Therefore, the error of approximation in the Simpson's rule becomes

$$R_2 = -\frac{(b-a)^5}{2880} f^{iv}(\eta) = -\frac{h^5}{90} f^{iv}(\eta). \tag{5.77}$$

When $n = 3$, the corresponding integration method is called **3/8th Simpson's rule**. The weights λ_k of the integration method (5.70) with $w(x) = 1$ for $n \le 6$ are given in Table 5.2.

Table 5.2. Weights of Newton-Cotes Integration Rule

$n\backslash\lambda$	λ_0	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	1/2	1/2					
2	1/3	4/3	1/3				
3	3/8	9/8	9/8	3/8			
4	14/45	64/45	24/45	64/45	14/45		
5	95/288	375/288	250/288	250/288	375/288	95/288	
6	41/140	216/140	27/140	272/140	27/140	216/140	41/140

Usually, for larger values of n, we get better approximation. However, for large $n\,(n \ge 8, n \ne 9)$ some of the weights become negative. This may cause loss of significant digits in the result, because of mutual cancellation. For this reason, higher order Newton-Cotes formulas are not commonly used.

The methods of the form (5.70) include the end points x_0 and x_n as abscissas. Such methods are also called **closed-type** methods.

The methods which do not include the end points as abscissas are often called **open-type** methods.

Open Type Integration Rules

We replace $f(x)$ in (5.59) by the Lagrange interpolating polynomial fitting the $n - 1$ data points (x_k, f_k), $k = 1(1)n - 1$ and integrate between the given limits. Some of the open-type integration methods $(w(x) = 1)$ together with the associated errors are listed below. The nodes are equispaced with $h = (b - a)/n$ and $x_0 = a$, $x_n = b$.

(i) *Mid-point rule* ($n = 2$), $x_0 = a$, $x_0 + h$, $x_0 + 2h = b$.

$$\int_a^b f(x)\,dx = 2hf(x_0 + h) + \frac{h^3}{3} f''(\xi_1). \tag{5.78}$$

(ii) *Two-point rule* ($n = 3$), $x_0 = a$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h = b$.

$$\int_a^b f(x)\,dx = \frac{3h}{2}[f(x_0 + h) + f(x_0 + 2h)] + \frac{3}{4} h^3 f''(\xi_2). \tag{5.79}$$

(iii) *Three-point rule* ($n = 4$), $x_0 = a$, $x_0 + h$, $x_0 + 2h$, $x_0 + 3h$, $x_0 + 4h = b$

$$\int_a^b f(x)\,dx = \frac{4h}{3}[2f(x_0 + h) - f(x_0 + 2h) + 2f(x_0 + 3h)]$$

$$+ \frac{14h^5}{45} f^{iv}(\xi_3). \tag{5.80}$$

where $a < \xi_1, \xi_2, \xi_3 < b$.

Chapter 5

Example 5.11 Find the approximate value of

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

using (i) trapezoidal rule, and (ii) Simpson's rule. Obtain a bound for the errors. The exact value of $I = \ln 2 = 0.693147$ correct to six decimal places.

Using the trapezoidal rule, we have

$$I \simeq \frac{1}{2}\left(1+\frac{1}{2}\right) = 0.75.$$

$$\text{Error} = 0.75 - 0.693147 = 0.056853.$$

The error in the trapezoidal rule is given by

$$|R_1| \le \frac{(b-a)^3}{12} \max_{0 \le x \le 1} |f''(x)| \le \frac{1}{12} \max_{0 \le x \le 1} \left| \frac{2}{(1+x)^3} \right| \le \frac{1}{6}.$$

Using the Simpson's rule, we have

$$I \simeq \frac{1}{6}\left(1+\frac{8}{3}+\frac{1}{2}\right) = \frac{25}{36} = 0.694444.$$

$$\text{Error} = 0.694444 - 0.693147 = 0.001297.$$

The error in the Simpson's rule is given by

$$|R_2| \le \frac{(b-a)^5}{2880} \max_{0 \le x \le 1} |f^{iv}(x)| \le \frac{1}{2880} \max_{0 \le x \le 1} \left| \frac{24}{(1+x)^5} \right| = 0.008333.$$

We note that in both cases, the actual error is much smaller than the error bounds obtained from theoretical considerations.

Example 5.12 Find the approximate value of

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

using (i) mid-point rule and (ii) two-point open type rule.

(i) *Mid-point rule.* We have $h = [(b-a)/2] = 1/2$ Therefore, $x_0 = 0$, $x_1 = 1/2$ and $x_2 = 1$.

$$I = \int_0^1 f(x)\, dx = 2hf(x_0 + h) = f\left(\frac{1}{2}\right) = 2\sin\left(\frac{1}{2}\right) = 0.9589.$$

(ii) *Two-point rule.* We have $h = [(b-a)/3] = 1/3$. Therefore, $x_0 = 0$, $x_1 = 1/3$, $x_2 = 2/3$ and $x_3 = 1$.

$$I = \int_0^1 f(x)\, dx = \frac{3h}{2}\, [f(x_0 + h) + f(x_0 + 2h)]$$

$$= \frac{1}{2}\left[f\left(\frac{1}{3}\right) + f\left(\frac{2}{3}\right)\right]$$

$$= \frac{1}{2}\left[3\sin\left(\frac{1}{3}\right) + \frac{3}{2}\sin\left(\frac{2}{3}\right)\right] = 0.9546.$$

Example 5.13 Find the remainder of the Simpson three-eighth rule

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\,[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

for equally spaced points $x_i = x_0 + ih$, $i = 1, 2, 3$. Use this rule to approximate the value of the integral

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

Also, find a bound on the error.

