# Chapter 6

# Numerical Differentiation and Integration

## 6.1 INTRODUCTION

In Chapter 3, we were concerned with the general problem of interpolation, viz., given the set of values $(x_0, y_0)$, $(x_1, y_1)$, …, $(x_n, y_n)$ of $x$ and $y$, to find a polynomial $\phi(x)$ of the lowest degree such that $y(x)$ and $\phi(x)$ agree at the set of tabulated points. In the present chapter, we shall be concerned with the problems of numerical differentiation and integration. That is to say, given the set of values of $x$ and $y$, as above, we shall derive formulae to compute:

(i) $\dfrac{dy}{dx}, \dfrac{d^2y}{dx^2}, \cdots$ for any value of $x$ in $[x_0, x_n]$, and

(ii) $\displaystyle\int_{x_0}^{x_n} y\, dx.$

## 6.2 NUMERICAL DIFFERENTIATION

The general method for deriving the numerical differentiation formulae is to differentiate the interpolating polynomial. Hence, corresponding to each of the formulae derived in Chapter 3, we may derive a formula for the derivative. We illustrate the derivation with Newton's forward difference formula only, the method of derivation being the same with regard to the other formulae.

Consider Newton's forward difference formula:

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots, \tag{6.1}$$

where

$$x = x_0 + uh. \tag{6.2}$$

Then

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} = \frac{1}{h}\left(\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \cdots\right). \tag{6.3}$$

This formula can be used for computing the value of $dy/dx$ for *non-tabular values* of $x$. For tabular values of $x$, the formula takes a simpler form, for by setting $x = x_0$ we obtain $u = 0$ from Eq. (6.2), and hence Eq. (6.3) gives

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right). \tag{6.4}$$

Differentiating Eq. (6.3) once again, we obtain

$$\frac{d^2 y}{dx^2} = \frac{1}{h^2}\left(\Delta^2 y_0 + \frac{6u-6}{6}\Delta^3 y_0 + \frac{12u^2-36u+22}{24}\Delta^4 y_0 + \cdots\right), \tag{6.5}$$

from which we obtain

$$\left[\frac{d^2 y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 + \cdots\right). \tag{6.6}$$

Formulae for computing higher derivatives may be obtained by successive differentiation. In a similar way, different formulae can be derived by starting with other interpolation formuale. Thus,

(a) Newton's backward difference formula gives

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left(\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \cdots\right) \tag{6.7}$$

and

$$\left[\frac{d^2 y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left(\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \cdots\right). \tag{6.8}$$

(b) Stirling's formula gives

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left(\frac{\Delta y_{-1} + \Delta y_0}{2} - \frac{1}{6}\frac{\Delta^3 y_{-2} + \Delta^3 y_{-1}}{2} + \frac{1}{30}\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \cdots\right) \tag{6.9}$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left(\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} - \cdots\right). \tag{6.10}$$

If a derivative is required near the end of a table, one of the following formulae may be used to obtain better accuracy

$$hy_0' = \left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \frac{1}{5}\Delta^5 - \frac{1}{6}\Delta^6 + \cdots\right)y_0 \tag{6.11}$$

$$= \left(\Delta + \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \frac{1}{12}\Delta^4 - \frac{1}{20}\Delta^5 + \frac{1}{30}\Delta^6 - \cdots\right)y_{-1} \tag{6.12}$$

$$h^2 y_0'' = \left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \frac{137}{180}\Delta^6 - \frac{7}{10}\Delta^7 + \frac{363}{560}\Delta^8 - \cdots\right)y_0 \tag{6.13}$$

$$= \left(\Delta^2 - \frac{1}{12}\Delta^4 + \frac{1}{12}\Delta^5 - \frac{13}{180}\Delta^6 + \frac{11}{180}\Delta^7 - \frac{29}{560}\Delta^8 + \cdots\right)y_{-1} \tag{6.14}$$

$$hy_n' = \left(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \frac{1}{5}\nabla^5 + \frac{1}{6}\nabla^6 + \frac{1}{7}\nabla^7 + \frac{1}{8}\nabla^8 + \cdots\right)y_n \tag{6.15}$$

