEWTON–COTES INTEGRATION FORMULAE

In this method, as in the case of numerical differentiation, we shall approximate the given tabulated function, by a polynomial $P_n(x)$ and then integrate this polynomial. Suppose, we are given the data (x_i, y_i), $i = 0\,(1)\,n$, at equispaced points with spacing $h = x_{i+1} - x_i$, we can represent the polynomial by any standard interpolation polynomial. Suppose, we use Lagrangian approximation given by Eq. (6.45), then we have

$$f(x) \approx \sum L_k(x) y(x_k) \tag{7.32}$$

with associated error given by

$$E(x) = \frac{\Pi(x)}{(n+1)!} y^{(n+1)}(\xi) \tag{7.33}$$

where

$$L_k(x) = \frac{\Pi(x)}{(x - x_k)\Pi'(x_k)} \tag{7.34}$$

and

$$\Pi(x) = (x - x_0)\,(x - x_1)\,\ldots\,(x - x_n) \tag{7.35}$$

Then, we obtain an equivalent integration formula to the definite integral (7.31) in the form

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{n} c_k\,y(x_k) \tag{7.36}$$

where c_k are the weighting coefficients given by

$$c_k = \int_a^b L_k(x)\,dx \tag{7.37}$$

which are also called *Cotes numbers*. Let the equispaced nodes are defined by

$$x_0 = a, \qquad x_n = b, \qquad h = \frac{b-a}{n}, \qquad x_k = x_0 + kh$$

so that $x_k - x_1 = (k-1)\,h$ etc. Now, we shall change the variable x to p such that, $x = x_0 + ph$, then we can rewrite Eqs. (7.35) and (7.34) respectively as

$$\Pi(x) = h^{n+1}p(p-1)\,.\,.\,.\,(p-n) \tag{7.38}$$

and

$$L_k(x) = \frac{(x-x_0)(x-x_1)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)(x_k-x_1)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)}$$

$$= \frac{(ph)(p-1)h\cdots(p-k+1)\,h\,(p-k-1)h\cdots(p-n)h}{(kh)(k-1)h\cdots(1)\,h\,(-1)h\cdots(k-n)h}$$

or

$$L_k(x) = (-1)^{(n-k)}\,\frac{p(p-1)\cdots(p-k+1)(p-k-1)\cdots(p-n)}{k\,!(n-k)!} \tag{7.39}$$

Also, noting that $dx = h\,dp$. The limits of the integral in Eq. (7.37) change from 0 to n and Eq. (7.37) reduces to

$$c_k = \frac{(-1)^{n-k}\,h}{k\,!(n-k)\,!}\int_0^n p(p-1)\,\ldots\,(p-k+1)(p-k-1)\,\ldots\,(p-n)dp \tag{7.40}$$

The error in approximating the integral (7.36) can be obtained by substituting (7.38) into Eq. (7.33) in the form

$$E_n = \frac{h^{n+2}}{(n+1)!} \int_0^n p(p-1)\cdots(p-n)y^{(n+1)}(\xi)\, dp \tag{7.41}$$

where $x_0 < \xi < x_n$. For illustration, let us consider the cases for $n = 1, 2$. From Eq. (7.40), we get

$$c_0 = -h\int_0^1 (p-1)\, dp = \frac{h}{2}, \qquad c_1 = h\int_0^1 p\, dp = \frac{h}{2}$$

and Eq. (7.41) gives

$$E_1 = \frac{h^3}{2} y''(\xi) \int_0^1 p(p-1)\, dp = -\frac{h^3}{12} y''(\xi)$$

Thus, the integration formula corresponding to integral (7.36) is found to be

$$\int_{x_0}^{x_1} f(x)\, dx = c_0 y_0 + c_1 y_1 + \text{Error} = \frac{h}{2}(y_0 + y_1) - \frac{h^3}{12} y''(\xi) \tag{7.42}$$

This equation represents the Trapezoidal rule in the interval $[x_0, x_1]$ with error term. Geometrically, it represents an area between the curve $y = f(x)$, the x-axis and the ordinates erected at $x = x_0\,(=a)$ and $x = x_1$ as shown in Fig. 7.2. This area is approximated by the trapezium formed by replacing the curve with its secant line drawn between the end points (x_0, y_0) and (x_1, y_1).

