7.10 Integration

It is well known that, if a function $f(x)$ is known completely, even then it is not always possible to evaluate the definite integral of it using analytic method. Again, in many real life problems, we are required to integrate a function between two given limits, but the function is not known explicitly, but, it is known in a tabular form (equally or unequally spaced). Then a method, known as **numerical integration or quadrature** can be used to solve all such problems.

The problem of numerical integration is stated below:

Given a set of data points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ *of a function* $y = f(x)$, *it is required to find the value of the definite integral* $\int_a^b f(x)\,dx$. *The function* $f(x)$ *is replaced by a suitable interpolating polynomial* $\phi(x)$.

Then the approximate value of the definite integral is calculated using the following formula

$$\int_a^b f(x)\,dx \simeq \int_a^b \phi(x)\,dx. \tag{7.64}$$

Thus, different integration formulae can be derived depending on the type of the interpolation formulae used.

A numerical integration formula is said to be of **closed type**, if the limits of integration a and b are taken as interpolating points. If a and b are not taken as interpolating points then the formula is known as **open type** formula.

7.11 General Quadrature Formula Based on Newton's Forward Interpolation

The Newton's forward interpolation formula for the equispaced points $x_i, i = 0, 1, \ldots, n$, $x_i = x_0 + ih$ is

$$\phi(x) = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots, \tag{7.65}$$

where $u = \dfrac{x - x_0}{h}$, h is the spacing.

Let the interval $[a, b]$ be divided into n equal subintervals such that $a = x_0 < x_1 < x_2 < \cdots < x_n = b$. Then

$$\begin{aligned} I &= \int_a^b f(x)\,dx \simeq \int_{x_0}^{x_n} \phi(x)\,dx \\ &= \int_{x_0}^{x_n} \left[y_0 + u\Delta y_0 + \frac{u^2 - u}{2!}\Delta^2 y_0 + \frac{u^3 - 3u^2 + 2u}{3!}\Delta^3 y_0 + \cdots\right] dx. \end{aligned}$$

Since $x = x_0 + uh$, $dx = h\,du$, when $x = x_0$ then $u = 0$ and when $x = x_n$ then $u = n$. Thus,

$$\begin{aligned} I &= \int_0^n \left[y_0 + u\Delta y_0 + \frac{u^2 - u}{2!}\Delta^2 y_0 + \frac{u^3 - 3u^2 + 2u}{3!}\Delta^3 y_0 + \cdots\right] h du \\ &= h\left[y_0[u]_0^n + \Delta y_0\left[\frac{u^2}{2}\right]_0^n + \frac{\Delta^2 y_0}{2!}\left[\frac{u^3}{3} - \frac{u^2}{2}\right]_0^n + \frac{\Delta^3 y_0}{3!}\left[\frac{u^4}{4} - u^3 + u^2\right]_0^n + \cdots\right] \\ &= nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{2n^2 - 3n}{12}\Delta^2 y_0 + \frac{n^3 - 4n^2 + 4n}{24}\Delta^3 y_0 + \cdots\right]. \end{aligned} \tag{7.66}$$

From this formula, one can generate different integration formulae by substituting $n = 1, 2, 3, \ldots$.

7.11.1 Trapezoidal Rule

Substituting $n = 1$ in the equation (7.66). In this case all differences higher than the first difference become zero. Then

$$\int_{x_0}^{x_n} f(x)\,dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}(y_0 + y_1). \tag{7.67}$$

The formula (7.67) is known as the **trapezoidal rule**.

In this formula, the interval $[a, b]$ is considered as a single interval, and it gives a very rough answer. But, if the interval $[a, b]$ is divided into several subintervals and this formula is applied to each of these subintervals then a better approximate result may be obtained. This formula is known as composite formula, deduced below.

Composite trapezoidal rule

Let the interval $[a, b]$ be divided into n equal subintervals by the points $a = x_0$, x_1, x_2, $\ldots$, $x_n = b$, where $x_i = x_0 + ih$, $i = 1, 2, \ldots, n$.

Applying the trapezoidal rule to each of the subintervals, one can find the composite formula as

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx \\ &\simeq \frac{h}{2}[y_0 + y_1] + \frac{h}{2}[y_1 + y_2] + \frac{h}{2}[y_2 + y_3] + \cdots + \frac{h}{2}[y_{n-1} + y_n] \\ &= \frac{h}{2}[y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]. \qquad (7.68)\end{aligned}$$

Error in trapezoidal rule

The error of trapezoidal rule is

$$E = \int_a^b f(x)\,dx - \frac{h}{2}(y_0 + y_1). \qquad (7.69)$$

Let $y = f(x)$ be continuous and possesses continuous derivatives of all orders. Also, it is assumed that there exists a function $F(x)$ such that $F'(x) = f(x)$ in $[x_0, x_1]$.

Then

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{x_0}^{x_1} F'(x)\,dx = F(x_1) - F(x_0) \\ &= F(x_0 + h) - F(x_0) = F(x_0) + hF'(x_0) + \frac{h^2}{2!}F''(x_0) \\ &\quad + \frac{h^3}{3!}F'''(x_0) + \cdots - F(x_0) \\ &= hf(x_0) + \frac{h^2}{2!}f'(x_0) + \frac{h^3}{3!}f''(x_0) + \cdots \\ &= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{6}y_0'' + \cdots \qquad (7.70)\end{aligned}$$

Again,

$$\begin{aligned}\frac{h}{2}(y_0+y_1) &= \frac{h}{2}[y_0+y(x_0+h)]\\ &= \frac{h}{2}[y_0+y(x_0)+hy'(x_0)+\frac{h^2}{2!}y''(x_0)+\cdots]\\ &= \frac{h}{2}[y_0+y_0+hy'_0+\frac{h^2}{2!}y''_0+\cdots].\end{aligned} \tag{7.71}$$

Using (7.70) and (7.71), equation (7.69) becomes

$$\begin{aligned}E &= h\Big[y_0+\frac{h}{2}y'_0+\frac{h^2}{6}y''_0+\cdots\Big]-\frac{h}{2}\Big[2y_0+hy'_0+\frac{h^2}{2!}y''_0+\cdots\Big]\\ &= -\frac{h^3}{12}y''_0+\cdots\\ &= -\frac{h^3}{12}f''(x_0)+\cdots \simeq -\frac{h^3}{12}f''(\xi),\end{aligned} \tag{7.72}$$

where $a = x_0 < \xi < x_1 = b$.