Using (5.61) and definition 5.2, we can show that the rule is exact for $f(x) = 1, x, x^2, x^3$. For example, for $f(x) = 1$, we get

$$\int_{x_0}^{x_3} dx = (x_3 - x_0) = \frac{3h}{8}\,[8] = 3h$$

which is true. The error constant is given by

$$C = \int_{x_0}^{x_3} x^4\,dx - \frac{3h}{8}\,[x_0^4 + 3x_1^4 + 3x_2^4 + x_3^4]$$

$$= \frac{1}{5}\,[(x_0 + 3h)^5 - x_0^5] - \frac{3h}{8}\,[x_0^4 + 3(x_0 + h)^4 + 3(x_0 + 2h)^4 + (x_0 + 3h)^4]$$

$$= \frac{1}{5}\,[x_0^5 + 15x_0^4 h + 90x_0^3 h^2 + 270x_0^2 h^3 + 405x_0 h^4 + 243h^5 - x_0^5]$$

$$- \frac{3h}{8}\,[x_0^4 + 3(x_0^4 + 4x_0^3 h + 6x_0^2 h^2 + 4x_0 h^3 + h^4)$$

$$+ 3(x_0^4 + 8hx_0^3 + 24x_0^2 h^2 + 32x_0 h^3 + 16h^4)$$

$$+ (x_0^4 + 12x_0^3 \quad + 54x_0^2 h^2 + 108x_0 h^3 + 81h^4)]$$

$$= \left[\frac{243}{5} - \frac{99}{2}\right] h^5 = -\frac{9}{10}\,h^5.$$

Therefore, the error term is given by

$$\boxed{E = \frac{C}{4!} f^{iv}(\eta) = -\frac{9h^5}{10 \times 24} f^{iv}(\eta) = -\frac{3}{80}\,h^5 f^{iv}(\eta),} \quad x_0 < \eta < x_3.$$

We have $x_0 = 0$, $x_1 = 1/3$, $x_2 = 2/3$, $x_3 = 1$, $h = 1/3$. Therefore,

$$I = \frac{3}{8}\left(\frac{1}{3}\right)\left[f(0)+3f\left(\frac{1}{3}\right)+3f\left(\frac{2}{3}\right)+f(1)\right]$$

$$= \frac{1}{8}\left[1+\frac{9}{4}+\frac{9}{5}+\frac{1}{2}\right] = 0.69375.$$

5.8 METHODS BASED ON UNDETERMINED COEFFICIENTS

The Newton-Cotes methods derived in the previous section can also be obtained using the approach of method of undetermined coefficients. The Newton-Cotes methods are given by

$$\int_a^b f(x)\, dx = \sum_{k=0}^{n} \lambda_k f_k .$$

We shall derive the Trapezoidal and Simpson methods using the method of undetermined coefficients.

Newton-Cotes Methods

Trapezoidal method

We have $n = 1$, $x_0 = a$, $x_1 = b$ and $h = x_1 - x_0$. We write

$$\int_{x_0}^{x_1} f(x)\, dx = \lambda_0 f(x_0) + \lambda_1 f(x_1).$$

Using (5.61) and definition 5.2, the rule can be made exact for polynomials of degree upto one. For $f(x) = 1$ and x, we get the system of equations

$$f(x) = 1: x_1 - x_0 = \lambda_0 + \lambda_1, \text{ or } h = \lambda_0 + \lambda_1$$

$$f(x) = x: \frac{1}{2}(x_1^2 - x_0^2) = \lambda_0 x_0 + \lambda_1 x_1.$$

We have $$\frac{1}{2}(x_1 - x_0)(x_1 + x_0) = \lambda_0 x_0 + \lambda_1 x_1$$

or $$\frac{1}{2} h (2x_0 + h) = \lambda_0 x_0 + \lambda_1 (x_0 + h)$$

or $$\frac{1}{2} h (2x_0 + h) = (\lambda_0 + \lambda_1) x_0 + \lambda_1 h = h x_0 + \lambda_1 h$$

or $$\lambda_1 h = \frac{h^2}{2}, \text{ or } \lambda_1 = \frac{h}{2}.$$

From the first equation, we get $\lambda_0 = h - \lambda_1 = h/2$. The method becomes

$$\boxed{\int_{x_0}^{x_1} f(x)\, dx = \frac{h}{2}[f(x_0) + f(x_1)].}$$

From (5.69), the error constant is given by

$$C = \int_{x_0}^{x_1} x^2\, dx - \frac{h}{2}[x_0^2 + x_1^2] = \frac{1}{3}[x_1^3 - x_0^3] - \frac{h}{2}[x_0^2 + x_1^2]$$

$$= \frac{1}{6}\,[2(x_0^3 + 3x_0^2 h + 3x_0 h^2 + h^3) - 2x_0^3 - 3x_0^2 h$$
$$-3h(x_0^2 + 2x_0 h + h^2)]$$
$$= -\frac{h^3}{6}.$$

The truncation error becomes

$$R_1 = \frac{C}{2} f''(\xi) = -\frac{h^3}{12} f''(\xi), \quad x_0 < \xi < x_1.$$

Simpson's method

We have $n = 2$, $x_0 = a$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h = b$, $h = (b - a)/2$. We write

$$\int_{x_0}^{x_2} f(x)\,dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2).$$

The rule can be made exact for polynomials of degree upto two.