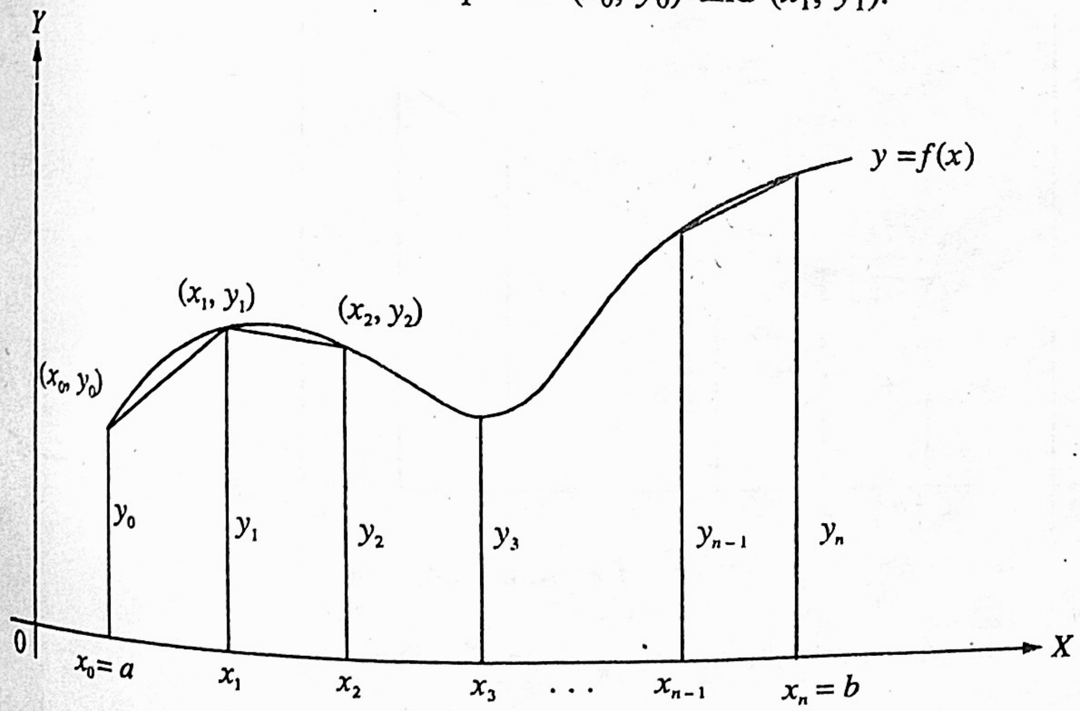

Fig. 7.2 Trapezoidal rule.

For $n = 2$, Eq. (7.40) gives

$$c_0 = \frac{h}{2}\int_0^2 (p-1)(p-2)\, dp = \frac{h}{3}$$

$$c_1 = -h\int_0^2 p(p-2)\,dp = \frac{4}{3}h$$

$$c_2 = \frac{h}{2}\int_0^2 p(p-1)\,dp = \frac{h}{3}$$

and the error term is given by

$$E_2 = -\frac{h^5}{90}y^{(iv)}(\xi)$$

Thus, for $n = 2$, the integration (7.36) takes the form

$$\int_{x_0}^{x_2} f(x)\,dx = c_0 y_0 + c_1 y_1 + c_2 y_2 + \text{Error}$$

$$= \frac{h}{3}(y_0 + 4y_1 + y_2) - \frac{h^5}{90}y^{(iv)}(\xi) \tag{7.43}$$

This is known as *Simpson's 1/3 rule*. Geometrically, this equation represents the area between the curve $y = f(x)$, the x-axis and the ordinates at $x = x_0$ and x_2 after replacing the arc of the curve between (x_0, y_0) and (x_2, y_2) by an arc of a quadratic polynomial as shown in Fig. 7.3. Thus Simpson's 1/3 rule is based on fitting three points with a quadratic.