Equation (7.72) gives the error in the interval $[x_0, x_1]$.

The total error in the composite rule is

$$E = -\frac{h^3}{12}(y''_0+y''_1+\cdots+y''_{n-1}).$$

If $y''(\xi)$ is the largest among the n quantities $y''_0, y''_1, \ldots, y''_{n-1}$ then

$$E \le -\frac{1}{12}h^3ny''(\xi) = -\frac{(b-a)}{12}h^2y''(\xi), \text{ as } nh = b-a.$$

Note 7.11.1 The error term shows that if the second and higher order derivatives of $f(x)$ vanish then the trapezoidal rule gives exact result of the integral. This means, the method gives exact result when $f(x)$ is linear.

Geometrical interpretation of trapezoidal rule

In this rule, the curve $y = f(x)$ is replaced by the line joining the points $A(x_0, y_0)$ and $B(x_1, y_1)$ (Figure 7.1). Thus the area bounded by the curve $y = f(x)$, the ordinates $x = x_0$, $x = x_1$ and the x-axis is then approximately equivalent to the area of the trapezium (ABCD) bounded by the line AB, $x = x_0$, $x = x_1$ and x-axis.

The geometrical significance of composite trapezoidal 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); $\ldots$, (x_{n-1}, y_{n-1}) and (x_n, y_n). Then the area bounded by the curve $y = f(x)$, the lines $x = x_0, x = x_n$ and the x-axis is then approximately equivalent to the sum of the area of n trapeziums (Figures 7.2).

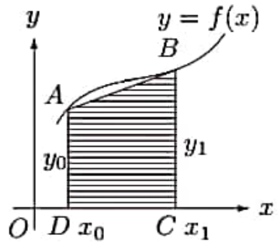

Figure 7.1: Geometrical interpretation of trapezoidal rule.

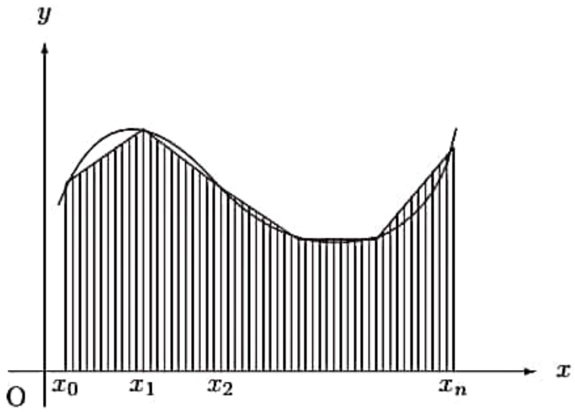

Figure 7.2: Composite trapezoidal rule.

Alternative deduction of trapezoidal rule

Let $f \in C^2[a,b]$, where $[a,b]$ is a finite interval. Now, transfer the interval $[a,b]$ to $[-1,1]$ using the relation $x = \frac{a+b}{2} + \frac{b-a}{2}t = p + qt$ (say).

Let $f(x) = f(p+qt) = g(t)$. When $x = a, b$ then $t = -1, 1$, i.e., $g(1) = f(b), g(-1) = f(a)$.

Thus

$$I = \int_a^b f(x)dx = \int_{-1}^{1} g(t)\; q\; dt = q\Big[\int_{-1}^{0} g(t)dt + \int_0^1 g(t)dt\Big]$$
$$= q\int_0^1 [g(t) + g(-t)]dt.$$

Now, applying integration by parts.

$$\begin{aligned}
I &= q\Big[\{g(t)+g(-t)\}t\Big]_0^1 - q\int_0^1 t[g'(t)-g'(-t)]dt \\
&= q[g(1)+g(-1)] - q\int_0^1 t.2tg''(c)dt, \text{ where } 0<c<1 \\
&\quad \text{[by Lagrange's MVT]} \\
&= q[f(a)+f(b)] - 2\,q\,g''(d)\int_0^1 t^2dt, 0<d<1, \\
&\quad \text{[by MVT of integral calculus]} \\
&= q[f(a)+f(b)] - \frac{2}{3}qg''(d) \\
&= q[f(a)+f(b)] - \frac{2}{3}q^3f''(p+qd) \\
&= q[f(a)+f(b)] - \frac{2}{3}q^3f''(\xi), \text{ where } a<\xi<b \\
&= \frac{b-a}{2}[f(a)+f(b)] - \frac{2}{3}\Big(\frac{b-a}{2}\Big)^3 f''(\xi) \\
&= \frac{h}{2}[f(a)+f(b)] - \frac{1}{12}h^3f''(\xi), \text{ as } h=b-a.
\end{aligned}$$

In this expression, the first term is the approximate integration obtained by trapezoidal rule and the second term represents the error.

Algorithm 7.3 (Trapezoidal). This algorithm finds the value of $\int_a^b f(x)dx$ based on the tabulated values $(x_i, y_i), y_i = f(x_i), i = 0, 1, 2, \ldots, n$, using trapezoidal rule.

