Lecture 25: Gaussian Quadrature

4.4 Gaussian quadrature.

It is clear that the trapezoid rule,

$$I(f) = \frac{b-a}{2}(f(a)+f(b)),$$

exactly integrates linear polynomials, but not all quadratics. In fact, one can show that *no* quadrature rule of the form

$$I(f) = w_a f(a) + w_b f(b)$$

will exactly integrate all quadratics over $[a,b]$, regardless of the choice of constants w_a and w_b.

4.4.1. A special 2-point rule.

Suppose we consider a more general class of 2-point quadrature rules, where we do not initially fix the points at which the integrand f is evaluated:

$$I(f) = w_0 f(x_0) + w_1 f(x_1)$$

for unknowns *nodes* $x_0, x_1 \in [a,b]$ and *weights* w_0 and w_1. We wish to pick x_0, x_1, w_0, and w_1 so that the quadrature rule exactly integrates all polynomials of the largest degree possible. Since this quadrature rule is linear, it will suffice to check that it is exact on monomials. There are four unknowns; to get four equations, we will require $I(f)$ to exactly integrate 1, x, x^2, x^3.

$$\begin{array}{lclcrcl}
f(x)=1: & \displaystyle\int_a^b 1\,\mathrm{d}x = I(1) & \Longrightarrow & b-a & = & w_0+w_1 \\
f(x)=x: & \displaystyle\int_a^b x\,\mathrm{d}x = I(x) & \Longrightarrow & \frac{1}{2}(b^2-a^2) & = & w_0x_0+w_1x_1 \\
f(x)=x^2: & \displaystyle\int_a^b x^2\,\mathrm{d}x = I(x^2) & \Longrightarrow & \frac{1}{3}(b^3-a^3) & = & w_0x_0^2+w_1x_1^2 \\
f(x)=x^3: & \displaystyle\int_a^b x^3\,\mathrm{d}x = I(x^3) & \Longrightarrow & \frac{1}{4}(b^4-a^4) & = & w_0x_0^3+w_1x_1^3
\end{array}$$

Three of these constraints are *nonlinear* equations of the unknowns x_0, x_1, w_0, and w_1: thus questions of existence and uniqueness of solutions becomes a bit more subtle than for the linear equations we so often encounter.

In this case, a solution *does* exist:

$$w_0 = w_1 = \tfrac{1}{2}(b-a), \qquad x_0 = \tfrac{1}{2}(b+a) - \tfrac{\sqrt{3}}{6}(b-a) \qquad x_1 = \tfrac{1}{2}(b+a) + \tfrac{\sqrt{3}}{6}(b-a).$$

Notice that $x_0, x_1 \in [a,b]$: If this were not the case, we could not use these points as quadrature nodes, since f might not be defined outside $[a,b]$. When $[a,b]=[-1,1]$, the interpolation points are $\pm 1/\sqrt{3}$, giving the quadrature rule

$$I(f) = f(-1/\sqrt{3}) + f(1/\sqrt{3}).$$

4.4.2. Generalization to higher degrees.

Emboldened by the success of this humble 2-point rule, we consider generalizations to higher degrees. If some two-point rule ($n+1$ integration nodes, for $n=1$) will exactly integrate all cubics ($3=2n+1$), one might anticipate the existence of rules based on $n+1$ points that exactly integrate all polynomials of degree $2n+1$, for general values of n. Toward this end, consider quadrature rules of the form

$$I(f) = \sum_{j=0}^{n} w_j f(x_j),$$

for which we will choose the nodes $\{x_j\}$ and weights $\{w_j\}$ (a total of $2n+2$ variables) to maximize the degree of polynomial that is integrated exactly.

The primary challenge is to find satisfactory quadrature nodes. Once these are found, the weights follow easily: in theory, one could obtain them by integrating the polynomial interpolant at the nodes, though better methods are available in practice. In particular, this procedure for assigning weights ensures, at a minimum, that $I(f)$ will exactly integrate all polynomials of degree n. This assumption will play a key role in the coming development.

Orthogonal polynomials, introduced in Lecture 20, will play a prominent role in this exposition. Let $\{\phi_j\}_{j=0}^{n+1}$ be a system of orthogonal polynomials with respect to the inner product

$$\langle f, g\rangle = \int_a^b f(x)g(x)w(x)\,\mathrm{d}x$$

for some weight function $w \in C(a,b)$ that is non-negative over (a,b) and takes the value of zero only on a set of measure zero. We wish to construct a quadrature rule of the form

$$I(f) = \sum_{j=0}^{n} w_j f(x_j) \approx \int_a^b f(x)w(x)\,\mathrm{d}x.$$

It is our aim to make $I(f)$ exact for all $p \in \mathcal{P}_{2n+1}$.