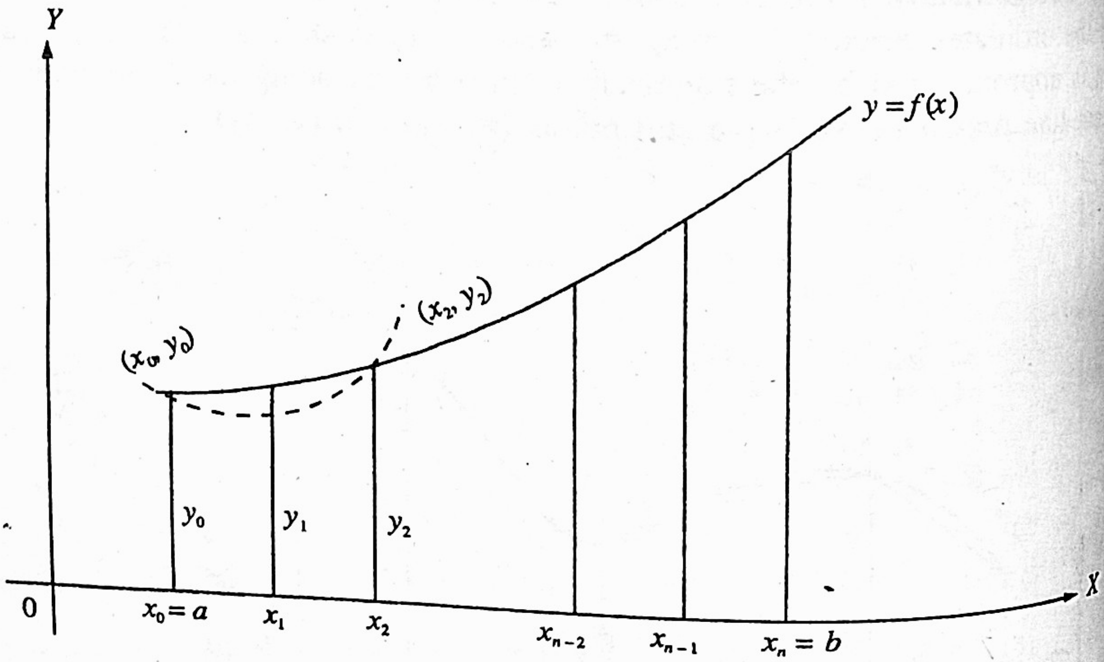

Fig. 7.3 Simpson's rule.

Similarly, for $n = 3$, the integration (7.36) is found to be

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{8}h(y_0 + 3y_1 + 3y_2 + y_3) - \frac{3}{80}h^5 y^{(iv)}(\xi) \tag{7.44}$$

This is known as *Simpson's 3/8 rule*, which is based on fitting four points by a cubic. Still higher order Newton–Cotes integration formulae can be derived for large values of n. But for all practical purposes, Simpson's 1/3 rule is found to be sufficiently accurate.

7.6.1 The Trapezoidal Rule (Composite Form)

The Newton–Cotes formula (7.42) is based on approximating $y = f(x)$ between (x_0, y_0) and (x_1, y_1) by a straight line, thus forming a trapezium, is called *trapezoidal rule*. In order to evaluate the definite integral

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

we divide the interval $[a, b]$ into n sub-intervals, each of size $h = (b - a)/n$ and denote the sub-intervals by $[x_0, x_1], [x_1, x_2], \ldots, [x_{n-1}, x_n]$, such that $x_0 = a$ and $x_n = b$ and $x_k = x_0 + kh$, $k = 1, 2, \ldots, n - 1$. Thus, we can write the above definite integral as a sum. Therefore,

$$I = \int_{x_0}^{x_n} f(x)\, dx = \int_{x_0}^{x_1} f(x)\, dx + \int_{x_1}^{x_2} f(x)\, dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\, dx \tag{7.45}$$

As shown in Fig. 7.2, the area under the curve in each sub-interval is approximated by a trapezium. The integral I, which represents an area between the curve $y = f(x)$, the x-axis and the ordinates at $x = x_0$ and $x = x_n$ is obtained by adding all the trapezoidal areas in each sub-interval.