Algorithm Trapezoidal
Input function $f(x)$;
Read a, b, n; //the lower and upper limits and number of subintervals.//
Compute $h = (b-a)/n$;

Set $sum = \frac{1}{2}[f(a) + f(a+nh)]$;

for $i = 1$ to $n-1$ do
    Compute $sum = sum + f(a+ih)$;
endfor;
Compute $result = sum * h$;
Print $result$;
end Trapezoidal

Program 7.3

```
/* Program Trapezoidal
   This program finds the value of integration of a function
   by trapezoidal rule.
   Here we assume that f(x)=x^3. */
#include<stdio.h>
void main()
{
 float a,b,h,sum; int n,i;
 float f(float);
 printf("Enter the values of a, b ");
 scanf("%f %f",&a,&b);
 printf("Enter the value of n ");
 scanf("%d",&n);
 h=(b-a)/n;
 sum=(f(a)+f(a+n*h))/2.;
 for(i=1;i<=n-1;i++) sum+=f(a+i*h);
 sum=sum*h;
 printf("The value of the integration is %8.5f ",sum);
}

/* definition of the function f(x) */
float f(float x)
 {
   return(x*x*x);
 }
```

A sample of input/output:

```
Enter the values of a, b 0 1
Enter the value of n 100
The value of the integration is  0.25002
```

7.11.2 Simpson's 1/3 rule

In this formula the interval $[a, b]$ is divided into two equal subintervals by the points x_0, x_1, x_2, where $h = (b - a)/2$, $x_1 = x_0 + h$ and $x_2 = x_1 + h$.

This rule is obtained by putting $n = 2$ in (7.66). In this case, the third and higher order differences do not exist.

The equation (7.66) is simplified as

$$\int_{x_0}^{x_n} f(x)\,dx \simeq 2h\left[y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right] = 2h[y_0 + (y_1 - y_0) + \frac{1}{6}(y_2 - 2y_1 + y_0)]$$
$$= \frac{h}{3}[y_0 + 4y_1 + y_2]. \qquad (7.73)$$

The above rule is known as **Simpson's 1/3 rule** or simply **Simpson's rule**.

Composite Simpson's 1/3 rule

Let the interval $[a, b]$ be divided into n (an *even number*) equal subintervals by the points $x_0, x_1, x_2, \ldots, x_n$, where $x_i = x_0 + ih$, $i = 1, 2, \ldots, n$. Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$
$$= \frac{h}{3}[y_0 + 4y_1 + y_2] + \frac{h}{3}[y_2 + 4y_3 + y_4] + \cdots + \frac{h}{3}[y_{n-2} + 4y_{n-1} + y_n]$$
$$= \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2}) + y_n]. \qquad (7.74)$$

This formula is known as **Simpson's 1/3 composite rule** for numerical integration.

Error in Simpson's 1/3 rule

The error in this formula is

$$E = \int_{x_0}^{x_n} f(x)\,dx - \frac{h}{3}[y_0 + 4y_1 + y_2]. \qquad (7.75)$$

Let the function $f(x)$ be continuous in $[x_0, x_2]$ and possesses continuous derivatives of all order. Also, let there exists a function $F(x)$ in $[x_0, x_2]$, such that $F'(x) = f(x)$. Then

$$\int_{x_0}^{x_2} f(x)\,dx = \int_{x_0}^{x_2} F'(x)\,dx = F(x_2) - F(x_0)$$
$$= F(x_0 + 2h) - F(x_0) = F(x_0) + 2hF'(x_0) + \frac{(2h)^2}{2!}F''(x_0)$$
$$+ \frac{(2h)^3}{3!}F'''(x_0) + \frac{(2h)^4}{4!}F^{iv}(x_0) + \frac{(2h)^5}{5!}F^{v}(x_0) + \cdots - F(x_0)$$
$$= 2hf(x_0) + 2h^2 f'(x_0) + \frac{4}{3}h^3 f''(x_0) + \frac{2}{3}h^4 f'''(x_0)$$
$$+ \frac{4}{15}h^5 f^{iv}(x_0) + \cdots. \qquad (7.76)$$

Again,

$$\begin{aligned}
\frac{h}{3}[y_0+4y_1+y_2] &= \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] \\
&= \frac{h}{3}[f(x_0)+4f(x_0+h)+f(x_0+2h)] \\
&= \frac{h}{3}\Bigg[f(x_0)+4\Big\{f(x_0)+hf'(x_0)+\frac{h^2}{2!}f''(x_0)+\frac{h^3}{3!}f'''(x_0) \\
&\quad +\frac{h^4}{4!}f^{iv}(x_0)+\cdots\Big\}+\Big\{f(x_0)+2hf'(x_0)+\frac{(2h)^2}{2!}f''(x_0) \\
&\quad +\frac{(2h)^3}{3!}f'''(x_0)+\frac{(2h)^4}{4!}f^{iv}(x_0)+\cdots\Big\}\Bigg] \\
&= 2hf(x_0)+2h^2f'(x_0)+\frac{4}{3}h^3f''(x_0)+\frac{2}{3}h^4f'''(x_0) \\
&\quad +\frac{5}{18}h^5f^{iv}(x_0)+\cdots. \qquad (7.77)
\end{aligned}$$

Using (7.76) and (7.77), equation (7.75) becomes,

$$E = \Big(\frac{4}{15}-\frac{5}{18}\Big)h^5f^{iv}(x_0)+\cdots \simeq -\frac{h^5}{90}f^{iv}(\xi), \qquad (7.78)$$

where $x_0 < \xi < x_2$.

This is the error in the interval $[x_0, x_2]$.

The total error in composite formula is

$$\begin{aligned}
E &= -\frac{h^5}{90}\{f^{iv}(x_0)+f^{iv}(x_2)+\cdots+f^{iv}(x_{n-2})\} \\
&= -\frac{h^5}{90}\frac{n}{2}f^{iv}(\xi) \\
&= -\frac{nh^5}{180}f^{iv}(\xi), \\
&\qquad \text{(where } f^{iv}(\xi) \text{ is the maximum among } f^{iv}(x_0), f^{iv}(x_2), \ldots, f^{iv}(x_{n-2})) \\
&= -\frac{(b-a)}{180}h^4f^{iv}(\xi). \qquad (7.79)
\end{aligned}$$

Geometrical interpretation of Simpson's 1/3 rule

In Simpson's 1/3 rule, the curve $y = f(x)$ is replaced by the second degree parabola passing through the points $A(x_0, y_0), B(x_1, y_1)$ and $C(x_2, y_2)$. Therefore, the area bounded by the curve $y = f(x)$, the ordinates $x = x_0, x = x_2$ and the x-axis is approximated to the area bounded by the parabola ABC, the straight lines $x = x_0, x = x_2$ and x-axis, i.e., the area of the shaded region ABCDEA.