$$= \left(\nabla - \frac{1}{2}\nabla^2 - \frac{1}{6}\nabla^3 - \frac{1}{12}\nabla^4 - \frac{1}{20}\nabla^5 - \frac{1}{30}\nabla^6 - \frac{1}{42}\nabla^7 - \frac{1}{56}\nabla^8 - \cdots\right)y_{n+1} \tag{6.16}$$

$$h^2 y_n'' = \left(\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{5}{6}\nabla^5 + \frac{137}{180}\nabla^6 + \frac{7}{10}\nabla^7 + \frac{363}{560}\nabla^8 + \cdots\right)y_n \tag{6.17}$$

$$= \left(\nabla^2 - \frac{1}{12}\nabla^4 - \frac{1}{12}\nabla^5 - \frac{13}{180}\nabla^6 - \frac{11}{180}\nabla^7 - \frac{29}{560}\nabla^8 - \cdots\right)y_{n+1}. \tag{6.18}$$

For more details, the reader is referred to Interpolation and Allied Tables. The following examples illustrate the use of the formulae stated above.

***Example 6.1*** From the following table of values of $x$ and $y$, obtain $dy/dx$ and $d^2y/dx^2$ for $x = 1.2$:

| $x$ | $y$ | $x$ | $y$ |
|---|---|---|---|
| 1.0 | 2.7183 | 1.8 | 6.0496 |
| 1.2 | 3.3201 | 2.0 | 7.3891 |
| 1.4 | 4.0552 | 2.2 | 9.0250 |
| 1.6 | 4.9530 | | |

The difference table is

| $x$ | $y$ | $\Delta$ | $\Delta^2$ | $\Delta^3$ | $\Delta^4$ | $\Delta^5$ | $\Delta^6$ |
|---|---|---|---|---|---|---|---|
| 1.0 | 2.7183 | | | | | | |
| | | 0.6018 | | | | | |
| 1.2 | 3.3201 | | 0.1333 | | | | |
| | | 0.7351 | | 0.0294 | | | |
| 1.4 | 4.0552 | | 0.1627 | | 0.0067 | | |
| | | 0.8978 | | 0.0361 | | 0.0013 | |
| 1.6 | 4.9530 | | 0.1988 | | 0.0080 | | 0.0001 |
| | | 1.0966 | | 0.0441 | | 0.0014 | |
| 1.8 | 6.0496 | | 0.2429 | | 0.0094 | | |
| | | 1.3395 | | 0.0535 | | | |
| 2.0 | 7.3891 | | 0.2964 | | | | |
| | | 1.6359 | | | | | |
| 2.2 | 9.0250 | | | | | | |

Here $x_0 = 1.2$, $y_0 = 3.3201$ and $h = 0.2$. Hence Eq. (6.11) gives

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.7351 - \frac{1}{2}(0.1627) + \frac{1}{3}(0.0361) - \frac{1}{4}(0.0080) + \frac{1}{5}(0.0014)\right]$$

$$= 3.3205.$$

If we use formula (6.12), then we should use the differences diagonally downwards from 0.6018 and this gives

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.6018 + \frac{1}{2}(0.1333) - \frac{1}{6}(0.0294) + \frac{1}{12}(0.0067) - \frac{1}{20}(0.0013\right]$$

$$= 3.3205, \text{ as before.}$$

Similarly, formula (6.13) gives

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1627 - 0.0361 + \frac{11}{12}(0.0080) - \frac{5}{6}(0.0014)\right] = 3.318.$$

Using formula (6.14), we obtain

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1333 - \frac{1}{12}(0.0067) + \frac{1}{12}(0.0013)\right] = 3.32.$$

***Example 6.2*** Calculate the first and second derivatives of the function tabulated in the preceding example at the point $x = 2.2$ and also $dy/dx$ at $x = 2.0$.