Now, using the trapezoidal rule as expressed in Eq. (7.42) into Eq. (7.45), we get

$$\int_{x_0}^{x_n} f(x)\, dx = \frac{h}{2}(y_0 + y_1) - \frac{h^3}{12} y''(\xi_1) + \frac{h}{2}(y_1 + y_2) - \frac{h^3}{12} y''(\xi_2)$$
$$+ \cdots + \frac{h}{2}(y_{n-1} + y_n) - \frac{h^3}{12} y''(\xi_n) \tag{7.46}$$

where $x_{k-1} < \xi_k < x_k$, for $k = 1, 2, \ldots, n - 1$.

Thus, we arrive at the result

$$\int_{x_0}^{x_n} f(x)\, dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + E_n \tag{7.47}$$

where the error term E_n is given by

$$E_n = -\frac{h^3}{12}[y''(\xi_1) + y''(\xi_2) + \cdots + y''(\xi_n)] \tag{7.48}$$

Equation (7.47) represents the trapezoidal rule over $[x_0, x_n]$, which is also called the *composite form of the trapezoidal rule.*

The error term given by Eq. (7.48) is called the *global error*. However, if we assume that $y''(x)$ is continuous over $[x_0, x_n]$ then there exists some ξ in $[x_0, x_n]$ such that $x_n = x_0 + nh$ and

$$E_n = -\frac{h^3}{12}[ny''(\xi)] = -\frac{x_n - x_0}{12} h^2 y''(\xi) \tag{7.49}$$

Then the global error can be conveniently written as $O(h^2)$.

7.6.2 Simpson's Rules (Composite Forms)

In deriving Eq. (7.43), the Simpson's 1/3 rule, we have used two sub-intervals of equal width. In order to get a composite formula, we shall divide the interval of integration $[a, b]$ into an even number of sub-intervals say $2N$, each of width $(b-a)/2N$, thereby we have $x_0 = a, x_1, \ldots, x_{2N} = b$ and $x_k = x_0 + kh, k = 1, 2, \ldots, (2N-1)$. Thus, the definite integral I can be written as

$$I = \int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{2N-2}}^{x_{2N}} f(x)\,dx \tag{7.50}$$

Applying Simpson's 1/3 rule as in Eq. (7.43) to each of the integrals on the right-hand side of Eq. (7.50), we obtain

$$I = \frac{h}{3}[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + \cdots$$

$$+ (y_{2N-2} + 4y_{2N-1} + y_{2N})] - \frac{N}{90}h^5 y^{(iv)}(\xi)$$

That is,

$$\int_{x_0}^{x_{2N}} f(x)\,dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{2N-1})$$

$$+ 2(y_2 + y_4 + \cdots + y_{2N-2}) + y_{2N}] + \text{Error term} \tag{7.51}$$

This formula is called *composite Simpson's 1/3 rule*. The error term E, which is also called *global error*, is given by

$$E = -\frac{N}{90}h^5 y^{(iv)}(\xi) = -\frac{x_{2N} - x_0}{180}h^4 y^{(iv)}(\xi) \tag{7.52}$$

for some ξ in $[x_0, x_{2N}]$. Thus, in Simpson's 1/3 rule, the global error is of $O(h^4)$.

