Chapter 5

Numerical Integration Methods

5.1 One-dimensional Integration

Consider the integral $I = \int_{x_1}^{x_2} g(x)\ dx$.

Many methods can be proposed to approximately evaluate this integral. Most of these methods are based on the idea that the value of an integral corresponds to the area under the graph of the integrand. These methods break the function up into a number of small steps and approximate the area under the graph in each case. Common examples include: the Rectangular Method, the Trapezoidal Method and Simpson's Method.

5.1.1 Rectangular Method

This method approximates the function as a piecewise constant over each small step. This means that each small region will be a rectangle and the integral can be approximated as the sum of these rectangles.

$$\int_{x_1}^{x_2} g(x)\ dx \approx \Delta x\left(g_1 + g_2 + \ldots + g_n\right) \tag{5.1}$$

where n is the number of piecewise regions, $\Delta x = \dfrac{x_2 - x_1}{n}$ and f_n is the function value at the start of the n^{th} step. Note that: (i) the approximation of the rectangular method is similar to that employed by Euler's method for solving ODEs; (ii) although Δx is shown here to be identical over the entire integration range, in practice it can vary if necessary.

5.1.2 Trapezoidal Method

This method approximates the function as a piecewise linear function over each small step. This means that each small region will be a trapezoid and the integral can be approximated as the sum of these trapezoids.

$$\int_{x_1}^{x_2} g(x)\ dx \approx \Delta x \left(\frac{1}{2} g_0 + g_1 + g_2 + \ldots + g_{n-1} + \frac{1}{2} g_n \right) \tag{5.2}$$

where $\Delta x = \dfrac{x_2 - x_1}{n}$.

5.1.3 Simpson's Method

This method approximates the function as a piecewise parabolic function over each small step.

$$\int_{x_1}^{x_2} g(x)\ dx \approx \frac{\Delta x}{3} \left(g_0 + 4g_1 + 2g_2 + 4g_3 + \ldots + 2g_{2n-2} + 4g_{2n-1} + g_{2n} \right) \tag{5.3}$$

where $\Delta x = \dfrac{x_2 - x_1}{2n}$.

Although these methods are often used, none are particularly accurate. Therefore, they will not be discussed further. A more accurate and flexible method called Gaussian quadrature will now be considered.

5.2 Gaussian Quadrature

Before we start discussing Gaussian quadrature in detail we wish to standardise the integration process. We can achieve this by normalising the integral.

We introduce the variable ξ such that $\xi = \dfrac{x - x_1}{x_2 - x_1}$ or $x = x_1 + (x_2 - x_1)\,\xi$. Using this definition at $x = x_1$ we have $\xi = 0$ and at $x = x_2$ we have $\xi = 1$. This implies $dx = (x_2 - x_1)\, d\xi = J d\xi$ (where J is called the Jacobian and is the function required to transform $dx \to d\xi$) and $g(x) = g(x_1 + (x_2 - x_1)\,\xi)$. Using this results allows us to rewrite the integral I in normalised form.

$$\int_{x_1}^{x_2} g(x)\ dx \to \int_{\xi=0}^{1} \bar{g}(\xi)\, J\, d\xi = \int_{\xi=0}^{1} f(\xi)\ d\xi \quad \text{where} \quad f(\xi) = g(x_1 + (x_2 - x_1)\,\xi)\,(x_2 - x_1) \tag{5.4}$$

Gaussian quadrature can be used to integrate an integral in normalised form. Gaussian quadrature approximates an integral as a weighted sum of the integrand at a number of specified points.

$$\int_0^1 f(\xi)\, d\xi \approx \sum_{g=1}^{G} w_g f\left(\xi^{(g)}\right) + E_G \tag{5.5}$$

$$= w_1 f\left(\xi^{(1)}\right) + w_2 f\left(\xi^{(2)}\right) + \ldots + w_G f\left(\xi^{(G)}\right) + E_G \tag{5.6}$$

where the sample locations $\xi^{(g)}$ are called Gauss points, w_g are called Gauss point weights and E_G is the error associated with the approximation. To implement this method we need to determine values for $\xi^{(g)}$ and w_g.