To begin, consider an arbitrary $p \in \mathcal{P}_{2n+1}$. Using polynomial division, we can always write

$$p(x) = \phi_{n+1}(x)q(x) + r(x)$$

for some $q, r \in \mathcal{P}_n$ that depend on p. Integrating this p, we obtain

$$\begin{aligned}\int_a^b p(x)w(x)\,\mathrm{d}x &= \int_a^b \phi_{n+1}(x)q(x)w(x)\,\mathrm{d}x + \int_a^b r(x)w(x)\,\mathrm{d}x\\ &= \int_a^b r(x)w(x)\,\mathrm{d}x.\end{aligned}$$

The second step is another consequence that important basic fact, proved in Lecture 20, that the orthogonal polynomial ϕ_{n+1} is orthogonal to all $q \in \mathcal{P}_n$.

Now apply the quadrature rule to p, and attempt to pick the interpolation nodes $\{x_j\}$ to yield the value of the exact integral computed above. In particular,

$$I(p) = \sum_{j=0}^{n} w_j p(x_j) = \sum_{j=0}^{n} w_j \phi_{n+1}(x_j)q(x_j) + \sum_{j=0}^{n} w_j r(x_j)$$

$$= \sum_{j=0}^{n} w_j \phi_{n+1}(x_j) q(x_j) + \int_a^b r(x) w(x)\,\mathrm{d}x.$$

This last statement is a consequence of the fact that $I(\cdot)$ will exactly integrate all $r \in \mathcal{P}_n$. This will be true regardless of our choice for the distinct nodes $\{x_j\} \subset [a,b]$. (Recall that the quadrature rule is constructed so that it exactly integrates a degree-n polynomial interpolant to the integrand, and in this case the integrand, r, is a degree n polynomial. Hence $I(r)$ will be exact.)

Notice that we can force agreement between $I(p)$ and $\int_a^b p(x)w(x)\,\mathrm{d}x$ provided

$$\sum_{j=0}^{n} w_j \phi_{n+1}(x_j) q(x_j) = 0.$$

We cannot make assumptions about $q \in \mathcal{P}_n$, as this polynomial will vary with the choice of p, but we can exploit properties of ϕ_{n+1}. Since ϕ_{n+1} has exact degree $n+1$ (recall this property of all orthogonal polynomials), it must have $n+1$ roots. If we choose the interpolation nodes $\{x_j\}$ to be the roots of ϕ_{n+1}, then $\sum_{j=0}^{n} w_j \phi_{n+1}(x_j) q(x_j) = 0$ as required, and we have a quadrature rule that is exact for all polynomials of degree $2n+1$.

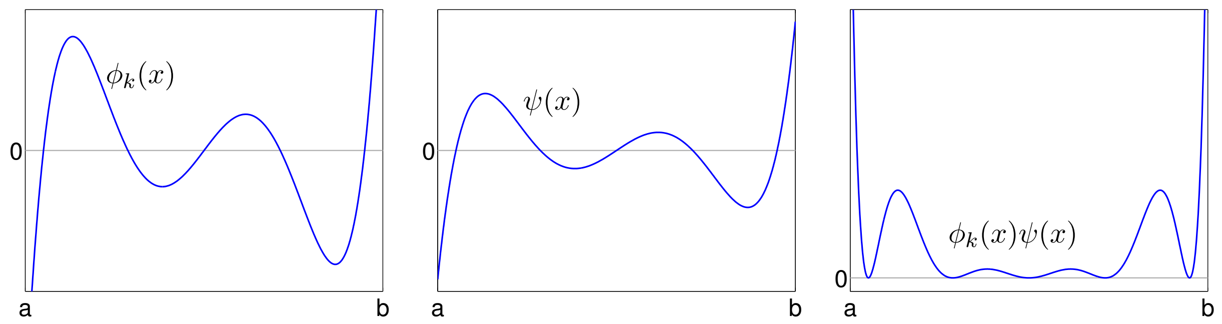
Before we can declare victory, though, we must exercise some caution. Perhaps ϕ_{n+1} has repeated roots (so that the nodes $\{x_j\}$ are not distinct), or perhaps these roots lie at points in the complex plane where f may not even be defined. Since we are integrating f over the interval $[a,b]$, it is crucial that ϕ_{n+1} has $n+1$ distinct roots in $[a,b]$. Fortunately, this is one of the many beautiful properties enjoyed by orthogonal polynomials.