Similarly in deriving composite Simpson's 3/8 rule, we divide the interval of integration into n sub-intervals, where n is divisible by 3, and applying the integration formula (7.44) to each of the integral given below

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_3} f(x)\,dx + \int_{x_3}^{x_6} f(x)\,dx + \cdots + \int_{x_{n-3}}^{x_n} f(x)\,dx$$

we obtain the composite form of Simpson's 3/8 rule as

$$\int_a^b f(x)\,dx = \frac{3}{8}h[y(a) + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots$$

$$+ 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y(b)] \tag{7.53}$$

with the global error E given by

$$E = -\frac{x_n - x_0}{80}h^4 y^{(iv)}(\xi) \tag{7.54}$$

It may be noted from Eqs. (7.52) and (7.54), the global error in Simpson's 1/3 and 3/8 rules are of the same order. However, if we consider the magnitudes of the error terms, we notice that Simpson's 1/3 rule is superior to Simpson's 3/8 rule. For illustration, we consider few examples.

Example 7.6 Find the approximate value of

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

using (i) trapezoidal rule, (ii) Simpson's 1/3 rule by dividing the range of integration into six equal parts. Calculate the percentage error from its true value in both the cases.

Solution We shall at first divide the range of integration $(0, \pi)$ into six equal parts so that each part is of width $\pi/6$ and write down the table of values:

x	0	$\pi/6$	$\pi/3$	$\pi/2$	$2\pi/3$	$5\pi/6$	π
$y = \sin x$	0.0	0.5	0.8660	1.0	0.8660	0.5	0.0

Applying trapezoidal rule, we have

$$\int_0^{\pi} \sin x \, dx = \frac{h}{2}[y_0 + y_6 + 2(y_1 + y_2 + y_3 + y_4 + y_5)]$$

Here, h, the width of the interval is $\pi/6$. Therefore,

$$y = \int_0^{\pi} \sin x dx = \frac{\pi}{12}[0 + 0 + 2(3.732)] = \frac{3.1415}{6} \times 3.732 = 1.9540$$

Applying Simpson's 1/3 rule (7.41), we have

$$\int_0^{\pi} \sin x dx = \frac{h}{3}[y_0 + y_6 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)]$$

$$= \frac{\pi}{18}[0 + 0 + (4 \times 2) + (2)(1.732)] = \frac{3.1415}{18} \times 11.464 = 2.0008$$

But the actual value of the integral is

$$\int_0^{\pi} \sin x \, dx = [-\cos x]_0^{\pi} = 2$$

Hence, in the case of trapezoidal rule

$$\text{The percentage of error} = \frac{2 - 1.954}{2} \times 100 = 2.3$$

While in the case of Simpson's rule the percentage error is

$$\frac{2 - 2.0008}{2} \times 100 = 0.04 \qquad \text{(sign ignored)}$$

Example 7.7 From the following data, estimate the value of

$$\int_1^5 \log x \, dx$$

using Simpson's 1/3 rule. Also, obtain the value of h, so that the value of the integral will be accurate up to five decimal places.

x	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
$y = \log x$	0.0000	0.4055	0.6931	0.9163	1.0986	1.2528	1.3863	1.5041	1.6094

Solution We have from the data, $n = 0, 1, \ldots, 8$, and $h = 0.5$. Now using Simpson's 1/3 rule,

$$\int_1^5 \log x \, dx = \frac{h}{3}[y_0 + y_8 + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6)]$$

$$= \frac{0.5}{3}[(0 + 1.6094) + 4(4.0787) + 2(3.178)]$$

$$= \frac{0.5}{3}(1.6094 + 16.3148 + 6.356)$$

$$= 4.0467$$

The error in Simpson's rule is given by

$$E = \frac{x_{2N} - x_0}{180} h^4 y^{(iv)}(\xi) \qquad \text{(ignoring the sign)}$$

Since

$$y = \log x, \quad y' = \frac{1}{x}, \quad y'' = -\frac{1}{x^2}, \quad y''' = \frac{2}{x^3}, \quad y^{(iv)} = -\frac{6}{x^4}$$

$$\max_{1 \le x \le 5} y^{(iv)}(x) = 6, \qquad \min_{1 \le x \le 5} y^{(iv)}(x) = 0.0096$$

Therefore, the error bounds are given by

$$\frac{(0.0096)(4)h^4}{180} < E < \frac{(6)(4)h^4}{180}$$

If the result is to be accurate up to five decimal places, then

$$\frac{24h^4}{180} < 10^{-5}$$

That is, $h^4 < 0.000075$ or $h < 0.09$. It may be noted that the actual value of integral is

$$\int_1^5 \log x \, dx = [x \log x - x]_1^5 = 5 \log 5 - 4$$

Example 7.8 Evaluate the integral

$$I = \int_0^1 \frac{dx}{1+x^2}$$

using (i) trapezoidal rule, (ii) Simpson's 1/3 rule by taking $h = 1/4$. Hence, compute the approximate value of π.