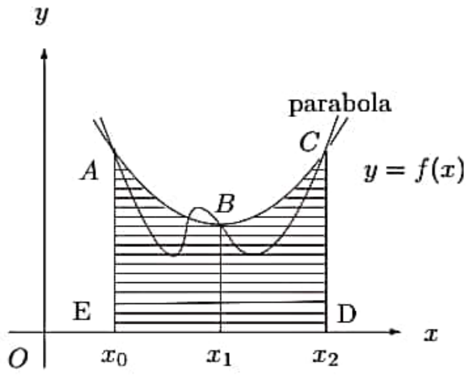

Figure 7.3: Geometrical interpretation of Simpson's 1/3 rule.

Example 7.11.1 Evaluate $\int_0^3 (2x - x^2)\,dx$, taking 6 intervals, by (i) Trapezoidal rule, and (ii) Simpson's 1/3 rule.

Solution. Here $n = 6, a = 0, b = 3, y = f(x) = 2x - x^2$.
So, $h = \dfrac{b-a}{n} = \dfrac{3-0}{6} = 0.5$.
The tabulated values of x and y are shown below.

	x_0	x_1	x_2	x_3	x_4	x_5	x_6
x_i :	0.0	0.5	1.0	1.5	2.0	2.5	3.0
y_i :	0.0	0.75	1.0	0.75	0.0	-1.25	-3.0
	y_0	y_1	y_2	y_3	y_4	y_5	y_6

(i) By Trapezoidal rule:

$$\int_0^3 (2x - x^2)\,dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + y_3 + y_4 + y_5) + y_6]$$
$$= \frac{0.5}{2}[0 + 2(0.75 + 1.0 + 0.75 + 0 - 1.25) - 3.0] = -0.125.$$

(ii) By Simpson's rule:

$$\int_0^3 (2x - x^2)\,dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4) + y_6]$$
$$= \frac{0.5}{3}[0 + 4(0.75 + 0.75 - 1.25) + 2(1.0 + 0.0) - 3.0]$$
$$= \frac{0.5}{3}[0 + 1 + 2 - 3] = 0.$$

Alternative deduction of Simpson's 1/3 rule

This rule can also be deduced by applying MVT of differential and of integral calculus. Let $f \in C^4[a,b]$ and $x = \frac{a+b}{2} + \frac{b-a}{2}z = p + qz, p = \frac{a+b}{2}, q = \frac{b-a}{2}$.

Then when $x = a, b$ then $z = -1, 1$.

Therefore,

$$\begin{aligned} I &= \int_a^b f(x)dx = q\int_{-1}^1 f(p+qz)dz \\ &= q\int_{-1}^1 g(z)dz, \text{ where } g(z) = f(p+qz) \\ &= q\left[\int_{-1}^0 g(z)dz + \int_0^1 g(z)dz\right] = q\int_0^1 [g(z)+g(-z)]dz \\ &= q\int_0^1 \phi(z)dz, \qquad (7.80) \end{aligned}$$

where $\phi(z) = g(z) + g(-z)$.

Note that $\phi(0) = 2g(0) = 2f(p) = 2f(\frac{a+b}{2}), \phi(1) = g(1)+g(-1) = f(a)+f(b), \phi'(0) = 0$.

To prove $\int_0^1 \phi(z)dz = (1+c)\phi(1) - c\phi(0) - \int_0^1 (z+c)\phi'(z)dz$, for arbitrary constant c.

$$\begin{aligned} \int_0^1 \phi(z)dz &= \int_0^1 \phi(z)d(z+c) = \int_c^{1+c} \phi(y-c)dy \qquad [\text{where } z+c=y] \\ &= \Big[y\phi(y-c)\Big]_c^{1+c} - \int_c^{1+c} y\phi'(y-c)dy \\ &= (1+c)\phi(1) - c\phi(0) - \int_0^1 (z+c)\phi'(z)d(z+c) \\ &= (1+c)\phi(1) - c\phi(0) - \int_0^1 (z+c)\phi'(z)dz. \qquad (7.81) \end{aligned}$$

Now, integrating (7.80) thrice

$$\int_0^1 \phi(z)dz = (1+c)\phi(1) - c\phi(0) - \int_0^1 (z+c)\phi'(z)dz$$

$$= (1+c)\phi(1) - c\phi(0) - \left[\Big(\frac{z^2}{2} + cz + c_1\Big)\phi'(z)\Big]_0^1 + \int_0^1 \Big(\frac{z^2}{2} + cz + c_1\Big)\phi''(z)dz\right.$$

$$= (1+c)\phi(1) - c\phi(0) - \Big(\frac{1}{2}+c+c_1\Big)\phi'(1) + c_1\phi'(0)$$
$$+\Big[\Big(\frac{z^3}{6}+c\frac{z^2}{2}+c_1z+c_2\Big)\phi''(z)\Big]_0^1 - \int_0^1 \Big(\frac{z^3}{6}+c\frac{z^2}{2}+c_1z+c_2\Big)\phi'''(z)dz$$
$$= (1+c)\phi(1) - c\phi(0) - \Big(\frac{1}{2}+c+c_1\Big)\phi'(1) + \Big(\frac{1}{6}+\frac{c}{2}+c_1+c_2\Big)\phi''(1)$$
$$-c_2\phi''(0) - \int_0^1 \Big(\frac{z^3}{6}+c\frac{z^2}{2}+c_1z+c_2\Big)\phi'''(z)dz, \qquad (7.82)$$

where c_1, c_2, c_3 are arbitrary constants and they are chosen in such a way that $\phi'(1), \phi''(1)$ and $\phi''(0)$ vanish. Thus

$$\frac{1}{2}+c+c_1 = 0, \qquad \frac{1}{6}+\frac{c}{2}+c_1+c_2 = 0, \qquad \text{and} \qquad c_2 = 0.$$

