7.9 GAUSSIAN QUADRATURE FORMULAE

The numerical integration technique associated with the natural coordinates (ξ, η) used in finite element method for evaluating the element matrices is the Gauss–Legendre quadrature. In Newton–Cotes formulae, the integral of a function is approximated by the sum of its functional values at a set of equally spaced points, multiplied by certain weighting coefficients. However, in Gaussian quadrature, we have the freedom to choose not only the weighting coefficients but also the location of abscissas also called 'sampling points' at which the function is to be evaluated. In fact, they are no longer equally-spaced and the number of functional evaluations are same in both the cases, while we can achieve better accuracy. To illustrate, the Gaussian quadrature, let us consider an integral for which the Gauss formulae is given as

$$\int_a^b W(x)f(x)dx = \sum_{i=1}^{n} W_i f(x_i) \tag{7.57}$$

where W_i are a set of weights and x_i are sampling points. We classify various Gauss formulae based on $W(x)$.*

Gauss–Chebyshev quadrature : $W(x) = (1 - x^2)^{-1/2}, \quad -1 < x < 1$
Gauss–Legendre quadrature : $W(x) = 1, \quad -1 < x < 1$
Gauss–Leguerre quadrature : $W(x) = x^{\alpha}e^{-x}, \quad 0 < x < \infty$
Gauss–Hermite quadrature : $W(x) = \exp(-x^2), \quad -\infty < x < \infty$

Thus, Gauss–Legendre quadrature formula can be expressed in the form

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} W_i f(x_i) \tag{7.58}$$

It may be noted that in case, the limits of integration is from a to b, they can be changed to from -1 to 1, using the transformation

$$x = \frac{1}{2}\xi(b-a) + \frac{1}{2}(b+a) \tag{7.59}$$

Now, consider Gauss–Legendre n-point formula as

$$\int_{-1}^{1} f(\xi)d\xi = \sum_{i=1}^{n} W_i f(\xi_i) = W_1 f(\xi_1) + W_2 f(\xi_2) + \cdots + W_n f(\xi_n) \tag{7.60}$$

where W_i are called weights and ξ_i are the sampling points or Gauss points. From Eq. (7.60), we can observe that there are n Gauss points and n weights, thus in all $2n$ arbitrary parameters. The formula (7.60) will be exact, if $f(\xi)$ is a polynomial of degree $(2n - 1)$ or less. Therefore, $f(\xi)$ is of the form

$$f(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \ldots + a_{2n-1}\xi^{2n-1} \tag{7.61}$$

*For more details, the reader may refer to Stroud and Secrest, 1966.

Substituting Eq. (7.61) into Eq. (7.60), its left-hand side becomes

$$\int_{-1}^{1} f(\xi)d\xi = \int_{-1}^{1}(a_0 + a_1\xi + a_2\xi^2 + \cdots + a_{2n-1}\xi^{2n-1})d\xi$$

$$= 2a_0 + \frac{2}{3}a_2 + \frac{2}{5}a_4 + \cdots \tag{7.62a}$$

By choosing, $\xi = \xi_i$, Eq. (7.61) changes to

$$f(\xi_i) = a_0 + a_1\xi_i + a_2\xi_i^2 + a_3\xi_i^3 + \cdots + a_{2n-1}\xi_i^{2n-1}$$

Using this expression, the right-hand side of Eq. (7.60) becomes

$$\int_{-1}^{1} f(\xi)d\xi = W_1(a_0 + a_1\xi_1 + a_2\xi_1^2 + a_3\xi_1^3 + \cdots + a_{2n-1}\xi_1^{2n-1})$$

$$+ W_2(a_0 + a_1\xi_2 + a_2\xi_2^2 + a_3\xi_2^3 + \cdots + a_{2n-1}\xi_2^{2n-1}) + \cdots$$

$$+ W_n(a_0 + a_1\xi_n + a_2\xi_n^2 + a_3\xi_n^3 + \cdots + a_{2n-1}\xi_n^{2n-1})$$

which on rewriting yields

$$\int_{-1}^{1} f(\xi)d\xi = a_0(W_1 + W_2 + W_3 + \cdots + W_n)$$

$$+ a_1(W_1\xi_1 + W_2\xi_2 + W_3\xi_3 + \cdots + W_n\xi_n)$$

$$+ a_2(W_1\xi_1^2 + W_2\xi_2^2 + W_3\xi_3^2 + \cdots + W_n\xi_n^2)$$

$$+ \cdots + a_{2n-1}(W_1\xi_1^{2n-1} + W_2\xi_2^{2n-1} + W_3\xi_3^{2n-1} + \cdots + W_n\xi_n^{2n-1}) \tag{7.62b}$$