Theorem (Roots of Orthogonal Polynomials). Let $\{\phi_k\}_{k=0}^{n}$ be a system of orthogonal polynomials on $[a,b]$ with respect to the weight function $w(x)$. Then ϕ_k has k distinct real roots, $\{x_j^{(k)}\}_{j=1}^{k}$, with $x_j^{(k)} \in [a,b]$ for $j = 1,\ldots,k$.

Proof. Suppose that ϕ_k, a polynomial of exact degree k, changes sign at $j < k$ distinct roots $\{x_\ell^{(k)}\}_{\ell=1}^{j}$, in the interval $[a,b]$. Then define

$$\psi(x) = (x - x_1^{(k)})(x - x_2^{(k)}) \cdots (x - x_j^{(k)}) \in \mathcal{P}_j.$$

This function changes sign at exactly the same points as ϕ_k does on $[a,b]$. Thus, the product of these two functions, $\phi_k\psi$, *does not change sign* on $[a,b]$. See the illustration below.



As the weight function $w(x)$ is nonnegative on $[a, b]$, it must also be that $\phi_k \psi w$ does not change sign on $[a, b]$. However, the fact that $\psi \in \mathcal{P}_j$ for $j < k$ implies that

$$\int_a^b \phi_k(x)\psi(x)w(x)\,\mathrm{d}x = 0,$$

since ϕ_k is orthogonal to all polynomials of degree $k-1$or lower. Thus, we conclude that the integral of some continuous nonzero function $\phi_k \psi w$ that never changes sign on $[a, b]$ must be zero. This is a contradiction, as the integral of such a function must always be positive. Thus, ϕ_k must have at least k distinct zeros in $[a, b]$. As ϕ_k is a polynomial of degree k, it can have no more than k zeros. ■

We have arrived at *Gaussian quadrature rules*: Integrate the polynomial that interpolates f at the roots of the orthogonal polynomial ϕ_{n+1}. What are the weights $\{w_j\}$? Write the interpolant, p_n, in the Lagrange basis,

$$p_n(x) = \sum_{j=0}^{n} f(x_j)\ell_j(x),$$

where the basis polynomials ℓ_j are defined as usual,

$$\ell_j(x) = \prod_{k=0,k\neq j}^{n} \frac{(x - x_k)}{(x_j - x_k)}.$$

Integrating this interpolant gives

$$I(f) = \int_a^b p_n(x)w(x)\,\mathrm{d}x = \int_a^b \sum_{j=0}^{n} f(x_j)\ell_j(x)w(x)\,\mathrm{d}x = \sum_{j=0}^{n} f(x_j)\int_a^b \ell_j(x)w(x)\,\mathrm{d}x,$$

revealing a formula for the quadrature weights:

$$w_j = \int_a^b \ell_j(x)w(x)\,\mathrm{d}x.$$

(There are better ways to compute these weights, but the values will be the same. In practice, one solves a symmetric tridiagonal eigenvalue problem with to get the nodes and weights.) By our construction, we have proved the following result.

Theorem. Suppose $I(f)$ is the Gaussian quadrature rule

$$I(f) = \sum_{j=0}^{n} w_j f(x_j),$$

where the nodes $\{x_j\}_{j=0}^n$ are the $n+1$ roots of a degree-$(n+1)$ orthogonal polynomial on $[a, b]$ with weight function $w(x)$, and $w_j = \int_a^b \ell_j(x)w(x)\,\mathrm{d}x$. Then $I(f)$ is exact for all polynomials of degree $2n + 1$.

Of course, in many circumstances we are not simply integrating polynomials, but more complicated functions. For that common situation, we have the following error bound, which we state without proof (see Süli and Mayers, pp. 282–283).

Theorem. Suppose $f \in C^{2n+2}[a,b]$ and let $I(f)$ be the usual $(n+1)$-point Gaussian quadrature rule on $[a,b]$ with weight function $w(x)$ and nodes $\{x_j\}_{j=0}^{n}$. Then

$$\int_a^b f(x)w(x)\,\mathrm{d}x - I(f) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\int_a^b \psi^2(x)w(x)\,\mathrm{d}x$$

for some $\xi \in [a,b]$ and $\psi(x) = \prod_{j=0}^{n}(x - x_j)$.