It can be shown that choosing G Gauss points allows a polynomial of degree $2G-1$ to be integrated exactly (G Gauss points have $2G$ unknownsand a polynomial of order $2G-1$ has $2G$ unknown coefficients). For example to exactly integrate a cubic polynomial of degree 3 ($f(\xi) = a + b\xi + c\xi^2 + d\xi^3$) we need two gauss points *i.e.*,

$$\int_0^1 f(x)\, d\xi = w_1 f\left(\xi^1\right) + w_2 f\left(\xi^2\right) \tag{5.7}$$

$$= \int_0^1 \left(a + b\xi + c\xi^2 + d\xi^3\right)\, d\xi \tag{5.8}$$

$$= a\int_0^1 1\, d\xi + b\int_0^1 \xi\, d\xi + c\int_0^1 \xi^2\, d\xi + d\int_0^1 \xi^3\, d\xi \tag{5.9}$$

Since each constant is arbitrary, in order for the entire integral to be exactly evaluated each of the individual integrals must be exactly evaluated by the Gauss point scheme. Therefore:

$$
\begin{aligned}
&\int_0^1 1\, d\xi = 1 = w_1 + w_2 \qquad \text{since } f(\xi) = 1 \\
&\int_0^1 \xi\, d\xi = \frac{1}{2} = w_1 \xi^{(1)} + w_2 \xi^{(2)} \qquad \text{since } f(\xi) = \xi \\
&\int_0^1 \xi^2\, d\xi = \frac{1}{3} = w_1 \xi^{(1)^2} + w_2 \xi^{(2)^2} \qquad \text{since } f(\xi) = \xi^2 \\
&\int_0^1 \xi^3\, d\xi = \frac{1}{4} = w_1 \xi^{(1)^3} + w_2 \xi^{(2)^3} \qquad \text{since } f(\xi) = \xi^3
\end{aligned}
\tag{5.10}
$$

This gives four equations in the four unknowns $\xi^{(1)}$, $\xi^{(2)}$. w_1 and w_2. Solving for these unknowns gives $\xi^{(1)} = \frac{1}{2} - \frac{1}{2\sqrt{3}}$, $\xi^{(2)} = \frac{1}{2} + \frac{1}{2\sqrt{3}}$, $w_1 = \frac{1}{2}$ and $w_2 = \frac{1}{2}$.

Similarly a fifth degree polynomial may be exactly integrated using the 3 Gauss points $\xi^{(1)} = \frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{5}}$, $\xi^{(2)} = \frac{1}{2}$, $\xi^{(3)} = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{3}{5}}$, $w_1 = \frac{5}{18}$, $w_2 = \frac{4}{9}$ and $w_3 = \frac{5}{18}$.

As a general characteristic for this type of Gauss quadrature scheme the $\xi^{(g)}$ positions are symmetric about $\frac{1}{2}$ and the w_g weights reflect this symmetry and sum to 1.

5.3 Gauss Quadrature in Two Dimensions

Consider the two-dimensional integral

$$
I = \int_{x_1}^{x_2} \int_{y_1}^{y_2} g(x, y)\; dy dx \tag{5.11}
$$

Before we can apply Gauss quadrature to evaluate this integral we need to rewrite it in normalised form using the variables $\xi_1 = \frac{x - x_1}{x_2 - x_1}$ and $\xi_2 = \frac{y - y_1}{y_2 - y_1}$. This can be achieved using the Jacobian J such that

$$
I = \int_{\xi_1=0}^{1} \int_{\xi_2=0}^{1} \bar{g}(\xi_1, \xi_2)\, J\, d\xi_2 d\xi_1 \tag{5.12}
$$

where

$$J = \det\left[\frac{\partial x_i}{\partial \xi_j}\right] = \det\begin{bmatrix} \dfrac{\partial x}{\partial \xi_1} & \dfrac{\partial x}{\partial \xi_2} \\ \dfrac{\partial y}{\partial \xi_1} & \dfrac{\partial y}{\partial \xi_2} \end{bmatrix} \tag{5.13}$$

