1. Gauss quadrature

Recall that the method of moments approach to numerical integration based upon sampling $\mathscr{D} = \{(x_i, y_i = f(x_i)), i = 0,..., n\}$,

$$\int_a^b \omega(t) f(t)\,\mathrm{d}t = \sum_{i=0}^n w_i y_i + e \cong \sum_{i=0}^n w_i y_i,$$

imposes exact results for a finite number of members of a basis set $\{\phi_0, \ldots, \phi_n, \ldots\}$

$$\int_a^b \omega(t) \phi_k(t)\,\mathrm{d}t = \sum_{i=0}^n w_i \phi_k(x_i), k = 0, 1, \ldots, n.$$

The trapezoid, Simpson formulas arise from the monomial basis set $\{1, t, t^2, \ldots\}$, in which case

$$\int_a^b \omega(t) t^k\,\mathrm{d}t = \sum_{i=0}^n w_i x_i^k, k = 0, 1, \ldots, n,$$

but any basis set can be chosen. Instead of prescribing the sampling points x_i *a priori*, which typically leads to an error $e = \mathscr{O}(\phi_{n+1}(t))$, the sampling points can be chosen to minimize the error e. For the monomial basis this leads to a system of $2(n+1)$ equations

$$\int_a^b \omega(t) t^k\,\mathrm{d}t = \sum_{i=0}^n w_i x_i^k, k = 0, 1, \ldots, 2n+1,$$

for the unknown $n+1$ quadrature weights w_i and the $n+1$ sampling points x_i. The system is nonlinear, but can be solved in an insightful manner exploiting the properties of orthogonal polynomials known as Gauss quadrature.

The basic idea is to consider a Hilbert function space with the scalar product

$$(f, g) = \int_a^b \omega(t) f(t)\, g(t)\,\mathrm{d}t,$$

and orthonormal basis set $\{\phi_0(t), \phi_1(t), \phi_2(t),, \ldots\}$,

$$(\phi_j, \phi_k) = \int_a^b \omega(t) \phi_j(t)\, \phi_k(t)\,\mathrm{d}t = \delta_{jk}.$$

Assume that $\phi_k(t)$ are polynomials of degree k. A polynomial p_{2n+1} of degree $2n+1$ can be factored as

$$p_{2n+1}(t) = q_n(t)\, \phi_{n+1}(t) + r_n(t),$$

where $q_n(t)$ is the quotient polynomial of degree n, and r_n is the remainder polynomial of degree n. The weighted integral of p_{2n+1} is therefore

$$\int_a^b \omega(t) p_{2n+1}(t)\,\mathrm{d}t = \int_a^b \omega(t) [q_n(t)\, \phi_{n+1}(t) + r_n(t)]\,\mathrm{d}t = (q_n, \phi_{n+1}) + \int_a^b \omega(t) r_n(t)\,\mathrm{d}t.$$

Since $\{\phi_0, \ldots, \phi_{n+1}\}$ is an orthonormal set, $(q_n, \phi_{n+1}) = 0$, and the integral becomes

$$\int_a^b \omega(t) p_{2n+1}(t)\,\mathrm{d}t = \int_a^b \omega(t) r_n(t)\,\mathrm{d}t.$$

The integral of the n^{th} remainder polynomial can be exactly evaluated through an $n+1$ point quadrature

$$\int_a^b \omega(t) r_n(t)\,\mathrm{d}t = \sum_{i=0}^n w_i\, r(x_i),$$

that however evaluates $r(t)$ rather than the original integrand $p_{2n+1}(t)$. However, evaluation of the factorization (1) at the roots x_i of ϕ_{n+1}, $\phi_{n+1}(x_i) = 0$, $i = 0, 1, \ldots, n$, gives

$$p_{2n+1}(x_i) = q_n(x_i)\, \phi_{n+1}(x_i) + r_n(x_i) = r_n(x_i),$$

stating that the values of the remainder at these nodes are the same as those of the p_{2n+1} polynomial. This implies that

$$\int_a^b \omega(t) p_{2n+1}(t)\,\mathrm{d}t = \sum_{i=0}^n w_i\, p_{2n+1}(x_i),$$

is an exact quadrature of order $2n+1$, $e = \mathcal{O}(t^{2n+1})$. The weights w_i can be determined through any of the previously outlined methods, e.g., method of moments

$$\int_a^b \omega(t) t^k \, \mathrm{d}t = \sum_{i=0}^{n} w_i x_i^k, k = 0, \ldots, n,$$

which is now a linear system that can be readily solved. Alternatively, the weights are also directly given as integrals of the Lagrange polynomials based upon the nodes that are roots of ϕ_{n+1}

$$w_i = \int_a^b \omega(t) \, \ell_i(t) \, \mathrm{d}t.$$