Quadrature

Numerical quadrature is the computation of the area (or volume, etc.) of a region bounded by one or more functions; in one variable it is the evaluation of

$$I \equiv \int_a^b f(x)dx.$$

Let's assume (i) that f is integrable on $[a, b]$ and (ii) that we can evaluate f at any point in (a, b). An important class of commonly used formulas for approximating I can be derived from the Lagrange interpolation result:

$$f(x) = P_n(x) + R_n(x), \quad \text{where} \quad R(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j),$$

$x_j \in (a, b),\ j = 0, 1, \ldots, n$, and $\xi = \xi(x) \in (a, b)$.

Integrating gives

$$\int_a^b f(x)dx = \int_a^b P_n(x)dx + \int_a^b R_n(x)dx,$$

which yields a family of quadrature formulae

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \sum_{i=0}^{n} c_i f(x_i),$$

where

$$c_i = \int_a^b L_{ni}(x)dx.$$

If f is smooth enough, the error in this approximation is $\int_a^b R_n(x)dx$.

If we discretize $[a, b]$ into $n + 1$ equally spaced nodes, the integrals giving the c_i can be evaluated analytically *a priori*, to give quadrature rules. If we let $h = (b - a)/n$ and $x_j = a + jh,\ j = 0, 1, \ldots, n$, then a few of the *closed Newton-Cotes* rules are

$$\begin{aligned} \int_a^b f(x)dx &= \tfrac{b-a}{2}(f(a) + f(b)) - \tfrac{h^3}{12} f''(\xi_1) && \text{(Trapezoidal Rule}, n = 1) \\ &= \tfrac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \tfrac{h^5}{90} f^{(4)}(\xi_2) && \text{(Simpson's Rule}, n = 2) \end{aligned}$$

If we let $h = (b - a)/(n + 2)$, and $x_j = a + (j + 1)h,\ j = 0, 1, \ldots, n$, we get the *open Newton-Cotes* formulae. This set of nodes does not include a or b and might be useful if there is a singularity at an endpoint:

$$\begin{aligned} \int_a^b f(x)dx &= \tfrac{b-a}{2}(f(x_0) + f(x_1)) + \tfrac{3h^3}{4} f''(\xi_1) && (n = 1) \\ &= \tfrac{b-a}{3}(2f(x_0) - f(x_1) + 2f(x_2)) + \tfrac{14h^5}{45} f^{(4)}(\xi_2) && (n = 2) \end{aligned}$$

The error terms have formulae that depend on the parity of n and whether open or closed, but they all look something like the closed rule with n-even:

$$R(f, n) = \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t \prod_{k=0}^{n} (t - k)\ dt, \quad \xi \in (a, b).$$