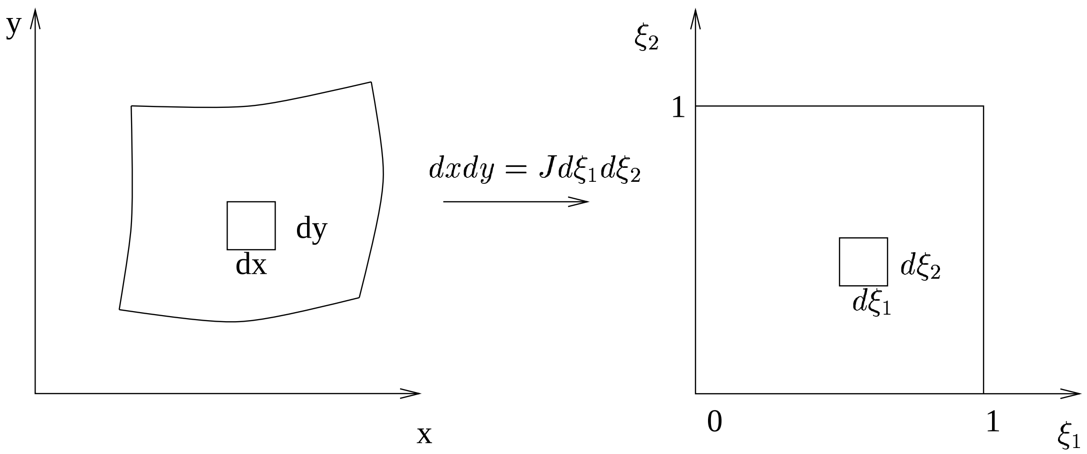

FIGURE 5.1:

To approximate the surface integral in normalised coordinates, one-dimensional quadrature schemes can be used in each direction (this formula uses the notation $f(\xi_1, \xi_2) = \bar{g}(\xi_1, \xi_2) J$).

$$\int_0^1\int_0^1 f(\xi_1, \xi_2)\, d\xi_2 d\xi_1 \approx \int_0^1 \left(\sum_{g=1}^{G} w_g f\left(\xi_1, \xi_2^{(g)}\right) + E_G\right) d\xi_1 \tag{5.14}$$

$$\approx \sum_{h=1}^{H}\sum_{g=1}^{G} w_g w_h f\left(\xi_1^{(h)}, \xi_2^{(g)}\right) + E_{GH} \tag{5.15}$$

where G Gauss points are used in the ξ_2 direction (at positions $\xi_2^{(g)}$ with weights w_g) and H Gauss points are used in the ξ_1 direction (at positions $\xi_1^{(h)}$ with weights w_h). The error term E_{GH} depends on the choice of quadrature schemes in the ξ_1 and ξ_2 directions separately (different schemes can be used in either direction).

For example, for a 2x2 Gaussian quadrature scheme we have:

Gauss Point	ξ_1	ξ_2	Weight
1	$\frac{1}{2} - \frac{1}{2\sqrt{3}}$	$\frac{1}{2} - \frac{1}{2\sqrt{3}}$	$\left(\frac{1}{2}\right)\left(\frac{1}{2}\right) = \frac{1}{4}$
2	$\frac{1}{2} + \frac{1}{2\sqrt{3}}$	$\frac{1}{2} - \frac{1}{2\sqrt{3}}$	$\left(\frac{1}{2}\right)\left(\frac{1}{2}\right) = \frac{1}{4}$
3	$\frac{1}{2} - \frac{1}{2\sqrt{3}}$	$\frac{1}{2} + \frac{1}{2\sqrt{3}}$	$\left(\frac{1}{2}\right)\left(\frac{1}{2}\right) = \frac{1}{4}$
4	$\frac{1}{2} + \frac{1}{2\sqrt{3}}$	$\frac{1}{2} + \frac{1}{2\sqrt{3}}$	$\left(\frac{1}{2}\right)\left(\frac{1}{2}\right) = \frac{1}{4}$

5.3.1 Examples

1. Analytic Direct Evaluation

$$
\begin{aligned}
I &= \int_{-2}^{1}\int_{1}^{3} xy \quad dxdy \\
&= \int_{-2}^{1}\left[\frac{1}{2}x^2 y\right]_1^3 \quad dy \\
&= \left[\frac{9}{2} - \frac{1}{2}\right]\int_{-2}^{1} y \quad dy \\
&= 4\left[\frac{1}{2}y^2\right]_{-2}^{1} \\
&= -6
\end{aligned}
$$

