

In this project, the Gaussian square is used which states that:

$$\int_{-1}^1 f(x)dx \approx \sum_{i=1}^n w_i f(x_i)$$

For the simplest integration problem stated above, i.e., $f(x)$ is well approximated by polynomials on $[-1, 1]$, the associated orthogonal polynomials are Legendre polynomials, denoted by $P_n(x)$. With the n -th polynomial normalized to give $P_n(1) = 1$, the i -th Gauss node, x_i , is the i -th root of P_n and the weights are given by the formula (Hildebrand 1956, p. 324).

$$w_i = \frac{2(1 - x_i^2)}{(n+1)^2 [P_{n+1}(x)]^2}$$

An integral over $[a, b]$ must be changed into an integral over $[-1, 1]$ before applying the Gaussian quadrature rule. This change of interval can be done in the following way:

$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}\xi + \frac{a+b}{2}\right)d\xi$$

Applying n point Gaussian quadrature (ξ, w) rule then results in the following approximation:

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{i=1}^n w_i f\left(\frac{b-a}{2}\xi_i + \frac{a+b}{2}\right)$$

The error of a Gaussian quadrature rule can be stated as follows (Stoer & Bulirsch 2002, Thm 3.6.24). For an integrand which has $2n$ continuous derivatives:

$$\int_a^b w(x)f(x)dx - \sum_{i=1}^n w_i f(x_i) = \frac{f^{(2n)}(\xi)}{(2n)!} (p_n, p_n)$$

For some ξ in (a, b) , where p_n is the monic (i.e. the leading coefficient is 1) orthogonal polynomial of degree n and where:

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

In the important special case of $w(x) = 1$, we have the error estimate (Kahaner, Moler & Nash 1989, p. 5.2)

$$\frac{(b-a)^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), \quad a < \xi < b$$

Stoer and Bulirsch remark that this error estimate is inconvenient in practice, since it may be difficult to estimate the order $2n$ derivative, and furthermore the actual error may be much less than a bound established by the derivative. Another approach is to use two Gaussian quadrature rules of different orders, and to estimate the error as the difference between the two results. For this purpose, Gauss–Kronrod quadrature rules can be useful.