For $f(x) = 1, x, x^2$, we get the following system of equations.

$$f(x) = 1: x_2 - x_0 = \lambda_0 + \lambda_1 + \lambda_2, \text{ or } 2h = \lambda_0 + \lambda_1 + \lambda_2 \tag{5.81 a}$$

$$f(x) = x: \frac{1}{2}(x_2^2 - x_0^2) = \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 \tag{5.81 b}$$

$$f(x) = x^2: \frac{1}{3}(x_2^3 - x_0^3) = \lambda_0 x_0^2 + \lambda_1 x_1^2 + \lambda_2 x_2^2. \tag{5.81 c}$$

From (5.81 *b*), we get

$$\frac{1}{2}(x_2 - x_0)(x_2 + x_0) = \lambda_0 x_0 + \lambda_1(x_0 + h) + \lambda_2(x_0 + 2h)$$

or

$$\frac{1}{2}(2h)(2x_0 + 2h) = (\lambda_0 + \lambda_1 + \lambda_2)x_0 + (\lambda_1 + 2\lambda_2)h$$
$$= 2h\,x_0 + (\lambda_1 + 2\lambda_2)h \quad \text{using (5.81 } a)$$

or

$$2h = \lambda_1 + 2\lambda_2. \tag{5.81 d}$$

From (5.81 *c*), we get

$$\frac{1}{3}\,[(x_0^3 + 6x_0^2 h + 12x_0 h^2 + 8h^3) - x_0^3] = \lambda_0 x_0^2 + \lambda_1 (x_0^2 + 2x_0 h + h^2)$$
$$+ \lambda_2(x_0^2 + 4x_0 h + 4h^2)$$

or

$$2x_0^2 h + 4x_0 h^2 + \frac{8}{3} h^3 = (\lambda_0 + \lambda_1 + \lambda_2)x_0^2 + 2(\lambda_1 + 2\lambda_2)x_0 h + (\lambda_1 + 4\lambda_2)h^2$$
$$= 2h\,x_0^2 + 4x_0 h^2 + (\lambda_1 + 4\lambda_2)h^2$$

Chapter 5

$$\text{or} \qquad \frac{8}{3}h = \lambda_1 + 4\lambda_2. \tag{5.81 e}$$

Solving (5.81*d*), (5.81*e*) and using (5.81 *a*), we obtain $\lambda_0 = h/3$, $\lambda_1 = 4h/3$, $\lambda_2 = h/3$. The method is given by

$$\boxed{\int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}\,[f(x_0) + 4f(x_1) + f(x_2)].}$$

From (5.76), the error constant is given by

$$C = -\frac{(b-a)^5}{120} = -\frac{4}{15}h^5$$

and

$$R_2 = \frac{C}{4!} f^{iv}(\eta) = -\frac{h^5}{90} f^{iv}(\eta), \quad x_0 < \eta < x_2.$$

The method of undetermined coefficients can be used to derive quadrature formulas of a given type. We illustrate such derivations through the following examples.

Example 5.14 Determine a, b and c such that the formula

$$\int_0^h f(x)\, dx = h\left\{af(0) + bf\left(\frac{h}{3}\right) + cf(h)\right\}$$

is exact for polynomials of as high order as possible, and determine the order of the truncation error.

(Uppsala Univ., Sweden, BIT 13(1973), 123)

Making the method exact for polynomials of degree upto 2, we obtain

for $f(x) = 1$: $\quad h = h(a + b + c)$, or $a + b + c = 1$.

for $f(x) = x$: $\quad \dfrac{h^2}{2} = h\left(\dfrac{bh}{3} + ch\right)$, or $\dfrac{1}{3}b + c = \dfrac{1}{2}$.

for $f(x) = x^2$: $\quad \dfrac{h^3}{3} = h\left(\dfrac{bh^2}{9} + ch^2\right)$, or $\dfrac{1}{9}b + c = \dfrac{1}{3}$.

Solving the above equations, we get

$$a = 0, \quad b = 3/4, \text{ and } \quad c = 1/4.$$

The truncation error of the formula is given by

$$TE = \frac{C}{3!} f'''(\xi), \quad 0 < \xi < h$$

and

$$C = \int_0^h x^3\, dx - h\left[\frac{bh^3}{27} + ch^3\right] = -\frac{h^4}{36}.$$

Hence, we have

$$TE = -\frac{h^4}{216} f'''(\xi) = O(h^4).$$

Example 5.15 Find the quadrature formula

$$\int_0^1 f(x) \frac{dx}{\sqrt{x(1-x)}} = \alpha_1 f(0) + \alpha_2 f\left(\frac{1}{2}\right) + \alpha_3 f(1)$$

which is exact for polynomials of highest possible degree. Then use the formula on

$$\int_0^1 \frac{dx}{\sqrt{x - x^3}}$$

and compare with the exact value.

(Oslo Univ., Norway, BIT 7(1967), 170)

Making the method exact for polynomials of degree upto 2, we obtain

$$\text{for} \quad f(x) = 1: \quad I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = \alpha_1 + \alpha_2 + \alpha_3$$

$$\text{for} \quad f(x) = x: \quad I_2 = \int_0^1 \frac{x\,dx}{\sqrt{x(1-x)}} = \frac{1}{2}\alpha_2 + \alpha_3$$

$$\text{for} \quad f(x) = x^2: \quad I_3 = \int_0^1 \frac{x^2\,dx}{\sqrt{x(1-x)}} = \frac{1}{4}\alpha_2 + \alpha_3$$

where

$$I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = 2\int_0^1 \frac{dx}{\sqrt{1-(2x-1)^2}} = \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \left[\sin^{-1} t\right]_{-1}^1 = \pi$$

$$I_2 = \int_0^1 \frac{x\,dx}{\sqrt{x(1-x)}} = 2\int_0^1 \frac{x\,dx}{\sqrt{1-(2x-1)^2}} = \int_{-1}^1 \frac{t+1}{2\sqrt{1-t^2}}\,dt$$

$$= \frac{1}{2}\int_{-1}^1 \frac{t\,dt}{\sqrt{1-t^2}} + \frac{1}{2}\int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \frac{\pi}{2}.$$