The solution of these equations is $c_2 = 0, c_1 = \frac{1}{6}, c = -\frac{2}{3}$.
Hence

$$I = q\Big[\frac{1}{3}\phi(1) + \frac{2}{3}\phi(0) - \int_0^1 \Big(\frac{z^3}{6}-\frac{z^2}{3}+\frac{z}{6}\Big)\phi'''(z)dz\Big]$$
$$= h\Big[\frac{1}{3}\Big\{f(a)+f(b)\Big\} + \frac{4}{3}f\Big(\frac{a+b}{2}\Big)\Big] - \frac{h}{6}\int_0^1 (z^3-2z^2+z)\phi'''(z)dz\Big]$$
$$\Big[\text{as } q = \frac{b-a}{2} = h\Big]$$
$$= \frac{h}{3}\Big[f(a) + 4f\Big(\frac{a+b}{2}\Big) + f(b)\Big] + E$$

where

$$E = -\frac{h}{6}\int_0^1 z(z-1)^2\phi'''(z)dz = -\frac{h}{6}\int_0^1 z(z-1)^2[g'''(z)-g'''(-z)]dz$$
$$= -\frac{h}{6}\int_0^1 z(z-1)^2.[2zg^{iv}(\xi)]dz, \qquad -z<\xi<z$$
$$\text{[by Lagrange's MVT]}$$
$$= -\frac{h}{3}g^{iv}(\xi_1)\int_0^1 z^2(z-1)^2dz \qquad \text{[by MVT of integral calculus]}$$
$$= -\frac{h}{3}g^{iv}(\xi_1).\frac{1}{30} = -\frac{h}{90}g^{iv}(\xi_1), \qquad 0<\xi_1<1.$$

Again, $g(z) = f(p+qz), g^{iv}(z) = q^4 f^{iv}(p+qt) = h^4 f^{iv}(\xi_2),\ a<\xi_2<b$.
Therefore,

$$E = -\frac{h^5}{90}f^{iv}(\xi_2).$$

Hence,

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{h^5}{90}f^{iv}(\xi_2).$$

Here, the first term is the value of the integration obtained from the Simpson's 1/3 rule and the second term is its error.

Algorithm 7.4 (Simpson's 1/3). This algorithm determines the value of $\int_a^b f(x)\,dx$ using Simpson's 1/3 rule.

Algorithm Simpson_One_Third
Input function $f(x)$;
Read a, b, n; //the lower and upper limits and number of subintervals.//
Compute $h = (b - a)/n$;
Set $sum = [f(a) - f(a + nh)]$;
for $i = 1$ to $n - 1$ step 2 do
    Compute $sum = sum + 4 * f(a + ih) + 2 * f(a + (i + 1)h)$;
endfor;
Compute $result = sum * h/3$;
Print $result$;
end Simpson_One_Third.

Program 7.4

```
/* Program Simpson's 1/3
   Program to find the value of integration of a function
   f(x) using Simpson's 1/3 rule. Here we assume that f(x)=x^3.*/
#include<stdio.h>
void main()
{
 float f(float);
 float a,b,h,sum;
 int i,n;
 printf("\nEnter the values of a, b ");
 scanf("%f %f",&a,&b);
 printf("Enter the value of subintervals n ");
 scanf("%d",&n);
 if(n%2!=0) {
     printf("Number of subdivision should be even");
     exit(0);
   }
 h=(b-a)/n;
 sum=f(a)-f(a+n*h);
```

```
  for(i=1;i<=n-1;i+=2)
     sum+=4*f(a+i*h)+2*f(a+(i+1)*h);
  sum*=h/3.;
  printf("Value of the integration is %f ",sum);
} /* main */

/* definition of the function f(x) */
float f(float x)
  {
   return(x*x*x);
  }
```

A sample of input/output:

```
Enter the values of a, b 0 1
Enter the value of subintervals n 100
Value of the integration is 0.250000
```

7.11.3 Simpson's 3/8 rule

Simpson's 3/8 rule can be obtained by substituting $n = 3$ in (7.66). Note that the differences higher than the third order do not exist here.

$$\begin{aligned}\int_a^b f(x)dx = \int_{x_0}^{x_3} f(x)dx &= 3h\left[y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right] \\ &= 3h\left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0)\right] \\ &= \frac{3h}{8}[y_0 + 3y_1 + 3y_2 + y_3]. \end{aligned} \tag{7.83}$$

This formula is known as **Simpson's 3/8 rule**.

Now, the interval $[a, b]$ is divided into n (divisible by 3) equal subintervals by the points $x_0, x_1, \ldots, x_n$ and the formula is applied to each of the intervals.

Then

$$\begin{aligned}\int_{x_0}^{x_n} f(x)dx &= \int_{x_0}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x_{n-3}}^{x_n} f(x)dx \\ &= \frac{3h}{8}[(y_0 + 3y_1 + 3y_2 + y_3) + (y_3 + 3y_4 + 3y_5 + y_6) \\ &\quad + \cdots + (y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)] \\ &= \frac{3h}{8}[y_0 + 3(y_1 + y_2 + y_4 + y_5 + y_7 + y_8 + \cdots + y_{n-2} + y_{n-1}) \\ &\quad + 2(y_3 + y_6 + y_9 + \cdots + y_{n-3}) + y_n]. \end{aligned} \tag{7.84}$$

This formula is known as **Simpson's 3/8 composite rule**.

Note 7.11.2 This method is not so accurate as Simpson's 1/3 rule. The error in this formula is $-\frac{3}{80}h^5 f^{iv}(\xi), x_0 < \xi < x_3$.