We use the table of differences of Example 6.1. Here $x_n = 2.2$, $y_n = 9.0250$ and $h = 0.2$. Hence formula (6.15) gives

$$\left[\frac{dy}{dx}\right]_{x=2.2} = \frac{1}{0.2}\left[1.6359 + \frac{1}{2}(0.2964) + \frac{1}{3}(0.0535) + \frac{1}{4}(0.0094) + \frac{1}{5}(0.0014)\right]$$

$$= 9.0228.$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=2.2} = \frac{1}{0.04}\left[0.2964 + 0.0535 + \frac{11}{12}(0.0094) + \frac{5}{6}(0.0014)\right] = 8.992.$$

To find $dy/dx$ at $x = 2.0$, we can use either (6.15) or (6.16). Formula (6.15) gives

$$\left[\frac{dy}{dx}\right]_{x=2.0} = \frac{1}{0.2}\left[1.3395 + \frac{1}{2}(0.2429) + \frac{1}{3}(0.0441) + \frac{1}{4}(0.0080) + \frac{1}{5}(0.0013) + \frac{1}{6}(0.0001)\right]$$

$$= 7.3896.$$

whereas from formula (6.16), we obtain

$$\left[\frac{dy}{dx}\right]_{x=2.0} = \frac{1}{0.2}\left[1.6359 - \frac{1}{2}(0.2964) - \frac{1}{6}(0.0535) - \frac{1}{12}(0.0094) - \frac{1}{20}(0.0014)\right]$$

$$= 7.3896.$$

***Example 6.3*** Find $dy/dx$ and $d^2y/dx^2$ at $x = 1.6$ for the tabulated function of Example 6.1.

Choosing $x_0 = 1.6$, formula (6.9) gives

$$\left[\frac{dy}{dx}\right]_{x=1.6} = \frac{1}{0.2}\left(\frac{0.8978 + 1.0966}{2} - \frac{1}{2}\,\frac{0.0361 + 0.0441}{2} + \frac{1}{30}\,\frac{0.0013 + 0.0014}{2}\right)$$

$$= 4.9530.$$

Similarly, formula (6.10) yields

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.6} = \frac{1}{0.04}\left[0.1988 - \frac{1}{12}(0.0080) + \frac{1}{90}(0.0001)\right] = 4.9525.$$

***Example 6.7*** From the following table, find $x$, correct to two decimal places, for which $y$ is maximum and find this value of $y$.

| $x$ | $y$ |
|---|---|
| 1.2 | 0.9320 |
| 1.3 | 0.9636 |
| 1.4 | 0.9855 |
| 1.5 | 0.9975 |
| 1.6 | 0.9996 |

The table of differences is

| $x$ | $y$ | $\Delta$ | $\Delta^2$ |
|---|---|---|---|
| 1.2 | 0.9320 | | |
| | | 0.0316 | |
| 1.3 | 0.9636 | | –0.0097 |
| | | 0.0219 | |
| 1.4 | 0.9855 | | –0.0099 |
| | | 0.0120 | |
| 1.5 | 0.9975 | | –0.0099 |
| | | 0.0021 | |
| 1.6 | 0.9996 | | |

Let $x_0$ = 1.2. Then formula (6.25), terminated after second differences, gives

$$0 = 0.0316 + \frac{2p-1}{2}(-0.0097)$$

from which we obtain $p$ = 3.8. Hence

$$x = x_0 + ph = 1.2 + (3.8)\,(0.1) = 1.58.$$

For this value of $x$, Newton's backward difference formula at $x_n = 1.6$ gives

$$\begin{aligned} y(1.58) &= 0.9996 - 0.2(0.0021) + \frac{-0.2(-0.2+1)}{2}(-0.0099) \\ &= 0.9996 - 0.0004 + 0.0008 \\ &= 1.0. \end{aligned}$$

## 6.4 NUMERICAL INTEGRATION

The general problem of numerical integration may be stated as follows. Given a set of data points $(x_0, y_0)$, $(x_1, y_1)$, …, $(x_n, y_n)$ of a function $y = f(x)$, where $f(x)$ is not known explicitly, it is required to compute the value of the definite integral

$$I = \int_a^b y\,dx. \tag{6.28}$$

As in the case of numerical differentiation, one replaces $f(x)$ by an interpolating polynomial $\phi(x)$ and obtains, on integration, an approximate value of the definite integral. Thus, different integration formulae can be obtained depending upon the type of the interpolation formula used. We derive in this section a general formula for numerical integration using Newton's forward difference formula.