Now, Eqs. (7.62a) and (7.62b) are one and the same and hence by equating the coefficients of a_i in them, we immediately get the following $2n$ equations:

$$W_1 + W_2 + W_3 + \cdots + W_n = 2$$

$$W_1\xi_1 + W_2\xi_2 + W_3\xi_3 + \cdots + W_n\xi_n = 0$$

$$W_1\xi_1^2 + W_2\xi_2^2 + W_3\xi_3^2 + \cdots + W_n\xi_n^2 = \frac{2}{3}$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots \tag{7.62c}$$

$$W_1\xi_1^{2n-1} + W_2\xi_2^{2n-1} + W_3\xi_3^{2n-1} + \cdots + W_n\xi_n^{2n-1} = 0$$

The solution of these equations gives us $2n$ unknows such as W_i, the weighting coefficients and ξ_i, the sampling points or Gauss points for $i = 1, 2, \ldots, n$ and they are presented in Table 7.1 for values of n equal to 1 through 6.

Table 7.1 Abscissas and Weights for Gauss Legendre Quadrature

$$\int_{-1}^{1} f(\xi)d\xi = \sum_{i=1}^{n} W_i f(\xi_i)$$

Number of points n	Location, ξ_i	Weights, W_i
1	0.0	2.0
2	$\pm 1/\sqrt{3} = \pm 0.577350$	1.0
3	0.0	8/9 = 0.888889
	± 0.774597	5/9 = 0.555556
4	± 0.339981	0.652145
	± 0.861136	0.347855
5	0.0	0.568889
	± 0.538469	0.478629
	± 0.906180	0.236927
6	± 0.238619	0.467914
	± 0.661209	0.360762
	± 0.932470	0.171325

It may be observed from the table that Gauss points are located symmetrically about the origin or the mid-point of the interval and that symmetrically-placed points have the same weights.

To have a feel for the method, let us consider one-point and two-point approximations in the following examples:

Example 7.14 Evaluate

$$\int_{-1}^{1} f(\xi)d\xi = W_1 f(\xi_1) \qquad (1)$$

Solution This is one-point Gauss-Legendre quadrature formula given by (7.60). Since there are only two parameters W_1 and ξ_1, the formula (1) will be exact if $f(\xi)$ is a polynomial of degree one. Thus, we may write $f(\xi) = a_0 + a_1\xi$. Then it is required that

$$\text{Error} = \int_{-1}^{1} (a_0 + a_1\xi)d\xi - W_1 f(\xi_1)$$

That is,

$$2a_0 - W_1(a_0 + a_1\xi_1) = 0$$

Equivalently,

$$a_0(2 - W_1) - W_1 a_1 \xi_1 = 0 \qquad (2)$$

Thus, error is zero if and only if

$$W_1 = 2 \text{ and } \xi_1 = 0 \qquad (3)$$

Therefore, for any general $f(\xi)$, we have

$$\int_{-1}^{1} f(\xi)\,d\xi = 2f(0) \tag{4}$$

Example 7.15 Evaluate

$$\int_{-1}^{1} f(\xi)\,d\xi = W_1 f(\xi_1) + W_2 f(\xi_2) \tag{1}$$

Solution This is a two-point Gauss–Legendre formula given by Eq. (7.60). since we have four parameters W_1, W_2, ξ_1 and ξ_2 to be computed, the formula (1) will be exact if $f(\xi)$ is a cubic polynomial. Thus, we may write

$$f(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3$$

Then, it is required that

$$\text{Error} = \int_{-1}^{1} (a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3)\,d\xi - [W_1 f(\xi_1) + W_2 f(\xi_2)] = 0 \tag{2}$$

That is,

$$2a_0 + \frac{2}{3}a_2 - W_1(a_0 + a_1\xi_1 + a_2\xi_1^2 + a_3\xi_1^3)$$
$$-W_2(a_0 + a_1\xi_2 + a_2\xi_2^2 + a_3\xi_2^3) = 0$$

Equivalently,

$$a_0(2 - W_1 - W_2) - a_1(W_1\xi_1 + W_2\xi_2)$$
$$+ a_2\left(\frac{2}{3} - W_1\xi_1^2 - W_2\xi_2^2\right) - a_3\left(W_1\xi_1^3 + W_2\xi_2^3\right) = 0 \tag{3}$$