$$I_3 = \int_0^1 \frac{x^2\,dx}{\sqrt{x(1-x)}} = 2\int_0^1 \frac{x^2\,dx}{\sqrt{1-(2x-1)^2}} = \frac{1}{4}\int_{-1}^1 \frac{(t+1)^2}{\sqrt{1-t^2}}\,dt$$

$$= \frac{1}{4}\int_{-1}^1 \frac{t^2}{\sqrt{1-t^2}}\,dt + \frac{1}{2}\int_{-1}^1 \frac{t}{\sqrt{1-t^2}}\,dt + \frac{1}{4}\int_{-1}^1 \frac{dt}{\sqrt{1-t^2}}$$

$$= \frac{3\pi}{8}.$$

Chapter 5

Hence, we have the equations

$$\alpha_1 + \alpha_2 + \alpha_3 = \pi$$

$$\frac{1}{2}\alpha_2 + \alpha_3 = \frac{\pi}{2}$$

$$\frac{1}{4}\alpha_2 + \alpha_3 = \frac{3\pi}{8}$$

which gives

$$\alpha_1 = \pi/4, \quad \alpha_2 = \pi/2, \quad \alpha_3 = \pi/4.$$

The quadrature formula is given by

$$\int_0^1 \frac{f(x)\,dx}{\sqrt{x(1-x)}} = \frac{\pi}{4}\left[f(0) + 2f\left(\frac{1}{2}\right) + f(1)\right]$$

We now use this formula to evaluate

$$I = \int_0^1 \frac{dx}{\sqrt{x - x^3}} = \int_0^1 \frac{dx}{\sqrt{1+x}\,\sqrt{x(1-x)}} = \int_0^1 \frac{f(x)\,dx}{\sqrt{x(1-x)}}$$

where $f(x) = 1/\sqrt{1+x}$.

We obtain

$$I = \frac{\pi}{4}\left[1 + \frac{2\sqrt{2}}{\sqrt{3}} + \frac{\sqrt{2}}{2}\right] \approx 2.62331.$$

The exact value is $I = 2.62205755$.

Gauss Quadrature Methods

In the integration method (5.70), the nodes x_k's and the weights λ_k's, $k = 0(1)n$ can also be obtained by making the formula exact for polynomials of degree upto m. When the nodes are known, that is, $m = n$, the corresponding methods are called Newton-Cotes methods. When the nodes are also to be determined, we have $m = 2n + 1$ and the methods are called **Gaussian integration methods.** Since any finite interval $[a, b]$ can always be transformed to $[-1, 1]$, using the transformation

$$x = \frac{b-a}{2}t + \frac{b+a}{2}$$

we consider the integral in the form

$$\int_{-1}^{1} w(x)\, f(x)\, dx = \sum_{k=0}^{n} \lambda_k f_k \tag{5.82}$$

where $w(x) > 0$, $-1 \le x \le 1$, is the weight function.

Gauss-Legendre Integration Methods

Let the weight function be $w(x) = 1$. Then, the method (5.82) reduces to

$$\int_{-1}^{1} f(x)\, dx = \sum_{k=0}^{n} \lambda_k f(x_k). \tag{5.83}$$

In this case, all the nodes x_k and weights λ_k are unknown. Consider the following cases.

1 *One-point formula* $n = 0$. The formula is given by

$$\int_{-1}^{1} f(x)\, dx = \lambda_0 f(x_0). \tag{5.84}$$

The method has two unknowns λ_0, x_0. Making the method exact for $f(x) = 1, x$, we get

$$f(x) = 1: \quad 2 = \lambda_0$$

$$f(x) = x: \quad 0 = \lambda_0 x_0 \text{ or } x_0 = 0.$$

Hence, the method is given by

$$\int_{-1}^{1} f(x)\, dx = 2f(0) \tag{5.85}$$

which is same as the mid-point formula. The error constant is given by

$$C = \int_{-1}^{1} x^2\, dx - 2[0] = \frac{2}{3}.$$

Hence,
$$R_1 = \frac{C}{2!} f''(\xi) = \frac{1}{3} f''(\xi), \quad -1 < \xi < 1.$$

2 *Two-point formula* $n = 1$. The formula is given by

$$\int_{-1}^{1} f(x)\, dx = \lambda_0 f(x_0) + \lambda_1 f(x_1). \tag{5.86}$$

The method has four unknowns, x_0, x_1, λ_0 and λ_1. Making the method exact for $f(x) = 1, x, x^2, x^3$, we get

$$f(x) = 1 \quad : \quad 2 = \lambda_0 + \lambda_1 \tag{5.87 a}$$

$$f(x) = x \quad : \quad 0 = \lambda_0 x_0 + \lambda_1 x_1 \tag{5.87 b}$$

$$f(x) = x^2 \quad : \quad \frac{2}{3} = \lambda_0 x_0^2 + \lambda_1 x_1^2 \tag{5.87 c}$$

$$f(x) = x^3 \quad : \quad 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3. \tag{5.87 d}$$

Eliminating λ_0 from (5.87 *b*), (5.87 *d*), we get

$$\lambda_1 x_1^3 - \lambda_1 x_1 x_0^2 = 0, \text{ or } \lambda_1 x_1 (x_1 - x_0)(x_1 + x_0) = 0.$$

Chapter 5

Since $\lambda_1 \neq 0$, $x_0 \neq x_1$, we get $x_1 + x_0 = 0$ or $x_1 = -x_0$. Note that if $x_1 = 0$, then from (5.87 *b*), we get $x_0 = 0$ since $\lambda_0 \neq 0$. Therefore, $x_1 \neq 0$.

Substituting in (5.87 *b*), we get $\lambda_0 - \lambda_1 = 0$, or $\lambda_0 = \lambda_1$.

Substituting in (5.87 *a*), we get $\lambda_0 = \lambda_1 = 1$.