Let the interval $[a, b]$ be divided into $n$ equal subintervals such that $a = x_0 < x_1 < x_2 < \cdots x_n = b$. Clearly, $x_n = x_0 + nh$. Hence the integral becomes

$$I = \int_{x_0}^{x_n} y\,dx.$$

Approximating $y$ by Newton's forward difference formula, we obtain

$$I = \int_{x_0}^{x_n} \left[ y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots \right] dx.$$

Since $x = x_0 + ph$, $dx = h\,dp$ and hence the above integral becomes

$$I = h\int_{0}^{n} \left[ y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots \right] dp,$$

which gives on simplification

$$\int_{x_0}^{x_n} y\,dx = nh\left[ y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots \right]. \qquad (6.29)$$

From this *general formula*, we can obtain different integration formulae by putting $n = 1, 2, 3, \ldots$, etc. We derive here a few of these formulae but it should be remarked that the trapezoidal and Simpson's 1/3-rules are found to give sufficient accuracy for use in practical problems.

### 6.4.1 Trapezoidal Rule

Setting $n = 1$ in the general formula (6.29), all differences higher than the first will become zero and we obtain

$$\int_{x_0}^{x_1} y\,dx = h\left( y_0 + \frac{1}{2}\Delta y_0 \right) = h\left[ y_0 + \frac{1}{2}(y_1 - y_0) \right] = \frac{h}{2}(y_0 + y_1). \qquad (6.30)$$

For the next interval $[x_1, x_2]$, we deduce similarly

$$\int_{x_1}^{x_2} y\,dx = \frac{h}{2}(y_1 + y_2) \qquad (6.31)$$

and so on. For the last interval $[x_{n-1}, x_n]$, we have

$$\int_{x_{n-1}}^{x_n} y\,dx = \frac{h}{2}(y_{n-1} + y_n). \tag{6.32}$$

Combining all these expressions, we obtain the rule

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n], \tag{6.33}$$

which is known as the *trapezoidal rule*.

The geometrical significance of this rule is that the curve $y = f(x)$ is replaced by $n$ straight lines joining the points $(x_0, y_0)$ and $(x_1, y_1)$; $(x_1, y_1)$ and $(x_2, y_2)$, …, $(x_{n-1}, y_{n-1})$ and $(x_n, y_n)$. The area bounded by the curve $y = f(x)$, the ordinates $x = x_0$ and $x = x_n$, and the $x$-axis is then approximately equivalent to the sum of the areas of the $n$ trapeziums obtained.

The error of the trapezoidal formula can be obtained in the following way. Let $y = f(x)$ be continuous, well-behaved, and possess continuous derivatives in $[x_0, x_n]$. Expanding $y$ in a Taylor's series around $x = x_0$, we obtain

$$\begin{aligned}\int_{x_0}^{x_1} y\,dx &= \int_{x_0}^{x_1}\left[y_0 + (x - x_0)y_0' + \frac{(x-x_0)^2}{2}y_0'' + \cdots\right]dx \\ &= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{6}y_0'' + \cdots \end{aligned} \tag{6.34}$$

Similarly,

$$\begin{aligned}\frac{h}{2}(y_0 + y_1) &= \frac{h}{2}\left(y_0 + y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{6}y_0''' + \cdots\right) \\ &= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{4}y_0'' + \cdots \end{aligned} \tag{6.35}$$

From Eqs. (6.34) and (6.35), we obtain

$$\int_{x_0}^{x_1} y\,dx - \frac{h}{2}(y_0 + y_1) = -\frac{1}{12}h^3 y_0'' + \cdots, \tag{6.36}$$

which is the error in the interval $[x_0, x_1]$. Proceeding in a similar manner we obtain the errors in the remaining subintervals, viz., $[x_1, x_2]$, $[x_2, x_3]$, … and $[x_{n-1}, x_n]$. We thus have

$$E = -\frac{1}{12} h^3 (y_0'' + y_1'' + \cdots + y_{n-1}''), \tag{6.37}$$

where $E$ is the *total error*. Assuming that $y''(\bar{x})$ is the largest value of the $n$ quantities on the right-hand side of Eq. (6.37), we obtain

$$E = -\frac{1}{12} h^3 n y''(\bar{x}) = -\frac{b-a}{12} h^2 y''(\bar{x}) \tag{6.38}$$

since $nh = b - a$.