7.11.4 Boole's rule

Substituting $n = 4$ in (7.66). The equation (7.66) reduces to

$$\begin{aligned}\int_a^b f(x)dx &= 4h\left[y_0 + 2\Delta y_0 + \frac{5}{3}\Delta^2 y_0 + \frac{2}{3}\Delta^3 y_0 + \frac{7}{90}\Delta^4 y_0\right] \\ &= 4h[y_0 + 2(y_1 - y_0) + \frac{5}{3}(y_2 - 2y_1 + y_0) + \frac{2}{3}(y_3 - 3y_2 + 3y_1 - y_0) \\ &\quad + \frac{7}{90}(y_4 - 4y_3 + 6y_2 - 4y_1 + y_0)] \\ &= \frac{2h}{45}[7y_4 + 32y_3 + 12y_2 + 32y_1 + 7y_0]. \end{aligned} \tag{7.85}$$

This rule is known as **Boole's rule**.

It can be shown that the error of this formula is $-\frac{8h^7}{945}f^{vi}(\xi), a < \xi < b$.

7.11.5 Weddle's rule

To find Weddle's rule, substituting $n = 6$ in (7.66). Then

$$\begin{aligned}&\int_a^b f(x)dx \\ &= 6h\left[y_0 + 3\Delta y_0 + \frac{9}{2}\Delta^2 y_0 + 4\Delta^3 y_0 + \frac{41}{20}\Delta^4 y_0 + \frac{11}{20}\Delta^5 y_0 + \frac{41}{840}\Delta^6 y_0\right] \\ &= 6h\left[y_0 + 3\Delta y_0 + \frac{9}{2}\Delta^2 y_0 + 4\Delta^3 y_0 + \frac{41}{20}\Delta^4 y_0 + \frac{11}{20}\Delta^5 y_0 + \frac{1}{20}\Delta^6 y_0\right] - \frac{h}{140}\Delta^6 y_0.\end{aligned}$$

If the sixth order difference is very small, then we may neglect the last term $\frac{h}{140}\Delta^6 y_0$. But, this rejection increases a negligible amount of error, though, it simplifies the integration formula. Then the above equation becomes

$$\begin{aligned}&\int_{x_0}^{x_6} f(x)dx \\ &= \frac{3h}{10}[20y_0 + 60\Delta y_0 + 90\Delta^2 y_0 + 80\Delta^3 y_0 + 41\Delta^4 y_0 + 11\Delta^5 y_0 + \Delta^6 y_0] \\ &= \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6]. \end{aligned} \tag{7.86}$$

This formula is known as **Weddle's rule** for numerical integration.

Composite Weddle's rule

In this rule, interval $[a, b]$ is divided into n (divisible by 6) subintervals by the points $x_0, x_1, \ldots, x_n$. Then

$$\begin{aligned}\int_{x_0}^{x_n} f(x)dx &= \int_{x_0}^{x_6} f(x)dx + \int_{x_6}^{x_{12}} f(x)dx + \cdots + \int_{x_{n-6}}^{x_n} f(x)dx \\ &= \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6] \\ &\quad + \frac{3h}{10}[y_6 + 5y_7 + y_8 + 6y_9 + y_{10} + 5y_{11} + y_{12}] + \cdots \\ &\quad + \frac{3h}{10}[y_{n-6} + 5y_{n-5} + y_{n-4} + 6y_{n-3} + y_{n-2} + 5y_{n-1} + y_n] \\ &= \frac{3h}{10}[y_0 + 5(y_1 + y_5 + y_7 + y_{11} + \cdots + y_{n-5} + y_{n-1}) \\ &\quad + (y_2 + y_4 + y_8 + y_{10} + \cdots + y_{n-4} + y_{n-2}) \\ &\quad + 6(y_3 + y_9 + y_{15} + \cdots + y_{n-3}) + 2(y_6 + y_{12} + \cdots + y_{n-6})].\end{aligned} \tag{7.87}$$

The above formula is known as **Weddle's composite rule**.

By the technique used in trapezoidal and Simpson's 1/3 rules one can prove that the error in Weddle's rule is $-\frac{h^7}{140} f^{vi}(\xi), x_0 < \xi < x_6$.

Degree of Precision

The degree of precision of a quadrature formula is a positive integer n such that the error is zero for all polynomials of degree $i \leq n$, but it is non-zero for some polynomials of degree $n + 1$.

The degree of precision of some quadrature formulae are given in Table 7.2.

Table 7.2: Degree of precision of some quadrature formulae.

Method	Degree of precision
Trapezoidal	1
Simpson's 1/3	3
Simpson's 3/8	3
Boole's	5
Weddle's	5

Comparison of Simpson's 1/3 and Weddle's rules

The Weddle's rule gives more accurate result than Simpson's 1/3 rule. But, Weddle's rule has a major disadvantage that it requires the number of subdivisions (n) as a multiple of six. In many cases, the value of $h = \frac{b-a}{n}$ (n is multiple of six) is not finite in decimal representation. For these reasons, the values of $x_0, x_1, \ldots, x_n$ can not be determined accurately and hence the values of y i.e., $y_0, y_1, \ldots, y_n$ become inaccurate. In Simpson's 1/3 rule, n, the number of subdivisions is even, so one can take n as 10, 20 etc. and hence h is finite in decimal representation. Thus the values of $x_0, x_1, \ldots, x_n$ and $y_0, y_1, \ldots, y_n$ can be computed correctly.

However, Weddle's rule should be used when Simpson's 1/3 rule does not give the desired accuracy.

7.12 Integration Based on Lagrange's Interpolation

Let the function $y = f(x)$ be known at the $(n+1)$ points $x_0, x_1, \ldots, x_n$ of $[a, b]$, these points need not be equispaced.

The Lagrange's interpolation polynomial is

$$\phi(x) = \sum_{i=0}^{n} \frac{w(x)}{(x - x_i)w'(x_i)} y_i \tag{7.88}$$

$$\text{where } w(x) = (x - x_0) \cdots (x - x_n)$$

and $\phi(x_i) = y_i, i = 0, 1, 2, \ldots, n$.

