A

Quadrature

The numerical evaluation of integrals, often called *quadrature*, is a central feature of many computational schemes. This appendix briefly reviews some of the ideas behind single and multiple dimensional quadrature rules.

A.1 ROMBERG INTEGRATION [1–3]

One of the simplest classical quadrature algorithms is the trapezoidal rule. Suppose the integral

$$I = \int_a^b f(x)\,dx \tag{A.1}$$

is to be evaluated based on integrand samples at the endpoints of $N = 2^{n-1}$ equal-sized intervals, treating the function as a trapezoid over each. The resulting approximation can be written as

$$I_{n,1} = \frac{h}{2}[f(a) + f(b)] + h\sum_{i=1}^{N-1} f(a + ih) \tag{A.2}$$

where

$$h = \frac{b-a}{2^{n-1}} \tag{A.3}$$

is the uniform interval size. In the event that this approximation of the integral is not accurate enough, the intervals can be halved, leading to a formula involving 2^n intervals

$$I_{n+1,1} = \frac{1}{2}I_{n,1} + h'\sum_{i=1}^{2^{n-1}} f(a + [2i-1]h') \tag{A.4}$$

where h' denotes the new interval size

$$h' = \frac{b-a}{2^n} \tag{A.5}$$

Observe that the integrand samples used to compute $I_{n,1}$ are reused in $I_{n+1,1}$, saving half the required function evaluations necessary if $I_{n,1}$ was not available. Since the integrands of interest often contain special functions, it is usually desirable to minimize the number of evaluations. Because of sample point reuse, a series of approximations $\{I_{1,1}, I_{2,1}, \ldots, I_{n,1}\}$ can be generated for the same number of function evaluations as $I_{n,1}$. The availability of successive approximations facilitates error estimation.

The error produced by successive applications of the trapezoidal rule has an interesting property, namely that it consists entirely of even powers of $1/N$ [1]. In other words,

$$I - I_{n,1} = \frac{\alpha}{N^2} + \frac{\beta}{N^4} + \frac{\gamma}{N^6} + \cdots \tag{A.6}$$

where $N = 2^{n-1}$. This property can be exploited by a form of Richardson extrapolation in order to obtain better estimates of I. Given two successive approximations for I, the fact that the dominant-error term behaves as $O(N^{-2})$ means that the error drops by a factor of 4, or in equation form

$$I \cong I_{n,1} + \frac{K}{N^2} \tag{A.7}$$

$$I \cong I_{n+1,1} + \frac{K}{4N^2} \tag{A.8}$$

An improved approximation should be possible by solving these two equations for the coefficient K and extrapolating to a better estimate by removing the $O(N^{-2})$ error, to obtain

$$I \cong I_{n+1,2} = \tfrac{4}{3} I_{n+1,1} - \tfrac{1}{3} I_{n,1} \tag{A.9}$$

In general, $I_{n+1,2}$ will be a better approximation to the integral than $I_{n+1,1}$, since its leading-order error term is reduced to $O(N^{-4})$. By successively increasing n and extrapolating, this process can be continued. For instance, the two estimates

$$I \cong I_{n,2} + \frac{L}{N^4} \tag{A.10}$$

$$I \cong I_{n+1,2} + \frac{L}{16N^4} \tag{A.11}$$

can be used to extrapolate to

$$I \cong I_{n+1,3} = \tfrac{16}{15} I_{n+1,2} - \tfrac{1}{15} I_{n,2} \tag{A.12}$$

whose leading-order error is $O(N^{-6})$. By continuing this procedure, one obtains the estimate

$$I_{n+1,m+1} = \frac{4^m}{4^m - 1} I_{n+1,m} - \frac{1}{4^m - 1} I_{n,m} \tag{A.13}$$

for the same number of integrand samples necessary to compute $I_{n+1,1}$. This process of combining trapezoidal rule with Richardson extrapolation is known as *Romberg integration*.

To summarize, Romberg integration requires the use of trapezoidal rule to compute the initial estimate

$$I_{1,1} = (b-a)\left[\frac{f(a)+f(b)}{2}\right] \tag{A.14}$$

and successive estimates $I_{n+1,1}$, according to (A.4). For each $n > 1$, (A.13) is used to extrapolate to $I_{n+1,n+1}$. These estimates can be monitored until the approximation for I appears to converge to desired accuracy.