### 6.4.2 Simpson's 1/3-Rule

This rule is obtained by putting $n = 2$ in Eq. (6.29), i.e. by replacing the curve by $n/2$ arcs of second-degree polynomials or parabolas. We have then

$$\int_{x_0}^{x_2} y\,dx = 2h\left(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right) = \frac{h}{3}(y_0 + 4y_1 + y_2).$$

Similarly,

$$\int_{x_2}^{x_4} y\,dx = \frac{h}{3}(y_2 + 4y_3 + y_4)$$

$$\vdots$$

and finally

$$\int_{x_{n-2}}^{x_n} y\,dx = \frac{h}{3}(y_{n-2} + 4y_{n-1} + y_n).$$

Summing up, we obtain

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1}) + 2(y_2 + y_4 + y_6 + \cdots + y_{n-2}) + y_n], \tag{6.39}$$

which is known as *Simpson's* 1/3-*rule*, or simply Simpson's rule. It should be noted that this rule requires the division of the whole range into an even number of subintervals of width $h$.

Following the method outlined in Section 6.4.1, it can be shown that the error in Simpson's rule is given by

$$\int_a^b y\,dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1}) + 2(y_2 + y_4 + y_6 + \cdots + y_{n-2}) + y_n]$$

$$= -\frac{b-a}{180} h^4 y^{\text{iv}}(\bar{x}), \tag{6.40}$$

where $y^{\text{iv}}(\bar{x})$ is the largest value of the fourth derivatives.

### 6.4.3 Simpson's 3/8-Rule

Setting $n = 3$ in Eq. (6.29), we observe that all the differences higher than the third will become zero and we obtain

$$\int_{x_0}^{x_3} y\,dx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right)$$

$$= 3h\left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0)\right]$$

$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3).$$

Similarly

$$\int_{x_3}^{x_6} y\,dx = \frac{3h}{8}(y_3 + 3y_4 + 3y_5 + y_6)$$

and so on. Summing up all these, we obtain

$$\int_{x_0}^{x_n} y\,dx = \frac{3h}{8}[(y_0 + 3y_1 + 3y_2 + y_3) + (y_3 + 3y_4 + 3y_5 + y_6) + \cdots$$

$$+ (y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)]$$

$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots$$

$$+ 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n) \tag{6.41}$$

This rule, called Simpson's (3/8)-rule, is not so accurate as Simpson's rule, the dominant term in the error of this formula being $-(3/80)\, h^5 y^{\text{iv}}(\bar{x})$.

### 6.4.4 Boole's and Weddle's Rules

If we wish to retain differences up to those of the fourth order, we should integrate between $x_0$ and $x_4$ and obtain Boole's formula

$$\int_{x_0}^{x_4} y\,dx = \frac{2h}{45}(7y_0 + 32y_1 + 12y_2 + 32y_3 + 7y_4) \tag{6.42}$$

The leading term in the error of this formula can be shown to be

$$-\frac{8h^7}{945} y^{\text{vi}}(\bar{x}).$$

If, on the other hand, we integrate between $x_0$ and $x_6$ retaining differences up to those of the sixth order, we obtain Weddle's rule

$$\int_{x_0}^{x_6} y\,dx = \frac{3h}{10}(y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6), \tag{6.43}$$

the error in which is given by $-(h^7/140)y^{\text{vi}}(\bar{x})$.

These two formulae can also be generalized as in the previous cases. It should, however, be noted that the number of strips will have to be a multiple of four in the case of Boole's rule and a multiple of six for Weddle's rule.