The error will be zero if and only if the following equations are satisfied:

$$\left.\begin{aligned} W_1 + W_2 &= 2 \\ W_1\xi_1 + W_2\xi_2 &= 0 \\ W_1\xi_1^2 + W_2\xi_2^2 &= \frac{2}{3} \\ W_1\xi_1^3 + W_2\xi_2^3 &= 0 \end{aligned}\right\} \tag{4}$$

These are non-linear equations, whose solution is found to be

$$W_1 = W_2 = 1 \quad \text{and} \quad \xi_1 = -\xi_2 = \frac{1}{\sqrt{3}} = 0.577350$$

Example 7.16 Evaluate the integral

$$\int_{-1}^{1} (3\xi^2 + \xi^3)\,d\xi$$

using Gauss–Legendre four-point quadrature formula.

Solution Here, the given data is $n = 4$. Therefore,

$$I = \int_{-1}^{1}(3\xi^2 + \xi^3)d\xi = \sum_{n=1}^{4} W_i f(\xi_i) \quad (1)$$

where

$$f(\xi_i) = 3\xi_i^2 + \xi_i^3 = \xi_i^2(\xi_i + 3)$$

Taking abscissas and weights from Table 7.1, we have

$$\begin{aligned} I = \int_{-1}^{1}(3\xi^2 + \xi^3)d\xi &= 0.347855\,(-0.861136)^2\,(3 - 0.861136) + 0.652145 \\ &\quad (-0.339981)^2\,(3 - 0.339981) + 0.347855 \\ &\quad (0.861136)^2\,(3 + 0.861136) + 0.652145 \\ &\quad (0.339981)^2\,(3 + 0.339981) \\ &= 0.551728 + 0.200511 + 0.995994 + 0.251766 \\ &= 1.999995 \end{aligned}$$

Integrals in two dimensions

One can easily extend the Gauss–Legendre quadrature formula to two-dimensional integrals of the form

$$I = \int_{-1}^{1}\int_{-1}^{1} f(\xi, \eta)\, d\eta\, d\xi \quad (7.63)$$

The above area integrals in the (ξ, η) coordinate system can be numerically evaluated by first evaluating the inner integral, assuming ξ constant and then evaluating the outer integral. Thus, the inner integral gives

$$\int_{-1}^{1} f(\xi, \eta)\, d\eta = \sum_{j=1}^{n} W_j f(\xi, \eta_j) = g(\xi) \quad (7.64)$$

where η_j and W_j are the Gauss–Legendre sampling points and weighting coefficients given in Table 7.1. Now the outer integral becomes

$$\int_{-1}^{1} g(\xi)\, d\xi = \sum_{i=1}^{m} W_i g(\xi_i) \quad (7.65)$$

Substituting the value of $g(\xi)$ from Eq. (7.64), we get

$$\int_{-1}^{1}\int_{-1}^{1} f(\xi, \eta)\, d\eta\, d\xi = \sum_{i=1}^{m}\sum_{j=1}^{n} W_i W_j f(\xi_i\, \eta_j) \quad (7.66)$$

The implementation of this equation is usually carried out as a single sum over $n \times m$ sampling points with $W_i W_j$-type products.

7.10 MULTIPLE INTEGRALS

For evaluating multiple integrals, we extend below the Gaussian quadrature formula as developed in Section 7.9. Thus, consider a formula of the type

$$I = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(x, y, z)\, dx\, dy\, dz$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} W_i W_j W_k\, f(x_i, y_j, z_k) \tag{7.67}$$

where $f(x, y, z)$ is a polynomial, containing a linear combination of terms of the type $x^r y^s z^t$. We further assume that r, s and t are non-negative integars. Suppose, we assume that

$$f(x, y, z) = x^r y^s z^t$$

In view of the fact that the limits of integration are constants and the integrand is factorable, we write

$$I = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} x^r y^s z^t\, dx\, dy\, dz$$

$$= \left[\int_{-1}^{1} x^r\, dx\right]\left[\int_{-1}^{1} y^s\, dy\right]\left[\int_{-1}^{1} z^t\, dz\right]$$

Now, using Gaussian quadrature formula given by Eq. (7.58) we shall be able to write the above equation as

$$I = \left[\sum_{i=1}^{n} W_i x_i^r\right]\left[\sum_{j=1}^{n} W_j y_j^s\right]\left[\sum_{k=1}^{n} W_k z_k^t\right]$$

or

$$I = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} W_i W_j W_k\, x_i^r y_j^s z_k^t \tag{7.68}$$

We shall illustrate this technique through the following example.

