10 Gaussian Quadrature

So far we have encountered the Newton-Cotes formulas

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

which are *exact* if f is a polynomial of degree at most n.

It is important to note that in the derivation of the Newton-Cotes formulas we assumed that the nodes x_i were equally spaced and fixed. The main idea for obtaining more accurate quadrature rules is to treat the nodes as additional degrees of freedom, and then hope to find "good" locations that ensure higher accuracy. Therefore, we now have $n+1$ nodes x_i in addition to $n+1$ polynomial coefficients for a total of $2n+2$ degrees of freedom. This should be enough to derive a quadrature rule that is exact for polynomials of degree up to $2n+1$. Gaussian quadrature, indeed accomplishes this:

Theorem 10.1 *Let q be a nonzero polynomial of degree $n+1$ and w a positive weight function such that*

$$\int_a^b x^k q(x)w(x)dx = 0, \qquad k = 0, \ldots, n. \tag{95}$$

If the nodes x_i, $i = 0, \ldots, n$, are the zeros of q, then

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i) \tag{96}$$

with

$$A_i = \int_a^b \ell_i(x)w(x)dx, \qquad i = 0, \ldots, n, \tag{97}$$

is exact for all polynomials of degree at most $2n+1$. Here ℓ_i, $i = 0, \ldots, n$, are the usual Lagrange interpolating polynomials of Chapter 1.

Proof Assume f is a polynomial of degree at most $2n+1$, and show

$$\sum_{i=0}^{n} A_i f(x_i) = \int_a^b f(x)w(x)dx.$$

Using long division we have

$$\underbrace{f(x)}_{\text{deg.}2n+1} = \underbrace{q(x)}_{\text{deg.}n+1} p(x) + r(x),$$

where p and r are both polynomials of degree at most n.

By taking x_i as the zeros of q we have

$$f(x_i) = r(x_i), \qquad i = 0, \ldots, n.$$

Now

$$\int_a^b f(x)w(x)dx = \int_a^b [q(x)p(x) + r(x)]\, w(x)dx$$

$$= \underbrace{\int_a^b q(x)p(x)w(x)dx}_{=0} + \int_a^b r(x)w(x)dx,$$

where the first integral on the right-hand side is zero by the orthogonality assumption (95).

We know that (for any set of nodes x_i) (96) is exact for polynomials of degree at most n. Therefore,

$$\begin{aligned} \int_a^b f(x)w(x)dx &= \int_a^b r(x)w(x)dx \\ &\stackrel{(96)}{=} \sum_{i=0}^{n} A_i r(x_i). \end{aligned}$$

However, since our special choice of nodes implies $f(x_i) = r(x_i)$ we have

$$\int_a^b f(x)w(x)dx = \sum_{i=0}^{n} A_i f(x_i)$$

for any polynomial f of degree at most $2n+1$.

Remark Usually, the classical orthogonal polynomials as discussed in the Maple worksheet `478578_GaussQuadrature.mws` are used to construct Gaussian quadrature rules with the appropriate weight function suggested by the integrand at hand.

Example If $[a,b] = [-1,1]$ and $w(x) = 1$ we use Legendre polynomials (since they are orthogonal with respect to this interval and weight function). The corresponding two-point formula ($n = 1$ — which is exact for cubic polynomials) is

$$\int_{-1}^{1} f(x)dx \approx A_0 f(x_0) + A_1 f(x_1)$$

with x_0 and x_1 as the roots of $q_2(x) = x^2 - \frac{1}{3}$, i.e.,

$$x_0 = \frac{\sqrt{3}}{3}, \quad x_1 = -\frac{\sqrt{3}}{3}.$$

A_0 and A_1 are then found by enforcing exactness for polynomials of degree at most $n = 1$:

$$\begin{aligned} \int_{-1}^{1} dx &= A_0 + A_1 \\ \int_{-1}^{1} x dx &= A_0 x_0 + A_1 x_1. \end{aligned}$$

These formulas ensure (for arbitrary nodes) exactness for constants, and linear polynomials, respectively. The preceding equations are equivalent to the 2×2 linear system

$$\begin{bmatrix} 1 & 1 \\ x_0 & x_1 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix},$$

which implies $A_0 = A_1 = 1$. Alternatively, we could have applied (97) directly to compute the coefficients A_0 and A_1. Therefore,

$$\int_{-1}^{1} f(x)dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

Remark 1. There are tables for the values of x_i and A_i for various choices of classical orthogonal polynomials q of modest degree. Many software packages also have functions implementing this.

2. If the integral is defined over the interval $[a, b]$ instead of $[-1, 1]$, then a simple transformation

$$x = \frac{b + a + t(b - a)}{2}, \qquad -1 \leq t \leq 1$$

can be used.

3. Note that without the theorem on Gaussian quadrature we would have to solve a 4×4 system of *nonlinear* equations with unknowns x_0, x_1, A_0 and A_1 (enforcing exactness for cubic polynomials) to obtain the two-point formula of the example above (see the Maple worksheet `478578_GaussQuadrature.mws`).