Using (5.87 *c*), we get $x_0^2 = 1/3$, or $x_0 = \pm 1/\sqrt{3}$, and $x_1 = \mp 1/\sqrt{3}$. Therefore, the two-point Gauss-Legendre method is given by

$$\boxed{\int_{-1}^{1} f(x)\, dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).} \tag{5.88}$$

The error constant is given by

$$C = \int_{-1}^{1} x^4\, dx - \left[\frac{1}{9} + \frac{1}{9}\right] = \frac{2}{5} - \frac{2}{9} = \frac{8}{45}.$$

The error term R_4 becomes

$$R_4 = \frac{C}{4!} f^{(4)}(\xi) = \frac{1}{135} f^{(4)}(\xi), \quad -1 < \xi < 1. \tag{5.89}$$

5 *Three-point formula* $n = 2$. The method is given by

$$\int_{-1}^{1} f(x)\, dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2).$$

There are six unknowns in the method and it can be made exact for polynomials of degree upto five. For $f(x) = x^i$, $i = 0(1)5$, we get the system of equations

$$f(x) = 1 \; : \; \lambda_0 + \lambda_1 + \lambda_2 = 2 \tag{5.90 a}$$

$$f(x) = x \; : \; \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 = 0 \tag{5.90 b}$$

$$f(x) = x^2 \; : \; \lambda_0 x_0^2 + \lambda_1 x_1^2 + \lambda_2 x_2^2 = \frac{2}{3} \tag{5.90 c}$$

$$f(x) = x^3 \; : \; \lambda_0 x_0^3 + \lambda_1 x_1^3 + \lambda_2 x_2^3 = 0 \tag{5.90 d}$$

$$f(x) = x^4 \; : \; \lambda_0 x_0^4 + \lambda_1 x_1^4 + \lambda_2 x_2^4 = \frac{2}{5} \tag{5.90 e}$$

$$f(x) = x^5 \; : \; \lambda_0 x_0^5 + \lambda_1 x_1^5 + \lambda_2 x_2^5 = 0. \tag{5.90 f}$$

Eliminating λ_0 from (5.90 *b*), (5.90 *d*) and (5.90 *d*), (5.90 *f*), we get

$$\lambda_1 x_1(x_1^2 - x_0^2) + \lambda_2 x_2(x_2^2 - x_0^2) = 0$$

$$\lambda_1 x_1^3(x_1^2 - x_0^2) + \lambda_2 x_2^3(x_2^2 - x_0^2) = 0.$$

Eliminating the first term from these two equations, we get

$$\lambda_2 x_2^3(x_2^2 - x_0^2) - \lambda_2 x_2 x_1^2 (x_2^2 - x_0^2) = 0$$

or

$$\lambda_2 x_2(x_2^2 - x_0^2)(x_2^2 - x_1^2) = 0.$$

Since x_0, x_1, x_2 are distinct, we get on cancelling the terms $(x_2 - x_0)$ and $(x_2 - x_1)$

$$\lambda_2\, x_2(x_2 + x_0)\,(x_2 + x_1) = 0.$$

We have $\lambda_2 \neq 0$ and let $x_2 \neq 0$. Then, we have either $x_2 = -\,x_0$ or $x_2 = -\,x_1$. Let $x_2 = -\,x_0$. Then, from (5.90 b), (5.90 d), we get

$$(\lambda_0 - \lambda_2)x_0 + \lambda_1\, x_1 = 0$$

$$(\lambda_0 - \lambda_2)x_0^3 + \lambda_1\, x_1^3 = 0.$$

Eliminating the first term, we get $\lambda_1 x_1\,(x_1^2 - x_0^2) = 0$. Since, $\lambda_1 \neq 0$, $x_1 \neq x_0$, $x_1 \neq -\,x_0$ (otherwise $x_1 = x_2$), we get $x_1 = 0$.

Hence, $(\lambda_0 - \lambda_2)\, x_0 = 0$, or $\lambda_0 = \lambda_2$ since $x_0 \neq 0$.

Now, (5.90 c), (5.90 e) give

$$2\lambda_0\, x_0^2 = \frac{2}{3},\quad 2\lambda_0\, x_0^4 = \frac{2}{5}.$$

Dividing, we get $x_0^2 = 3/5$, or $x_0 = \pm\sqrt{3/5}$. Then $x_2 = \mp\sqrt{3/5}$.

Now, $\lambda_0\, x_0^2 = 1/3$ gives $\lambda_0 = 5/9$ and $\lambda_2 = \lambda_0 = 5/9$. From (5.90$a$), we get $\lambda_1 = 2 - 2\lambda_2 = 8/9$.

Therefore, the three-point Gauss-Legendre method is given by

$$\boxed{\int_{-1}^{1} f(x)\, dx = \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right]} \qquad (5.91)$$

If we take $x_2 = -\,x_1$, then we get $x_0 = 0$ and $x_2 = \pm\sqrt{3/5}$ giving the same method. The nodes are symmetrically placed about $x = 0$.

The error constant is given by

$$C = \int_{-1}^{1} x^6\, dx - \frac{1}{9}\left[5\left(-\sqrt{\frac{3}{5}}\right)^6 + 0 + 5\left(\sqrt{\frac{3}{5}}\right)^6\right]$$

$$= \frac{2}{7} - \frac{6}{25} = \frac{8}{175}.$$

The error in the method becomes

$$\boxed{R_6 = \frac{C}{6!}\, f^{(6)}(\xi) = \frac{8}{(6!)175}\, f^{(6)}(\xi) = \frac{1}{15750}\, f^{(6)}(\xi),\ -1 < \xi < 1.}$$

In the later part of this section, we shall prove that the abscissas of the above formulas are the zeros of the Legendre polynomials of the corresponding order. Hence, they are called the Gauss-Legendre quadrature methods.