Example 7.17 Evaluate

$$I = \int_{0}^{1}\int_{0}^{2}\int_{-1}^{0} x^3 y z^2\, dx\, dy\, dz$$

Using Gaussian quadrature formula and a two-term formulas for x, y and z.

Solution: We know that any finite range $a \le y \le b$ can be mapped onto the range $-1 \le x \le 1$ using the linear transformation $y = (b - a)x/2 + (b + a)/2$. Thus, the given integral becomes

$$I = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \frac{1}{4} \times \frac{1}{8}(u-1)^3(v+1)(w+1)^2 \frac{du}{2} dv \frac{dw}{2}$$

where, we have used

$$x = \frac{1}{2}(u-1),\ y = v+1,\ z = \frac{1}{2}(w+1)$$

or

$$I = \frac{1}{128}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} (u-1)^3(v+1)(w+1)^2\, du\, dv\, dw \qquad (1)$$

We also know from Section 7.9 that the two and three point Gaussian quadrature formulae are

$$\int_{-1}^{1} f(x)\,dx = [(1)f(-0.5774) + (1)f(0.5774)] \qquad (2)$$

and

$$\int_{-1}^{1} f(x)\,dx = \left[\frac{5}{9}f(-0.7746) + \frac{8}{9}f(0) + \frac{5}{9}f(0.7746)\right] \qquad (3)$$

Thus, using two-term formula (2) for x, y and z or for u, v and w, the integral (1) becomes

$$I = \frac{1}{128}\sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{2} W_i W_j W_k (u_i - 1)^3 (v_j + 1)(W_k + 1)^2 \qquad (4)$$

observe that $W_1 = 1$, $W_2 = 1$. Now writing down all the terms explicitly, we have

$$\begin{aligned}
I = \frac{1}{128}[&(1)(1)(1)(-0.5774-1)^3(-0.5774+1)(-0.5774+1)^2\\
&+(1)(1)(1)(-0.5774-1)^3(-0.5774+1)(0.5774+1)^2\\
&+(1)(1)(1)(-0.5774-1)^3(0.5774+1)(-0.5774+1)^2\\
&+(1)(1)(1)(-0.5774-1)^3(0.5774+1)(0.5774+1)^2\\
&+(1)(1)(1)(0.5774-1)^3(-0.5774+1)(-0.5774+1)^2\\
&+(1)(1)(1)(0.5774-1)^3(-0.5774+1)(0.5774+1)^2\\
&+(1)(1)(1)(0.5774-1)^3(0.5774+1)(-0.5774+1)^2\\
&+(1)(1)(1)(0.5774-1)^3(0.5774+1)(0.5774+1)^2]
\end{aligned}$$

$$= \frac{1}{128}[-0.2963 - 4.1271 - 1.1057 - 15.4048$$
$$-0.005698 - 0.07939 - 0.02127 - 0.2963]$$

or

$$I = \frac{1}{128}[-21.3366] = -0.16669 \qquad (5)$$

However, the exact solution is

$$I = \int_0^1 \int_0^2 \int_{-1}^0 x^3 y z^2 \, dx\, dy\, dz$$

$$= -\frac{1}{4} \int_0^1 \int_0^2 y z^2 dy\, dz$$

$$= -\frac{1}{2} \int_0^1 z^2 \, dz = -\frac{1}{6} = -0.1667 \qquad (6)$$

Comparing the numerical solution with the exact solution given by Eqs. (5) and (6) we observe that the numerical solution is four decimal accurate.

EXERCISES

7.1 Define shift operator E, average operator μ and differential operator D. Hence, show that

$$D^2 = \frac{1}{h^2}\left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \cdots\right)$$

7.2 Derive the formula

$$D^3 = \mu\left[\delta^3 - \left(\frac{1}{12} + \frac{1}{6}\right)\delta^5 + \cdots\right]$$

7.3 Find the first derivative of $f(x)$ at $x = 0.4$ from the following table:

x	0.1	0.2	0.3	0.4
$f(x)$	1.10517	1.22140	1.34986	1.49182

7.4 From the following table of values, estimate $y'(1.10)$ and $y''(1.10)$:

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
y	1.0000	1.0247	1.0488	1.0724	1.0954	1.1180	1.1402

7.5 A slider in a machine moves along a fixed straight rod. Its distance x c along the rod is given below for various values of time t (seconds). Fi the velocity of the slider and its acceleration when $t = 0.3$ s.

t	0.0	0.1	0.2	0.3	0.4	0.5	0.6
x	3.013	3.162	3.287	3.364	3.395	3.381	3.324

Use both the forward difference formula and the central difference formu to find the velocity and compare the results.