If the function $f(x)$ is replaced by the polynomial $\phi(x)$ then

$$\int_a^b f(x)dx \simeq \int_a^b \phi(x)dx = \sum_{i=0}^{n} \int_a^b \frac{w(x)}{(x - x_i)w'(x_i)} y_i dx. \tag{7.89}$$

The above equation can be written as

$$\int_a^b f(x)dx \simeq \sum_{i=0}^{n} C_i y_i, \tag{7.90}$$

$$\text{where } C_i = \int_a^b \frac{w(x)}{(x - x_i)w'(x_i)} dx, \qquad i = 0, 1, 2, \ldots, n. \tag{7.91}$$

It may be noted that the coefficients C_i are independent of the choice of the function $f(x)$ for a given set of points.

7.13 Newton-Cotes Integration Formulae (Closed type)

Let the interpolation points $x_0, x_1, \ldots, x_n$ be equispaced, i.e., $x_i = x_0 + ih$, $i = 1, 2, \ldots, n$. Also, let $x_0 = a, x_n = b, h = (b-a)/n$ and $y_i = f(x_i), i = 0, 1, 2, \ldots, n$. Then the definite integral $\int_a^b f(x)dx$ can be determined on replacing $f(x)$ by Lagrange's interpolation polynomial $\phi(x)$ and then the approximate integration formula is given by

$$\int_a^b f(x)dx \simeq \sum_{i=0}^{n} C_i y_i, \tag{7.92}$$

where C_i are some constant coefficients.

Now, the explicit expressions for C_i's are evaluated in the following.

The Lagrange's interpolation polynomial is

$$\phi(x) = \sum_{i=0}^{n} L_i(x) y_i, \tag{7.93}$$

where

$$L_i(x) = \frac{(x - x_0)(x - x_1)\cdots(x - x_{i-1})(x - x_{i+1})\cdots(x - x_n)}{(x_i - x_0)(x_i - x_1)\cdots(x_i - x_{i-1})(x_i - x_{i+1})\cdots(x_i - x_n)}. \tag{7.94}$$

Introducing $x = x_0 + sh$. Then $x - x_i = (s - i)h$ and $x_i - x_j = (i - j)h$. Therefore,

$$\begin{aligned} L_i(x) &= \frac{sh(s-1)h\cdots(s-\overline{i-1})h(s-\overline{i+1})h\cdots(s-n)h}{ih(i-1)h\cdots(i-\overline{i-1})h(i-\overline{i+1})h\cdots(i-n)h} \\ &= \frac{(-1)^{n-i}}{i!(n-i)!}\frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)}. \end{aligned} \tag{7.95}$$

Then (7.92) becomes

$$\int_{x_0}^{x_n} f(x)dx \simeq \sum_{i=0}^{n} C_i y_i$$

$$\text{or,} \quad \int_{x_0}^{x_n} \sum_{i=0}^{n} \frac{(-1)^{n-i}}{i!(n-i)!}\frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)} y_i dx = \sum_{i=0}^{n} C_i y_i$$

$$\text{or,} \quad \sum_{i=0}^{n}\left\{\int_{x_0}^{x_n} \frac{(-1)^{n-i}}{i!(n-i)!}\frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)}dx\right\} y_i = \sum_{i=0}^{n} C_i y_i. \tag{7.96}$$

Now, comparing both sides to find the expression for C_i in the form

$$\begin{aligned} C_i &= \int_{x_0}^{x_n} \frac{(-1)^{n-i}}{i!(n-i)!}\frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)}dx \\ &= \frac{(-1)^{n-i}h}{i!(n-i)!}\int_0^n \frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)}ds, \end{aligned} \tag{7.97}$$

$i = 0, 1, 2, \ldots, n$ and $x = x_0 + sh$.

Since $h = \dfrac{b-a}{n}$, substituting

$$C_i = (b-a)H_i, \tag{7.98}$$

where

$$H_i = \frac{1}{n}\frac{(-1)^{n-i}}{i!(n-i)!}\int_0^n \frac{s(s-1)(s-2)\cdots(s-n)}{(s-i)}ds, i = 0, 1, 2, \ldots, n. \tag{7.99}$$

These coefficients H_i are called **Cotes coefficients**.

Then the integration formula (7.92) becomes

$$\int_a^b f(x)dx \simeq (b-a)\sum_{i=0}^{n} H_i y_i, \tag{7.100}$$

where H_i's are given by (7.99).

Note 7.13.1 The cotes coefficients H_i's do not depend on the function $f(x)$.

7.13.1 Some results on Cotes coefficients

(i) $\sum_{i=0}^{n} C_i = (b-a)$.

By the property of Lagrangian functions, $\sum_{i=0}^{n} \dfrac{w(x)}{(x-x_i)w'(x_i)} = 1$

$$\text{That is, } \int_a^b \sum_{i=0}^{n} \frac{w(x)}{(x-x_i)w'(x_i)}dx = \int_a^b dx = (b-a). \tag{7.101}$$

Again,

$$\begin{aligned}\int_a^b \sum_{i=0}^{n} \frac{w(x)}{(x-x_i)w'(x_i)}dx &= \sum_{i=0}^{n}\int_0^n h(-1)^{n-i}\frac{s(s-1)(s-2)\cdots(s-n)}{i!(n-i)!(s-i)}ds \\ &= \sum_{i=0}^{n} C_i. \end{aligned} \tag{7.102}$$

Hence from (7.101) and (7.102),

$$\sum_{i=0}^{n} C_i = b-a. \tag{7.103}$$

(ii) $\sum_{i=0}^{n} H_i = 1$.
From the relation (7.98),
$C_i = (b-a)H_i$

or, $\sum_{i=0}^{n} C_i = (b-a)\sum_{i=0}^{n} H_i$

or, $(b-a) = (b-a)\sum_{i=0}^{n} H_i$. [using (7.103)]

Hence,

$$\sum_{i=0}^{n} H_i = 1. \tag{7.104}$$

That is, sum of cotes coefficients is one.

