Lecture 15
Angular Quadratures

1 Introduction

Angular quadratures play a critical role in the S_n method. The purpose of this lecture is to describe the basic properties of 1-D angular quadratures. An N-point quadrature set consists of N points and weights, $\{\mu_m, \omega_m\}_{m=1}^{N}$, such that

$$\sum_{m=1}^{N} f(\mu_m) w_m \approx \int_{-1}^{+1} f(\mu)\, d\mu \,. \tag{1}$$

Perhaps the simplest quadrature set is that corresponding to the rectangle rule:

$$\sum_{m=1}^{N} f(\mu_m) w_m \approx \int_{-1}^{+1} f(\mu)\, d\mu \,, \tag{2}$$

where

$$w_m = \frac{2}{N}\,, \quad m = 1, N, \tag{3a}$$

and

$$\mu_m = -1 + \frac{2}{N}(m - \frac{1}{2})\,, \quad m = 1, N. \tag{3b}$$

Assuming that $f(\mu)$ is integrable, the rectangle-rule quadrature yields the exact integral in the limit as $N \to \infty$, but for any finite N, the formula is exact only for linear functions.

2 Gauss Quadratures

The Gauss N-point quadrature formula is exact for all polynomials of degree $2N-1$ or less. Both the directions and weights are chosen to optimize accuracy (N directions and N weights). Thus Gauss quadratures are the most accurate of all 1-D quadratures. Given any N distinct quadrature points, one can always find N weights so that the corresponding quadrature formula is exact for polynomials of degree N-1 or less. Specifically, the weights must satisfy the following linear system of equations:

$$\sum_{m=1}^{N} P_{\ell}(\mu_m) w_m = 2\delta_{\ell,0}\,, \quad \ell = 0, N-1. \tag{4}$$

A potential problem with this approach is that the weights may turn out to be negative. Why is this undesirable? In principle, a combination of positive and negative weights can lead to roundoff problems, but in practice, this is not usually a problem. However, negative weights do represent a problem from the viewpoint of interpolation. For instance, let us expand a polynomial of degree $N-1$ in terms of the Lagrange interpolatory polynomials:

$$g(\mu) = \sum_{m=1}^{N} g(\mu_m) B_m(\mu)\,, \tag{5}$$

where

$$B_m(\mu) = \frac{(\mu-\mu_1)(\mu-\mu_2)\cdots(\mu-\mu_{m-1})(\mu-\mu_{m+1})\cdots(\mu-\mu_N)}{(\mu_m-\mu_1)(\mu_m-\mu_2)\cdots(\mu_m-\mu_{m-1})(\mu_m-\mu_{m+1})\cdots(\mu_m-\mu_N)}\,. \tag{6}$$

Integrating Eq. (5), we get

$$\int_{-1}^{+1} g(\mu)\, d\mu = \sum_{m=1}^{N} g(\mu_m) \int_{-1}^{+1} B_m(\mu)\, d\mu\,. \tag{7}$$

Since any polynomial of degree N-1 can be represented according to Eq. (5), it follows from Eq. (7) that any such polynomial is exactly integrated with the following quadrature formula:

$$\int_{-1}^{+1} g(\mu)\, d\mu = \sum_{m=1}^{N} g(\mu_m) w_m \quad , \tag{8}$$

where

$$w_m = \int_{-1}^{+1} B_m(\mu)\, d\mu\,. \tag{9}$$

Thus the w_m given by Eq. (9) are those that satisfy Eq. (4). If any particular w_k is negative, it implies that $B_k(\mu)$ has a negative area. The function, $B_k(\mu)$, represents the interpolant for the discrete function that is unity at μ_k and zero at the other quadrature points. If the integral of $B_k(\mu)$ is negative, it clearly indicates that this interpolation is quite poor. The accuracy of the interpolation is essentially unrelated to the accuracy of the integration, but it is important if one uses a trial space representation for $\psi(\mu)$ that is consistent with the quadrature formula, i.e.,

$$\psi(\mu) = \sum_{m=1}^{N} \psi(\mu_m) B_m(\mu)\,. \tag{10}$$

This is done in the discrete-ordinates or S_n method, which is one of the most popular numerical methods for solving the transport equation.

This positivity problem can be avoided by choosing the N quadrature points to be the roots of the Legendre polynomial of degree N, $P_N(\mu)$. For instance, any polynomial of degree $2N-1$ can be expressed in the following form:

$$g(\mu) = h(\mu)P_N(\mu) + q(\mu)\,, \tag{11}$$

where $h(\mu)$ and $q(\mu)$ are polynomials of degree $N-1$ or less. Integrating Eq. (11) we find that

$$\begin{aligned} \int_{-1}^{+1} g(\mu)\,d\mu &= \int_{-1}^{+1} h(\mu)P_N(\mu)\,d\mu + \int_{-1}^{+1} q(\mu)\,d\mu\,, \\ &= \int_{-1}^{+1} q(\mu)\,d\mu\,. \end{aligned} \tag{12}$$

If the quadrature points are chosen to be the roots of $P_N(\mu)$ then

$$\begin{aligned} \sum_{m=1}^{N} g(\mu_m)w_m &= \sum_{m=1}^{N} h(\mu_m)P_N(\mu_m)w_m + \sum_{m=1}^{N} q(\mu_m)w_m\,, \\ &= \sum_{m=1}^{N} q(\mu_m)w_m\,. \end{aligned} \tag{13}$$

The weights defined by (6a) give an exact integration of any polynomial of degree N-1 or less regardless of the value of μ_m that are chosen. Since $q(\mu)$ is such a polynomial, it follows that

$$\int_{-1}^{+1} g(\mu)\,d\mu = \sum_{m=1}^{N} g(\mu_m)w_m\,, \tag{14}$$

where the $\{\mu_m\}_{m=1}^{N}$ are the roots of $P_N(\mu)$ and the weights are defined by Eq. (9). This particular quadrature set is known as the Gauss N–point set, and it is exact for all polynomials of degree $2N-1$ or less. Furthermore, the Gauss weights are positive. This can be shown as follows. For any k,

$$\int_{-1}^{+1} B_k(\mu)\, d\mu = \sum_{m=1}^{N} B_k(\mu_m) w_m \,. \tag{15}$$

From Eq. (6) it can be seen that

$$B_k(\mu_m) = \delta_{k,m} \,. \tag{16}$$

Thus from Eq. (16) we find that

$$\int_{-1}^{+1} B_k(\mu)\, d\mu = w_k \,. \tag{17}$$

However, since $B_k(\mu)$ is a polynomial of degree N–1 or less, it follows that the Gauss formula can also integrate $B_k^2(\mu)$:

$$\int_{-1}^{+1} B_k^2(\mu)\, d\mu = \sum_{m=1}^{N} B_k^2(\mu_m)\omega_m = \omega_k \,. \tag{18}$$

Since the left side of (14) must be positive, it follows that the Gauss weights are indeed positive. Finally, we note that the roots of $P_N(x)$ always lie on the open interval $(-1, +1)$.

There are many variations on Gauss quadrature in which one gives up accuracy in return for placing quadrature points at specific locations. For instance, every N-point Labatto quadrature has quadrature points at $\mu = \pm 1$. The remaining free parameters (N weights and $N-2$ points) are chosen to maximize integration accuracy. Thus an N-point Lobatto set exactly integrates all polynomials of degree $2N-3$ or less.