2. Analytic Evaluation in Normalised Form

$$I = \int_{-2}^{1}\int_{1}^{3} xy \quad dxdy$$

Transformation from $(x, y) \rightarrow (\xi_1, \xi_2)$:

$$
\begin{aligned}
\xi_1 &= \frac{x-1}{3-1} & \qquad \xi_2 &= \frac{y+2}{1+2} \\
\Rightarrow x &= 2\xi_1 + 1 & \qquad \Rightarrow y &= 3\xi_2 - 2
\end{aligned}
$$

Note that in general:

$$x = f(\xi_1, \xi_2) \qquad \text{and} \qquad y = g(\xi_1, \xi_2)$$

Jacobian for the transformation from $dxdy \rightarrow Jd\xi_1 d\xi_2$:

$$J = \begin{vmatrix} \frac{\partial x}{\partial \xi_1} & \frac{\partial x}{\partial \xi_2} \\ \frac{\partial y}{\partial \xi_1} & \frac{\partial y}{\partial \xi_2} \end{vmatrix} = \begin{vmatrix} 2 & 0 \\ 0 & 3 \end{vmatrix} = 6$$

Transformed limits of integration:

upper limit on x: $x = 3 \rightarrow \xi_1 = 1$
lower limit on x: $x = 1 \rightarrow \xi_1 = 0$
upper limit on y: $x = 1 \rightarrow \xi_2 = 1$
lower limit on y: $x = -2 \rightarrow \xi_2 = 0$

The integral in normalised form:

$$\begin{aligned} I &= \int_0^1 \int_0^1 x(\xi_1, \xi_2) y(\xi_1, \xi_2) J d\xi_1 d\xi_2 \\ &= \int_0^1 \int_0^1 (2\xi_1 + 1)(3\xi_2 - 2) 6 d\xi_1 d\xi_2 \\ &= 6 \int_0^1 \left[\frac{6}{2}{\xi_1}^2 \xi_2 + 3\xi_1\xi_2 - \frac{4}{2}{\xi_1}^2 - 2\xi_1 \right]_0^1 d\xi_2 \\ &= 6 \int_0^1 \left[6\xi_1 - 4 \right] d\xi_2 \\ &= -6 \qquad \text{(4WR)} \end{aligned}$$

3. Approximate Evaluation using Gaussian Quadrature

   (a) One Gauss Point

$$\boldsymbol{\xi}_1 = \left(\frac{1}{2}, \frac{1}{2} \right) \qquad w_1 = 1$$

$$
\begin{aligned}
I &= 6\int_0^1\int_0^1 (2\xi_1+1)(3\xi_2-2)d\xi_1 d\xi_2 \\
&\approx 6w_1(2\xi_{11}+1)(3\xi_{12}-2) \\
&= 6\times 1\times 2\times \frac{-1}{2} \\
&= -6 \qquad \text{(4WR)}
\end{aligned}
$$

(b) Four Gauss Points

$$
\begin{aligned}
\boldsymbol{\xi}_1 &= (0.2113, 0.2113) \qquad w_1 = 0.25 \\
\boldsymbol{\xi}_2 &= (0.7887, 0.2113) \qquad w_2 = 0.25 \\
\boldsymbol{\xi}_3 &= (0.2113, 0.7887) \qquad w_3 = 0.25 \\
\boldsymbol{\xi}_4 &= (0.7887, 0.7887) \qquad w_4 = 0.25
\end{aligned}
$$

$$
\begin{aligned}
I &= 6\int_0^1\int_0^1 (2\xi_1+1)(3\xi_2-2)d\xi_1 d\xi_2 \\
&\approx 6(0.25\times 1.4226\times -1.3661 + 0.25\times 2.5774\times -1.3661 + \\
&\qquad 0.25\times 1.4226\times 0.3661 + 0.25\times 2.5774\times 0.3661) \\
&= -6 \qquad \text{(4WR)}
\end{aligned}
$$