(iii) $C_i = C_{n-i}$.
From the definition of C_i, one can find

$$C_{n-i} = \frac{(-1)^i h}{(n-i)!i!}\int_0^n \frac{s(s-1)(s-2)\cdots(s-n)}{s-(n-i)}ds.$$

Substituting $t = n - s$, we obtain

$$\begin{aligned} C_{n-i} &= -\frac{(-1)^i h(-1)^n}{i!(n-i)!}\int_n^0 \frac{t(t-1)(t-2)\cdots(t-n)}{t-i}dt \\ &= \frac{(-1)^{n-i} h}{i!(n-i)!}\int_0^n \frac{s(s-1)(s-2)\cdots(s-n)}{s-i}dt = C_i. \end{aligned}$$

Hence,

$$C_i = C_{n-i}. \tag{7.105}$$

(iv) $H_i = H_{n-i}$.
Multiplying (7.105) by $(b-a)$ and hence obtain

$$H_i = H_{n-i}. \tag{7.106}$$

7.13.2 Deduction of quadrature formulae

Trapezoidal rule

Substituting $n = 1$ in (7.100), we get

$$\int_a^b f(x)dx = (b-a)\sum_{i=0}^{1} H_i y_i = (b-a)(H_0 y_0 + H_1 y_1).$$

Now H_0 and H_1 are obtained from (7.99) by substituting $i = 0$ and 1. Therefore,

$$H_0 = -\int_0^1 \frac{s(s-1)}{s} ds = \frac{1}{2} \text{ and } H_1 = \int_0^1 s ds = \frac{1}{2}.$$

Here, $h = (b-a)/n = b-a$ for $n = 1$.

Hence, $\displaystyle\int_a^b f(x)dx = \frac{(b-a)}{2}(y_0 + y_1) = \frac{h}{2}(y_0 + y_1).$

Simpson's 1/3 rule

For $n = 2$, $H_0 = \dfrac{1}{2}\cdot\dfrac{1}{2}\displaystyle\int_0^2 (s-1)(s-2)ds = \frac{1}{6}$

$H_1 = -\dfrac{1}{2}\displaystyle\int_0^2 s(s-2)ds = \frac{2}{3},\qquad H_2 = \frac{1}{2}\cdot\frac{1}{2}\int_0^2 s(s-1)ds = \frac{1}{6}.$

In this case $h = (b-a)/2$.

Hence equation (7.100) gives the following formula.

$$\begin{aligned}\int_a^b f(x)dx &= (b-a)\sum_{i=0}^{2} H_i y_i = (b-a)(H_0 y_0 + H_1 y_1 + H_2 y_2)\\ &= \frac{h}{3}(y_0 + 4y_1 + y_2).\end{aligned}$$

Weddle's rule

To deduce the Weddle's rule, $n = 6$ is substituted in (7.100).

$$\begin{aligned}\int_a^b f(x)dx &= (b-a)\sum_{i=0}^{6} H_i y_i\\ &= 6h(H_0 y_0 + H_1 y_1 + H_2 y_2 + H_3 y_3 + H_4 y_4 + H_5 y_5 + H_6 y_6)\\ &= 6h[H_0(y_0 + y_6) + H_1(y_1 + y_5) + H_2(y_2 + y_4) + H_3 y_3].\end{aligned}$$

To find the values of H_i's one may use the result $H_i = H_{n-i}$. Also the value of H_3 can be obtained by the formula

$H_3 = 1 - (H_0 + H_1 + H_2 + H_4 + H_5 + H_6) = 1 - 2(H_0 + H_1 + H_2)$.

Now, $H_0 = \frac{1}{6} \cdot \frac{1}{6!} \int_0^6 \frac{s(s-1)(s-2)\cdots(s-6)}{s} ds = \frac{41}{840}$.

Similarly, $H_1 = \frac{216}{840}, H_2 = \frac{27}{840}, H_3 = \frac{272}{840}$.

Hence,

$$\int_a^b f(x)dx = \frac{h}{140}[41y_0 + 216y_1 + 27y_2 + 272y_3 + 27y_4 + 216y_5 + 41y_6]. \quad (7.107)$$

Again, we know that $\Delta^6 y_0 = y_0 - 6y_1 + 15y_2 - 20y_3 + 15y_4 - 6y_5 + y_6$,
i.e., $\frac{h}{140}[y_0 - 6y_1 + 15y_2 - 20y_3 + 15y_4 - 6y_5 + y_6] - \frac{h}{140}\Delta^6 y_0 = 0$.

Adding left hand side of above identity (as it is zero) to the right hand side of (7.107). After simplification the equation (7.107) finally reduces to

$$\int_a^b f(x)dx = \frac{3h}{10}[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6] - \frac{h}{140}\Delta^6 y_0.$$

The first term is the well known Weddle's rule and the last term is the error in addition to the truncation error.

Table 7.3: Weights of Newton-Cotes integration rule for different n.

n							
1	$\frac{1}{2}$	$\frac{1}{2}$					
2	$\frac{1}{3}$	$\frac{4}{3}$	$\frac{1}{3}$				
3	$\frac{3}{8}$	$\frac{9}{8}$	$\frac{9}{8}$	$\frac{3}{8}$			
4	$\frac{14}{45}$	$\frac{64}{45}$	$\frac{24}{45}$	$\frac{64}{45}$	$\frac{14}{45}$		
5	$\frac{95}{288}$	$\frac{375}{288}$	$\frac{250}{288}$	$\frac{250}{288}$	$\frac{375}{288}$	$\frac{95}{288}$	
6	$\frac{41}{140}$	$\frac{216}{140}$	$\frac{27}{140}$	$\frac{272}{140}$	$\frac{27}{140}$	$\frac{216}{140}$	$\frac{41}{140}$