The nodes and the corresponding weights for the **Gauss-Legendre integration method** (5.83) for $n = 1(1)5$ are given in Table 5.3.

Chapter 5

Scanned with CamScanner

Table 5.3 Nodes and Weights for Gauss-Legendre Integration Method (5.83).

n	nodes x_k	weights λ_k
1	±0.5773502692	1.0000000000
2	0.0000000000	0.8888888889
	±0.7745966692	0.5555555556
3	±0.3399810436	0.6521451549
	±0.8611363116	0.3478548451
4	0.0000000000	0.5688888889
	±0.5384693101	0.4786286705
	±0.9061798459	0.2369268851
5	±0.2386191861	0.4679139346
	±0.6612093865	0.3607615730
	±0.9324695142	0.1713244924

Example 5.16 Evaluate the integral

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

using Gauss-Legendre three-point formula.

First we transform the interval [0, 1] to the interval [–1, 1]. Let $t = ax + b$. We have

$$-1 = b, \quad 1 = a + b$$

$$a = 2, \quad b = -1, \text{ and } t = 2x - 1.$$

or

$$I = \int_0^1 \frac{dx}{1+x} = \int_{-1}^1 \frac{dt}{t+3}.$$

Using Gauss-Legendre three-point rule (corresponding to $n = 2$), we get

$$I = \frac{1}{9}\left[\overset{5}{\cancel{8}}\left(\frac{1}{0+3}\right) + \overset{8}{\cancel{5}}\left(\frac{1}{3+\sqrt{3/5}}\right) + 5\left(\frac{1}{3-\sqrt{3/5}}\right)\right]$$

$$= \frac{131}{189} = 0.693122.$$

The exact solution is $I = \ln 2 = 0.693147$.

Example 5.17 Evaluate the integral $I = \int_1^2 \frac{2x\,dx}{1+x^4}$, using the Gauss-Legendre 1-point, 2-point and 3-point quadrature rules. Compare with the exact solution

$$I = \tan^{-1}(4) - (\pi/4).$$

To use the Gauss-Legendre rules, the interval [1, 2] is to be reduced to [−1, 1]. Writing $x = at + b$, we get

$$1 = -a + b, \quad 2 = a + b$$

whose solution is $b = 3/2$, $a = 1/2$. Therefore, $x = (t + 3)/2$, $dx = dt/2$ and

$$I = \int_{-1}^{1} \frac{8(t+3)\,dt}{[16+(t+3)^4]} = \int_{-1}^{1} f(t)dt.$$

Using the 1-point rule, we get

$$I = 2\,f(0) = 2\left[\frac{24}{16+81}\right] = 0.4948.$$

Using the 2-point rule, we get

$$I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = 0.3842 + 0.1592 = 0.5434.$$

Using the 3-point rule, we get

$$I = \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right]$$

$$= \frac{1}{9}\,[5(0.4393) + 8(0.2474) + 5(0.1379)] = 0.5406.$$

The exact solution is $I = 0.5404$.

Gauss-Chebyshev Integration

5.9 COMPOSITE INTEGRATION METHODS

As the order of the integration method (5.60) is increased, the order of the derivative in the error term associated with the method, also increases. For any method to produce meaningful results, these higher order derivatives must remain continuous in the interval of interest. Also, Newton-Cotes type methods of higher order sometimes produce diverging results. An alternative to obtain accurate results, while using lower order methods is the use of composite integration methods. We subdivide the given interval $[a, b]$ or $[-1, 1]$ into a number of subintervals and evaluate the integral in each subinterval by a particular method.

Trapezoidal Rule

We divide the interval $[a, b]$ into N subintervals, each of length $h = (b - a)/N$. We denote the subintervals as (x_0, x_1), (x_1, x_2), $\cdots$, (x_{N-1}, x_N) where $x_0 = a$, $x_N = b$ and $x_i = x_0 + ih$, $i = 1(1)N - 1$. We write

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

$$= \int_{x_0}^{x_1} f(x)\, dx + \int_{x_1}^{x_2} f(x)\, dx + \cdots + \int_{x_{N-1}}^{x_N} f(x)\, dx. \quad (5.141)$$

Evaluating each of the integrals on the right hand side of (5.141) by the trapezoidal rule (5.73), we get

$$I = \frac{h}{2}\, [(f_0 + f_1) + (f_1 + f_2) + \cdots + (f_{N-1} + f_N)]$$

$$= \frac{h}{2}[f_0 + 2(f_1 + f_2 + \cdots + f_{N-1}) + f_N] \quad (5.142)$$

where $f_k = f(x_k)$, $k = 0(1)N$. The formula (5.142) is called the **composite trapezoidal rule**. The error in the integration method (5.142) becomes

$$R_1 = -\frac{h^3}{12}\, [f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_N)] \quad (5.143)$$

where $x_{i-1} \le \xi_i \le x_i$, $i = 1, 2, \cdots, N$.
If $f''(x)$ is constant for all x in $[a, b]$ or if

$$f''(\eta) = \max_{a \le x \le b} |f''(x)|, \quad a < \eta < b$$

we may write (5.143) as

$$|R_1| \le \frac{h^3 N}{12} f''(\eta).$$

Since $h = (b - a)/N$, we have

$$|R_1| \le \frac{(b-a)^3}{12N^2} f''(\eta) = \frac{(b-a)}{12} h^2 f''(\eta). \quad (5.144)$$

The factor N in the denominator in the error term (5.144) reduces the error considerably for large N. The number of intervals may be odd or even in this case.