7.6 Given the table of values, estimate $y''(1.3)$:

x	1.3	1.5	1.7	1.9	2.1	2.3
y	2.9648	2.6599	2.3333	1.9922	1.6442	1.2969

7.7 The following divided difference table is for $y = 1/x$. Use it to find $y'(0.75)$ (i) from a quadratic polynomial fit (ii) from a cubic polynomial fit. What degree polynomial fit gives the most accurate value of $y'(0.75)$.

x	$y = 1/x$	1st divided difference	2nd divided difference	3rd divided difference	4th divided difference
0.25	4.0000				
		−8.0000			
0.50	2.0000		10.6664		
		−2.6668		−14.2219	
0.75	1.3333		2.6672		12.0875
		−1.3332		−2.1344	
1.00	1.0000		1.0664		1.4240
		−0.8000		−0.7104	
1.25	0.8000		0.5336		
		−0.5332			
1.50	0.6667				

7.8 Evaluate the integral

$$\int_{1.0}^{1.8} \frac{e^x + e^{-x}}{2}\, dx$$

using Simpson's 1/3 rule, by taking $h = 0.2$.

7.9 Evaluate the integral

$$\int_0^6 [f(x)]^2\, dx$$

using Simpson's 1/3 rule, given that

x	0	1	2	3	4	5	6
$f(x)$	1	0	1	4	9	16	25

7.10 Using Simpson's 1/3 rule, Evaluate the integral

$$\int_0^{\pi/2} \frac{dx}{\sin^2 x + \frac{1}{4}\cos^2 x}$$

7.11 Compute the integral,

$$\int_1^2 \frac{dx}{x}$$

using Simpson's 1/3 rule, and also obtain the error bounds by taking $h = 0.25$.

7.12 Evaluate the integral

$$\int_0^1 e^x\, dx$$

using Simpson's 1/3 rule, by dividing the interval of integration into eight equal parts.

7.13 Using the Richardson extrapolation limit, find $y''(0.6)$ of the following tabulated function by applying the formula

$$F(x) = \frac{1}{h^2}[y(x+h) - 2y(x) + y(x-h)]$$

with $h = 0.4, 0.2, 0.1$.

x	0.2	0.4	0.5	0.6	0.7	0.8	1.0
$y(x)$	1.42007	1.88124	2.12815	2.38676	2.65797	2.94289	3.55975

7.14 Apply Romberg's integration method to evaluate

$$\int_{1.0}^{1.8} \cosh\, dx$$

by applying trapezoidal rule with $h = 0.8, 0.4, 0.2, 0.1$.

7.15 Evaluate the integral

$$\int_1^2 \frac{dx}{x}$$

using Romberg's method of integration starting with trapezoidal rule, taking $h = 1, 0.5, 0.25, 0.0125$.

7.16 Evaluate the double integral

$$I = \int_0^1 \int_0^2 \frac{2xy}{(1+x^2)(1+y^2)}\, dy\, dx$$

using Simpson's 1/3 rule, with step length $h = k = 0.25$.

7.17 Compute numerically

$$I = \iint_D \frac{dx\, dy}{x^2 + y^2}$$

where D is the square with corners at (1, 1), (2, 1), (2, 2), (1, 2).

7.18 Evaluate

$$I = \int_0^1 \int_1^2 (x^2 + y^2)\, dx\, dy$$

using Simpson's 1/3 rule.

7.19 The velocity v m/s of a particle at a time t seconds is given in the following table:

t	0	2	4	6	8	10	12
v	4	6	16	34	60	94	136

Find the distance travelled by the particle in 12 s and also the acceleration at $t = 2$ s.

7.20 Find y' and y'' of the function which is tabulated below at the point $x = 2.03$.

x	1.96	1.98	2.00	2.02	2.04
y	0.7825	0.7739	0.7651	0.7563	0.7473

7.21 A body is in the form of a solid of revolution, whose diameter d in cm of its sections at various distances x cm from one end is given in the table below. Compute the volume of the solid using Simpson's 1/3 rule.

x	0.0	2.5	5.0	7.5	10.0	12.5	15.0
d	5.00	5.50	6.00	6.75	6.25	5.50	4.00

7.22 Evaluate the following triple integral

$$I = \int_0^1 \int_{-1}^0 \int_{-1}^1 yz\, e^x\, dx$$

Using Gaussian quadrature formula and taking a three-term formula for x and two-term formula for y and z.