

# Lecture 12

## 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

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

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

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

where

$$\omega_m = \frac{2}{N}, \quad m = 1, N, \quad (3a)$$

and

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

Assuming that  $f(\mu)$  is integrable, the rectangle-rule quadrature yields the exact integral in the limit as  $N \rightarrow \infty$ , 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:

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

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:

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

where

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

Integrating Eq. (5), we get

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

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:

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

where

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

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  $\mu_k$  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.,

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

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:

$$g(\mu) = h(\mu)P_N(\mu) + q(\mu), \quad (11)$$

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

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

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

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

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

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

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 poly-

nomials of degree  $2N - 1$  or less. Furthermore, the Gauss weights are positive. This can be shown as follows. For any  $k$ ,

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

From Eq. (6) it can be seen that

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

Thus from Eq. (16) we find that

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

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

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

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 Lobatto 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.