Chapter 5

Simpson's Rule

In using the Simpson's rule of integration (5.75), we need three abscissas. We divide the interval $[a, b]$ into an even number of subintervals of equal length giving an odd number of abscissas. If we divide the interval $[a, b]$ into $2N$ subintervals each of length $h = (b - a)/(2N)$, then we get $2N + 1$ abscissas $x_0, x_1, \cdots, x_{2N}, x_0 = a, x_{2N} = b, x_i = x_0 + ih, i = 1, 2, \cdots, 2N - 1$. We write

$$I = \int_a^b f(x)\, dx = \int_{x_0}^{x_2} f(x)\, dx + \int_{x_2}^{x_4} f(x)\, dx + \cdots$$

$$+ \int_{x_{2N-2}}^{x_{2N}} f(x)\, dx. \tag{5.145}$$

Evaluating each of the integrals on the right hand side of (5.145) by the Simpson's rule (5.75), we get

$$I = \frac{h}{3} [(f_0 + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + \cdots + (f_{2N-2} + 4f_{2N-1} + f_{2N})]$$

$$= \frac{h}{3} [(f_0 + 4(f_1 + f_3 + \cdots + f_{2N-1}) + 2(f_2 + f_4 + \cdots + f_{2N-2}) + f_{2N}] \tag{5.146}$$

The formula (5.146) is called the **composite Simpson's rule**. The error in the integration method (5.146) becomes

$$R_2 = -\frac{h^5}{90} [f^{iv}(\xi_1) + f^{iv}(\xi_2) + \cdots + f^{iv}(\xi_N)] \tag{5.147}$$

where $x_{2i-2} < \xi_i < x_{2i}, \quad i = 1, 2, \cdots, N$.
Using

$$f^{iv}(\eta) = \max_{a \le x \le b} |f^{iv}(x)|, \quad a < \eta < b$$

we can write (5.147) in the form

$$|R_2| \le \frac{Nh^5}{90} f^{iv}(\eta) = \frac{(b-a)^5}{2880N^4} f^{iv}(\eta)$$

$$= \boxed{\frac{(b-a)}{180} h^4 f^{iv}(\eta).} \tag{5.148}$$

Similarly, composite rules in other cases may be obtained.

Example 5.26 Evaluate the integral

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

using (i) composite trapezoidal rule, (ii) composite Simpson's rule, with 2, 4 and 8 equal subintervals.

When $N = 2$, we have $h = 1/2$ and three nodes, 0, 1/2 and 1. Let I_T and I_S represent the values obtained by using the trapezoidal rule and Simpson's rule respectively. We have two subintervals for trapezoidal rule and only one interval for Simpson's rule.

We have

$$I_T = \frac{1}{4}\left[f(0) + 2f\left(\frac{1}{2}\right) + f(1)\right] = \frac{1}{4}\left(1 + \frac{4}{3} + \frac{1}{2}\right) = \frac{17}{24}$$

$$= 0.708333.$$

$$I_S = \frac{1}{6}\left[f(0) + 4f\left(\frac{1}{2}\right) + f(1)\right] = \frac{1}{6}\left(1 + \frac{8}{3} + \frac{1}{2}\right) = \frac{25}{36}$$

$$= 0.694444.$$

When $N = 4$, we have $h = 1/4$ and five nodes 0, 1/4, 2/4, 3/4 and 1. We have four subintervals for trapezoidal rule and two subintervals for Simpson's rule. We get

$$I_T = \frac{1}{8}\left[f(0) + 2\left(f\left(\frac{1}{4}\right) + f\left(\frac{1}{2}\right) + f\left(\frac{3}{4}\right)\right) + f(1)\right]$$

$$= 0.697024.$$

$$I_S = \frac{1}{12}\left[f(0) + 4f\left(\frac{1}{4}\right) + 2f\left(\frac{1}{2}\right) + 4f\left(\frac{3}{4}\right) + f(1)\right]$$

$$= 0.693254.$$

When $N = 8$ we have $h = 1/8$ and nine nodes 0, 1/8, 2/8, $\cdots$, 1. We have eight subintervals for trapezoidal rule and four subintervals for Simpson's rule. We get

$$I_T = \frac{1}{16}\left[f(0) + 2\sum_{i=1}^{7} f\left(\frac{i}{8}\right) + f(1)\right]$$

$$= 0.694122.$$

$$I_S = \frac{1}{24}\left[f(0) + 4\sum_{i=1}^{4} f\left(\frac{2i-1}{8}\right) + 2\sum_{i=1}^{3} f\left(\frac{2i}{8}\right) + f(1)\right]$$

$$= 0.693155.$$

The exact value of the integral is $I = 0.693147$.

Example 5.27 Evaluate the integral

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

by subdividing the interval [0, 1] into two equal parts and then applying the Gauss-Legendre three-point formula

$$\int_{-1}^{1} f(x)\,dx = \frac{1}{9}\left[5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right)\right]$$

We write

$$\int_0^1 \frac{dx}{1+x} = \int_0^{1/2} \frac{dx}{1+x} + \int_{1/2}^1 \frac{dx}{1+x} = I_1 + I_2.$$

The transformations $t = 4x - 1$ and $y = 4x - 3$ in the first and second integrals respectively, change the limits of integration to [–1, 1]. Thus we have

$$I = \int_{-1}^{1} \frac{dt}{t+5} + \int_{-1}^{1} \frac{dy}{y+7} = I_1 + I_2.$$

Evaluating each of the integrals I_1 and I_2 by the Gauss-Legendre three-point formula, we get

$$I_1 = \frac{1}{9}\left[\frac{5}{5-\sqrt{3/5}} + \frac{8}{5} + \frac{5}{5+\sqrt{3/5}}\right] = 0.405464.$$

$$I_2 = \frac{1}{9}\left[\frac{5}{7-\sqrt{3/5}} + \frac{8}{7} + \frac{5}{7+\sqrt{3/5}}\right] = 0.287682.$$

Therefore,

$$\begin{aligned} I &= I_1 + I_2 \\ &= 0.405464 + 0.287682 = 0.693146. \end{aligned}$$

The exact value of I is 0.693147.