### 6.4.5 Use of Cubic Splines

If $s(x)$ is the cubic spline in the interval $(x_{i-1}, x_i)$, then we have

$$I = \int_{x_0}^{x_n} y\,dx \approx \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} s(x)\,dx$$

$$= \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} \left\{ \frac{1}{6h}[(x_i - x)^3 M_{i-1} + (x - x_{i-1})^3 M_i] \right.$$

$$\left. + \frac{1}{h}(x_i - x)\left( y_{i-1} - \frac{h^2}{6} M_{i-1} \right) + \frac{1}{h}(x - x_{i-1})\left( y_i - \frac{h^2}{6} M_i \right) \right\} dx,$$

using Eq. (5.27). On carrying out the integration and simplifying, we obtain

$$I = \sum_{i=1}^{n} \left[ \frac{h}{2}(y_{i-1} + y_i) - \frac{h^3}{24}(M_{i-1} + M_i) \right], \tag{6.44}$$

where $M_i$, the spline second-derivatives, are calculated from the recurrence relation

$$M_{i-1} + 4M_i + M_{i+1} = \frac{6}{h^2}(y_{i-1} - 2y_i + y_{i+1}), \qquad i = 1, 2, \ldots, n-1.$$

The use of the cubic spline method is demonstrated in Example 6.13.

### 6.4.6 Romberg Integration

This method can often be used to improve the approximate results obtained by the finite-difference methods. Its application to the numerical evaluation of definite integrals, for example in the use of trapezoidal rule, can be described, as follows. We consider the definite integral

We know that

$$\text{Area} = \int_{7.47}^{7.52} f(x)\,dx$$

with $h = 0.01$, the trapezoidal rule given in Eq. (6.32) gives

$$\text{Area} = \frac{0.01}{2}[1.93 + 2(1.95 + 1.98 + 2.01 + 2.03) + 2.06] = 0.0996.$$

***Example 6.9*** A solid of revolution is formed by rotating about the $x$-axis the area between the $x$-axis, the lines $x = 0$ and $x = 1$, and a curve through the points with the following coordinates:

| $x$ | $y$ |
|---|---|
| 0.00 | 1.0000 |
| 0.25 | 0.9896 |
| 0.50 | 0.9589 |
| 0.75 | 0.9089 |
| 1.00 | 0.8415 |

Estimate the volume of the solid formed, giving the answer to three decimal places.

If $V$ is the volume of the solid formed, then we know that

$$V = \pi \int_0^1 y^2 dx$$

Hence we need the values of $y^2$ and these are tabulated below, correct to four decimal places

| $x$ | $y^2$ |
|---|---|
| 0.00 | 1.0000 |
| 0.25 | 0.9793 |
| 0.50 | 0.9195 |
| 0.75 | 0.8261 |
| 1.00 | 0.7081 |

With $h = 0.25$, Simpson's rule gives

$$V = \frac{\pi(0.25)}{3}[1.0000 + 4(0.9793 + 0.8261) + 2(0.9195) + 0.7081]$$

$$= 2.8192.$$

***Example 6.10*** Evaluate

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

correct to three decimal places.

We solve this example by both the trapezoidal and Simpson's rules with $h = 0.5, 0.25$ and $0.125$ respectively.

(i) $h = 0.5$: The values of $x$ and $y$ are tabulated below:

| $x$ | $y$ |
|---|---|
| 0.0 | 1.0000 |
| 0.5 | 0.6667 |
| 1.0 | 0.5000 |

(a) Trapezoidal rule gives

$$I = \frac{1}{4}[1.0000 + 2(0.6667) + 0.5] = 0.70835.$$

(b) Simpson's rule gives

$$I = \frac{1}{6}[1.0000 + 4(0.6667) + 0.5] = 0.6945.$$

(ii) $h = 0.25$: The tabulated values of $x$ and $y$ are given below:

| $x$ | $y$ |
|---|---|
| 0.00 | 1.0000 |
| 0.25 | 0.8000 |
| 0.50 | 0.6667 |
| 0.75 | 0.5714 |
| 1.00 | 0.5000 |

(a) Trapezoidal rule gives

$$I = \frac{1}{8}[1.0 + 2(0.8000 + 0.6667 + 0.5714) + 0.5] = 0.6970.$$

(b) Simpson's rule gives

$$I = \frac{1}{12}[1.0 + 4(0.8000 + 0.5714) + 2(0.6667) + 0.5] = 0.6932.$$

(iii) Finally, we take $h = 0.125$: The tabulated values of $x$ and $y$ are

| $x$ | $y$ | $x$ | $y$ |
|---|---|---|---|
| 0 | 1.0 | 0.625 | 0.6154 |
| 0.125 | 0.8889 | 0.750 | 0.5714 |
| 0.250 | 0.8000 | 0.875 | 0.5333 |
| 0.375 | 0.7273 | 1.0 | 0.5 |
| 0.5 | 0.6667 | | |