Computer programs for Romberg integration are widely available [1–3].

A.2 GAUSSIAN QUADRATURE

Romberg integration is based on a uniform subdivision of the interval (a, b). A more efficient type of numerical integration, known as Gaussian quadrature, involves nonuniform intervals. Referring to Equation (A.1), the integral estimate

$$I \cong \sum_{i=1}^{N} w_i f(x_i) \tag{A.15}$$

can be developed so that both the weights $\{w_i\}$ and the abscissas $\{x_i\}$ are selected to optimize the procedure. A common approach is to select these parameters so that the estimate is exact for polynomials up to degree p. For instance, consider a polynomial of degree 3:

$$f(x) = \alpha + \beta x + \gamma x^2 + \delta x^3 \tag{A.16}$$

For simplicity, we restrict our attention to the interval $-1 < x < 1$ and impose left-to-right symmetry on the weights and abscissas.

A rule with the form of (A.15) can be found involving only two sample points, $x = \pm x_1$. These can be determined by equating the rule (A.15) with the exact evaluation of (A.1) for each term in (A.16). This general constraint

$$\int_{-1}^{1} f(x)\,dx = w_{-1}f(x_{-1}) + w_1 f(x_1) = w_1 f(-x_1) + w_1 f(x_1) \tag{A.17}$$

yields the equations

$$2\alpha = w_1\alpha + w_1\alpha \tag{A.18}$$

$$\tfrac{2}{3}\gamma = w_1\gamma x_1^2 + w_1\gamma x_1^2 \tag{A.19}$$

Equations (A.18) and (A.19) can be solved to produce

$$w_{-1} = 1 \qquad x_{-1} = -\sqrt{\tfrac{1}{3}} \tag{A.20}$$

$$w_1 = 1 \qquad x_1 = \sqrt{\tfrac{1}{3}} \tag{A.21}$$

as the weights and samples. If it is desired to integrate a polynomial of degree 4, a third sample point at $x = x_0 = 0$ can be added, producing a set of constraints

$$2\alpha = w_1\alpha + w_0\alpha + w_1\alpha \tag{A.22}$$

$$\tfrac{2}{3}\gamma = w_1\gamma x_1^2 + w_1\gamma x_1^2 \tag{A.23}$$

$$\tfrac{2}{5}\varepsilon = w_1\varepsilon x_1^4 + w_1\varepsilon x_1^4 \tag{A.24}$$

leading to the set of weights and samples

$$w_{-1} = \tfrac{5}{9} \qquad x_{-1} = -\sqrt{\tfrac{3}{5}} \tag{A.25}$$

$$w_0 = \tfrac{8}{9} \qquad x_0 = 0 \tag{A.26}$$

$$w_1 = \tfrac{5}{9} \qquad x_1 = \sqrt{\tfrac{3}{5}} \tag{A.27}$$

Thus, with only three integrand samples, this quadrature rule can exactly integrate fourth-order polynomial functions.

The weights and samples derived above are known as Gauss–Legendre rules. Tables of weights and samples for Gauss–Legendre rules of various orders can be found in most numerical methods textbooks. In practice, higher order rules are developed based on the theory of orthogonal polynomials rather than the cumbersome simultaneous solution of nonlinear equations, used here for illustration. Additional information on Gaussian quadrature is available in the literature [1, 3–5].

A.3 GAUSS–KRONROD RULES

When integrating analytic (smooth) functions, Gaussian quadrature is more efficient than Romberg integration in the sense that it generally produces more accurate estimates for a given number of integrand samples. However, Romberg integration permits complete reuse of integrand samples when doubling the number of sample points. Thus, in a situation where no a priori knowledge of the necessary number of samples is available, Romberg integration provides a sequence of integral approximations, at no extra cost, from which convergence can be estimated.

Although a similar sequence cannot be obtained as efficiently with Gaussian quadrature, a partial remedy was provided in 1964 when Kronrod developed $(2n + 1)$-point Gaussian quadrature rules that reused the sample points from an n-point Gauss–Legendre formula [6]. This provides two estimates of the integral, one more accurate than the other, for $2n + 1$ samples. Since then, similar ideas have been applied to other forms of Gaussian quadrature [7] and incorporated into software libraries such as QUADPACK [8]. Because of the improved efficiency of Gaussian quadrature, the Gauss–Kronrod rules have usually superseded Romberg integration in practice.