Solution At first, we shall tabulate the function as

x	0	1/4	1/2	3/4	1
$y = \dfrac{1}{1+x^2}$	1	0.9412	0.8000	0.6400	0.5000

using trapezoidal rule, and taking $h = 1/4$

$$I = \frac{h}{2}[y_0 + y_4 + 2(y_1 + y_2 + y_3)] = \frac{1}{8}[1.5 + 2(2.312)] = 0.7828 \qquad (1)$$

using Simpson's 1/3 rule, and taking $h = 1/4$, we have

$$I = \frac{h}{3}[y_0 + y_4 + 4(y_1 + y_3) + 2y_2] = \frac{1}{12}[1.5 + 4(1.512) + 1.6] = 0.7854 \qquad (2)$$

But the closed form solution to the given integral is

$$\int_0^1 \frac{dx}{1+x^2} + [\tan^{-1} x]_0^1 = \frac{\pi}{4} \qquad (3)$$

Equating (2) and (3), we get $\pi = 3.1416$.

Example 7.9 Compute the integral

$$I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} \, dx$$

using Simpson's 1/3 rule, taking $h = 0.125$.

Solution At the outset, we shall construct the table of the function as required.

x	0	0.125	0.250	0.375	0.5	0.625	0.750	0.875	1.0
$y = \sqrt{\frac{2}{\pi}} e^{-x^2/2}$	0.7979	0.7917	0.7733	0.7437	0.7041	0.6563	0.6023	0.5441	0.4839

Using Simpson's 1/3 rule, we have

$$I = \frac{h}{3}[y_0 + y_8 + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6)]$$

$$= \frac{0.125}{3}[0.7979 + 0.4839 + 4(0.7917 + 0.7437 + 0.6563 + 0.5441)$$

$$+ 2(0.7733 + 0.7041 + 0.6023)]$$

$$= \frac{0.125}{3}(1.2818 + 10.9432 + 4.1594) = 0.6827$$

Hence, $I = 0.6827$.

Example 7.10 A missile is launched from a ground station. The acceleration during its first 80 seconds of flight, as recorded, is given in the following table:

t (s)	0	10	20	30	40	50	60	70	80
a (m/s^2)	30	31.63	33.34	35.47	37.75	40.33	43.25	46.69	50.67

compute the velocity of the missile when $t = 80$ s, using Simpson's 1/3 rule.

Solution Since acceleration is defined as the rate of change of velocity, we have

$$\frac{dv}{dt} = a \quad \text{or} \quad v = \int_0^{80} a\,dt$$

Using Simpson's 1/3-rule, we have

$$v = \frac{h}{3}[(y_0 + y_8) + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6)]$$

$$= \frac{10}{3}[(30 + 50.67) + 4(31.63 + 35.47 + 40.33 + 46.69)$$

$$+ 2(33.34 + 37.75 + 43.25)]$$

$$= 3086.1 \text{ m/s}$$

Therefore, the required velocity is given by $v = 3.0861$ km/s.

7.7 ROMBERG'S INTEGRATION

In Section 7.6, we have observed that the trapezoidal rule of integration of a definite integral is of $O(h^2)$, while that of Simpson's 1/3 and 3/8 rules are of fourth-order accurate. We can improve the accuracy of trapezoidal and Simpson's rules using Richardson's extrapolation procedure as described in Section 7.4, which is also called *Romberg's integration method*. For example, the error in trapezoidal rule of a definite integral

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