(a) Trapezoidal rule gives

$$I = \frac{1}{16}[1.0 + 2(0.8889 + 0.8000 + 0.7273 + 0.6667 + 0.6154 + 0.5714 + 0.5333) + 0.5]$$

$$= 0.6941.$$

(b) Simpson's rule gives

$$I = \frac{1}{24}[1.0 + 4(0.8889 + 0.7273 + 0.6154 + 0.5333) + 2(0.8000 + 0.6667 + 0.5714) + 0.5]$$

$$= 0.6932.$$

Hence the value of $I$ may be taken to be equal to 0.693, correct to three decimal places. The exact value of $I$ is $\log_e 2$, which is equal to 0.693147…. This example demonstrates that, in general, Simpson's rule yields more accurate results than the trapezoidal rule.

***Example 6.11*** Use Romberg's method to compute

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

correct to three decimal places.

We take $h = 0.5$, 0.25 and 0.125 successively and use the results obtained in the previous example. We therefore have

$$I(h) = 0.7084, \quad I\left(\frac{1}{2}h\right) = 0.6970, \quad \text{and} \quad I\left(\frac{1}{4}h\right) = 0.6941$$

Hence, using Eq. (6.49), we obtain

$$I\left(h, \frac{1}{2}h\right) = 0.6970 + \frac{1}{3}(0.6970 - 0.7084) = 0.6932.$$

Hence formula (i) takes the form

$$\int_{-h}^{h} y\,dx = \frac{h}{3}(y_{-1} + 4y_0 + y_1),$$

which is the Simpson's 1/3-rule given in Section 6.4.2.

## 6.5 EULER–MACLAURIN FORMULA

Consider the expansion of $1/(e^x - 1)$ in ascending powers of $x$, obtained by writing the Maclaurin expansion of $e^x$ and simplifying

$$\frac{1}{e^x - 1} = \frac{1}{x} - \frac{1}{2} + B_1 x + B_3 x^3 + B_5 x^5 + \cdots, \tag{6.57}$$

where

$$B_{2r} = 0, \qquad B_1 = \frac{1}{12}, \qquad B_3 = -\frac{1}{720,} \qquad B_5 = \frac{1}{30,240}, \quad \text{etc.}$$

In Eq. (6.57), if we set $x = hD$ and use the relation $E \equiv e^{hD}$ (see Section 3.3.4), we obtain the identity

$$\frac{1}{E-1} \equiv \frac{1}{hD} - \frac{1}{2} + B_1 hD + B_3 h^3 D^3 + B_5 h^5 D^5 + \cdots$$

or equivalently

$$\frac{E^n - 1}{E - 1} = \frac{1}{hD}(E^n - 1) - \frac{1}{2}(E^n - 1) + B_1 hD(E^n - 1) + B_3 h^3 D^3 (E^n - 1) + \cdots \tag{6.58}$$

Operating this identity on $y_0$, we obtain

$$\begin{aligned}
\frac{E^n - 1}{E - 1} y_0 &= \frac{1}{hD}(E^n - 1) y_0 - \frac{1}{2}(E^n - 1) y_0 + B_1 hD(E^n - 1) y_0 + \cdots \\
&= \frac{1}{hD}(y_n - y_0) - \frac{1}{2}(y_n - y_0) + B_1 h(y'_n - y'_0) + B_3 h^3 (y'''_n - y'''_0) \\
&\quad + B_5 h^5 (y_n^{\mathrm{v}} - y_0^{\mathrm{v}}) + \cdots
\end{aligned} \tag{6.59}$$

It can be easily shown that the left-hand side denotes the sum $y_0 + y_1 + y_2 + \cdots + y_{n-1}$, whereas the term

$$\frac{1}{hD}(y_n - y_0)$$

on the right side can be written as

$$\frac{1}{h} \int_{x_0}^{x_n} y\,dx$$

since $1/D$ can be interpreted as an integration operator.