5.10 ROMBERG INTEGRATION

Richardson's extrapolation procedure described in section 5.4, applied to the integration methods, is called **Romberg integration**. First, we find the power series expansion of the error term in the integration method. Then, by eliminating the leading terms in the error expansion by using the computed results, we obtain new methods which are of higher order than the previous methods. Consider the integral

$$I = \int_a^b f(x)\ dx. \tag{5.149}$$

The errors in the composite trapezoidal rule (5.142) and the composite Simpson's rule (5.146) can be obtained as

$$I = I_T + c_1 h^2 + c_2 h^4 + c_3 h^6 + \cdots \tag{5.150}$$

$$I = I_S + d_1 h^4 + d_2 h^6 + d_3 h^8 + \cdots \tag{5.151}$$

where c's and d's are constants independent of h.

The extrapolation procedure for the trapezoidal rule as given by (5.52) becomes

$$I_T^{(m)}(h) = \frac{4^m I_T^{(m-1)}(h/2) - I_T^{(m-1)}(h)}{4^m - 1}, \quad m = 1, 2, \cdots \tag{5.152}$$

The extrapolation procedure for the Simpson's rule becomes

$$I_S^{(m)}(h) = \frac{4^{m+1} I_S^{(m-1)}(h/2) - I_S^{(m-1)}(h)}{4^{m+1} - 1}, \quad m = 1, 2, \cdots \tag{5.153}$$

Example 5.28 Find the approximate value of the integral

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

using (i) composite trapezoidal rule with 2, 3, 5, 9 nodes and Romberg integration, (ii) composite Simpson's rule with 3, 5, 9 nodes and Romberg integration. Obtain the number of function evaluations required to get an accuracy of 10^{-6} when the integral is evaluated directly by using the trapezoidal and Simpson's rules.

Using the composite trapezoidal rule

$$I = \int_a^b f(x)\,dx = \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{N-1} f_i + f_N \right]$$

where $x_0 = a$, $x_N = b$, $h = (b - a)/N$, $x_i = x_0 + ih$, we get

$$N = 1,\ h = 1,\ I_T = \frac{h}{2}\,[f_0 + f_1] = 0.750000.$$

$$N = 2,\ h = \frac{1}{2},\ I_T = \frac{h}{2}\,[f_0 + 2f_1 + f_2] = 0.708333.$$

$$N = 4,\ h = \frac{1}{4},\ I_T = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + 2f_3 + f_4] = 0.697024.$$

$$N = 8,\ h = \frac{1}{8},\ I_T = \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{7} f_i + f_8 \right] = 0.694122.$$

Using Romberg integration we obtain the results as given in Table 5.8.

Table 5.8 Trapezoidal Rule with Romberg Integration

h	*Second order method*	*Fourth order method*	*Sixth order method*	*Eighth order method*
1	0.750000			
		0.694444		
1/2	0.708333		0.693175	
		0.693254		0.693148
1/4	0.697024		0.693148	
		0.693155		
1/8	0.694122			

Since the exact solution is 0.693147, we require only nine function evaluations using trapezoidal rule with Romberg integration to achieve the accuracy of 10^{-6}.

The error in the trapezoidal rule is given by

$$R_1 = \frac{h^2}{12} f''(\xi), \quad 0 < \xi < 1.$$

Since $f(x) = 1/(1 + x)$, for $0 \le x \le 1$, $(1/4) \le |f''(x)| \le 2$. Therefore, we have

$$\frac{h^2}{48} \le \frac{h^2}{12}|f''(\xi)| \le \frac{h^2}{6}.$$

For achieving accuracy of 10^{-6}, we require

$$\frac{h^2}{48} \le 10^{-6}$$

which gives $h = 0.007$.

Hence, we require at least $(1 - 0)/0.007 = 145$ function evaluations to achieve this accuracy if trapezoidal rule is used directly.

Similarly, using the composite Simpson's rule

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

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

$$x_0 = 0,\ x_{2N} = b,\ h = \frac{b-a}{2N},\ \text{we get}$$

$$N = 1,\ h = \frac{1}{2}:\ I_S = \frac{h}{3}(f_0 + 4f_1 + f_2) = 0.694444.$$

$$N = 2,\ h = \frac{1}{4}:\ I_S = \frac{h}{3}[f_0 + 4(f_1 + f_3) + 2f_2 + f_4] = 0.693254.$$

$$N = 4,\ h = \frac{1}{8}:\ I_S = \frac{h}{3}[f_0 + 4(f_1 + f_3 + f_5 + f_7)$$

$$+ 2(f_2 + f_4 + f_6) + f_8] = 0.693155.$$

Using Romberg integration, we obtain the results as given in Table 5.9.

Table 5.9 Simpson's Rule with Romberg Integration

h	*Fourth order method*	*Sixth order method*	*Eighth order method*
1/2	0.694444		
		0.693175	
1/4	0.693254		0.693148
		0.693148	
1/8	0.693155		

In this case also, we require nine function evaluations to achieve the required accuracy. Also, when Simpson's rule is applied directly, we have for $0 \le x \le 1$, $(3/4) \le |f^{iv}(x)| \le 24$ and therefore

$$\frac{3h^4}{720} \le \frac{h^4}{180} \, |f^{iv}(\xi)| \le \frac{24}{180} \, h^4.$$

For getting an accuracy of 10^{-6}, we must have

$$\frac{3h^4}{720} \le 10^{-6}, \text{ or } h \approx 0.1245$$

which gives at least $(1 - 0)/0.1245 \approx 9$ function evaluations.