A.4 INCORPORATION OF LOGARITHMIC SINGULARITIES

Although standard Gauss–Legendre rules yield relatively poor accuracy if the integrand contains a singularity, generalized Gaussian quadrature rules can be developed for integrals of the form

$$I = \int_a^b w(x) f(x)\, dx \tag{A.28}$$

where $w(x)$ might be singular. For instance, quadrature rules have been developed for a logarithmic singularity [9, 10]. In this case, a quadrature rule using n samples permits the exact integration of functions containing the $2n$ terms $\{1, \ln x, x, x \ln x, \ldots, x^{n-1}, x^{n-1} \ln x\}$.

When high accuracy is required, rules of this type are more efficient than the "singularity subtraction" approach introduced in Chapter 2. For illustration, a FORTRAN subroutine capable of treating a logarithmic singularity is provided in Appendix C.

A.5 GAUSSIAN QUADRATURE FOR TRIANGLES [11]

For evaluating multidimensional integrals, one possible approach is to create "product rules" by nesting single-dimensional quadrature rules. However, these algorithms are far from optimal. Gaussian quadrature rules can be developed specifically for multidimensional domains using ideas similar to those outlined in Section A.2. For triangular regions, consider the quadratic function

$$f(L_1, L_2) = \alpha L_1^2 + \beta L_2^2 + \gamma L_1 L_2 + \delta L_1 + \varepsilon L_2 + \zeta \tag{A.29}$$

where L_1 and L_2 denote two linearly independent simplex coordinates (L_1, L_2, L_3) within the triangle. By imposing triangular symmetry on the sample points and weights, a rule is sought involving the three sample points (η, ξ, ξ), (ξ, η, ξ), and (ξ, ξ, η), each of which is associated with the same weight. After imposing symmetry conditions, the quadrature rule must satisfy the four constraints

$$\iint dA = A \tag{A.30}$$

$$\iint L_1 \, dA = \tfrac{1}{3}A \tag{A.31}$$

$$\iint L_1^2 \, dA = \tfrac{1}{6}A \tag{A.32}$$

$$\iint L_1 L_2 \, dA = \tfrac{1}{12}A \tag{A.33}$$

where A denotes the triangle area. By equating the rule

$$I \cong A \sum_i w_i f(L_{1i}, L_{2i}, L_{3i}) \tag{A.34}$$

with the exact evaluations in (A.30)–(A.33), one obtains a system of four nonlinear equations, from which it is possible to extract the three sample points

$$w = \tfrac{1}{3} \qquad (L_1, L_2, L_3) = \left(\tfrac{2}{3}, \tfrac{1}{6}, \tfrac{1}{6}\right) \tag{A.35}$$

$$w = \tfrac{1}{3} \qquad (L_1, L_2, L_3) = \left(\tfrac{1}{6}, \tfrac{2}{3}, \tfrac{1}{6}\right) \tag{A.36}$$

$$w = \tfrac{1}{3} \qquad (L_1, L_2, L_3) = \left(\tfrac{1}{6}, \tfrac{1}{6}, \tfrac{2}{3}\right) \tag{A.37}$$

Similar rules can be developed for higher order representations, and the literature contains Gaussian quadrature rules sufficient for integrating polynomials up to degree 20 on triangles [12–14].

In the single-dimensional case, orthogonal polynomials can be used to simplify the development of higher order quadrature rules. The lack of an analogous theory for multidimensional orthogonal polynomials has hampered the systematic development of multidimensional Gaussian quadrature rules, and most of the existing rules [13, 14] appear to be the result of numerical solutions of the nonlinear equations.

A.6 GAUSSIAN QUADRATURE FOR TETRAHEDRONS

A few quadrature formulas have been developed for tetrahedral domains using ideas similar to those outlined above. For instance, Keast presents rules up to polynomial degree 9 [14, 15]. The table of coefficients in [15] appears to contain an error for the eighth-degree rule for the weight associated with the sample point in the centroid of the tetrahedron. The correct weight should be negative ($-0.039327\ldots$).

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