Hence, Eq. (6.59) becomes

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) - \frac{h^2}{12}(y_n' - y_0')$$

$$+\frac{h^4}{720}(y_n''' - y_0''') - \frac{h^6}{30,240}(y_n^{\mathrm{v}} - y_0^{\mathrm{v}}) + \cdots \tag{6.60}$$

which is called the *Euler–Maclaurin's formula* for integration. The first expression on the right-hand side of Eq. (6.60) denotes the approximate value of the integral obtained by using trapezoidal rule and the other expressions represent the successive *corrections* to this value. It should be noted that this formula may also be used to find the sum of a series of the form $y_0 + y_1 + y_2 + \cdots + y_n$. The use of this formula is illustrated by the following examples.

***Example 6.15*** Evaluate

$$I = \int_0^{\pi/2} \sin x\,dx$$

using the Euler–Maclaurin's formula.

In this case, formula (6.60) simplifies to

$$\int_0^{\pi/2} \sin x\,dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + \frac{h^2}{12} + \frac{h^4}{720} + \frac{h^6}{30,240} + \cdots \tag{i}$$

To evaluate the integral, we take $h = \pi/4$. Then we obtain

$$\int_0^{\pi/2} \sin x\,dx = \frac{\pi}{8}(0 + 2 + 0) + \frac{\pi^2}{192} + \frac{\pi^4}{1,84,320} + \cdots$$

$$= \frac{\pi}{4} + \frac{\pi^2}{192} + \frac{\pi^4}{1,84,320}, \text{ approximately}$$

$$= 0.785398 + 0.051404 + 0.000528$$

$$= 0.837330.$$

On the other hand with $h = \pi/8$, we obtain

$$\int_0^{\pi/2} \sin x\,dx = \frac{\pi}{16}[(0 + 2(0.382683) + .707117 + 0.923879 + 1.000000)]$$

$$= 0.987119 + 0.012851 + 0.000033$$

$$= 1.000003.$$

***Example 6.16*** Use the Euler–Maclaurin formula to prove

$$\sum_{1}^{n} x^2 = \frac{n(n+1)(2n+1)}{6}.$$

In this case, rewrite Eq. (6.60) as

$$\frac{1}{2}y_0 + y_1 + y_2 + \cdots + y_{n-1} + \frac{1}{2}y_n = \frac{1}{h}\int_{x_0}^{x_n} y\,dx + \frac{h}{12}(y_n' - y_0') - \frac{h^3}{720}(y_n''' - y_0''')$$

$$+\frac{h^5}{30,240}(y_n^{\text{v}} - y_0^{\text{v}}) - \cdots \qquad \text{(i)}$$

Here $y(x) = x^2$, $y'(x) = 2x$ and $h = 1$.

Hence Eq. (i) gives

$$\text{Sum} = \int_1^n x^2\,dx + \frac{1}{2}(n^2+1) + \frac{1}{12}(2n-2)$$

$$= \frac{1}{3}(n^3-1) + \frac{1}{2}(n^2+1) + \frac{1}{6}(n-1)$$

$$= \frac{1}{6}(2n^3 + 3n^2 + n)$$

$$= \frac{n(n+1)(2n+1)}{6}.$$

## 6.6 NUMERICAL INTEGRATION WITH DIFFERENT STEP SIZES

We have so far considered integration formulae which use equally spaced abscissae. In practical problems, however, we often come across situations which require the use of different step-sizes while solving a problem. This would be so if the interval in question contains parts over which the function varies too rapidly or too slowly. For better accuracy and efficiency, it would be desirable to take a smaller size in parts of the interval over which the function variation is large. Similarly, it would be efficient to take larger step sizes over parts in which the function varies too slowly. A numerical integration procedure which *adopts* automatically a suitable step-size to solve an integration problem numerically is called *adaptive quadrature method*. We describe below an 'adaptive quadrature method' based on Simpson's (1/3)-rule.

Suppose that we wish to approximate the integral

$$I = \int_a^b y(x)\,dx \qquad (6.61)$$