AM205: Gaussian quadrature

In the lectures, we discussed the accuracy of different quadrature schemes for numerically evaluating integrals of the form

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

Let Q_n be a quadrature scheme that integrates polynomials up to degree n exactly. Then we derived that the error between $Q_n[f]$ and the true integral satisfies the bound

$$|I[f] - Q_n[f]| \le C_n \min_{p\in\mathbb{P}_n} \|p - f\|_\infty, \tag{2}$$

where $\mathbb{P}_n$ is the family of all polynomials of degree n. Here $C_n = b - a + \sum_{k=0}^{n} |w_k|$, where w_k are the quadrature weights. As n increases, the accuracy of approximation of f by polynomials will increase. Indeed, by the Weierstraß approximation theorem, we know that for a continuous function f, then $\min_{p\in\mathbb{P}_n} \|p - f\| \to 0$ as $n \to \infty$. Hence, to improve accuracy, it is generally desirable to search for quadrature schemes that maximize the degree of polynomial that they integrate exactly.

Given any set of $n + 1$ quadrature points $x_0, x_1, \ldots, x_n$, the associated quadrature scheme is based upon constructing a Lagrange interpolating polynomial of degree n through the function f at those points. Hence any choice of quadrature points will integrate all polynomials of up to order n exactly, since the Lagrange interpolant will simply match the polynomial itself. However, we can ask whether it is possible to do better via a judicious choice of points. A quadrature scheme is defined by the points $x_0, x_1, \ldots, x_n$ plus the associated weights $w_0, w_1, \ldots, w_n$, providing $2n + 2$ total degrees of freedom.

Amazingly, it is possible to construct an $(n+1)$-point quadrature scheme that integrates polynomials up to degree $2n + 1$ exactly. Since polynomials in $\mathbb{P}_{2n+1}$ have $2n + 2$ degrees of freedom, this is the maximum that we could hope to achieve. These quadrature schemes are called *Gaussian quadrature*. The points of the $(n + 1)$-point Gaussian quadrature scheme are given by the roots of the $(n + 1)$th *Legendre polynomial*, discussed in the next section. Once the roots are known, the weights are given by integrating the associated Lagrange polynomial basis. A further useful property of Gaussian quadrature is that the weights always work out to be positive, which is not true for other schemes such as Newton–Cotes.

At first sight, it is not obvious why Gaussian quadrature schemes are able to integrate double the expected order of polynomials. This document explains why.

Orthogonal polynomials

The Legendre polynomials are an example of an orthogonal polynomial set. To define an orthogonal polynomial set, an inner product of the form

$$\langle p, q\rangle = \int_a^b p(x)q(x)w(x)dx \tag{3}$$

is first introduced, where $w(x)$ is a positive weight function. This inner product can be viewed as a generalization of the scalar product for vectors.[1] An orthogonal polynomial set is then given by a family of polynomials $u_0, u_1, u_2, \ldots$ such that

$$\langle u_j, u_k \rangle = 0 \qquad \text{for } j \neq k. \tag{4}$$

Many different families of orthogonal polynomials are used in mathematics, depending on the choice of weight function $w(x)$ and interval $[a, b]$. The two of most relevance to AM205 are:

- The Chebyshev polynomials, given by $w(x) = (1 - x^2)^{-1/2}$ and the interval $[-1, 1]$, which are optimal in some sense for function interpolation.
- The Legendre polynomials given by $w(x) = 1$ and the interval $[-1, 1]$, which form the basis of Gaussian quadrature.

However, many other examples exist, such as

- The Hermite polynomials, given by $w(x) = e^{-x^2}$ and the interval $(-\infty, \infty)$.
- The Laguerre polynomials, given by $w(x) = e^{-x}$ and the interval $[0, \infty)$.
- The Jacobi polynomials, given by $w(x) = (1 - x)^\alpha (1 + x)^\beta$ and the interval $[-1, 1]$. Here α and β are free parameters. Note that the Chebyshev and Legendre polynomials are special cases when $(\alpha, \beta) = (-1/2, -1/2)$ and $(\alpha, \beta) = (0, 0)$, respectively.

In each polynomial set, the polynomials have increasing order, so that u_k has degree k. Furthermore, for any k, the set $\{u_0, u_1, \ldots, u_k\}$ forms a basis for $\mathbb{P}_k$. Note that for the polynomials specified over a finite interval, the range $[-1, 1]$ is typically used by convention, but the polynomials can be applied to any other interval by an appropriate rescaling. Orthogonal polynomials have many useful properties. Here, we focus particularly on the Legendre polynomials $P_k(x)$, the first several of which are given by

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = \tfrac{1}{2}(3x^2 - 1). \tag{5}$$

They can be calculated using Rodrigues' formula,

$$P_k(x) = \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2 - 1)^k, \tag{6}$$

and they satisfy the recurrence relation

$$(k + 1) P_{k+1}(x) = (2k + 1) x P_k(x) - k P_{k-1}(x). \tag{7}$$

[1]Let $\mathbf{p} = (p_1, p_2, \ldots, p_m)$ and $\mathbf{q} = (q_1, q_2, \ldots, q_m)$ be m-dimensional vectors. The scalar product is $\mathbf{p} \cdot \mathbf{q} = \sum_{i=1}^m p_i q_i$, and as m gets large, this sum becomes similar to taking an integral like Eq. 3, for the special case of $w(x) = 1$.

Gaussian quadrature

We now establish the main result that the $(n+1)$-point Gaussian quadrature scheme can integrate polynomials of degree $2n+1$ exactly. For maximum generality, we keep $w(x)$ as an arbitrary weight function and let $u_0, u_1, \ldots$ be the associated orthogonal polynomial set. Let u_{n+1} be the associated orthogonal polynomial of degree $n+1$. Consider a monomial x^l where $l \leq n$. Then using the basis property of orthogonal polynomials, there is an expansion $x^l = \sum_{i=0}^{l} \gamma_i u_i(x)$ and hence

$$\int_a^b x^l u_{n+1}(x) w(x) dx = \int_a^b \left(\sum_{i=0}^{l} \gamma_i u_i(x) \right) u_{n+1}(x) w(x) dx = \sum_{i=0}^{l} \gamma_i \langle u_i, u_{n+1} \rangle = 0 \tag{8}$$

where the inner products vanish from the orthogonality relations. Let the points of the quadrature scheme $x_0, x_1, \ldots, x_n$ be the roots of $u_{n+1}(x)$, and define associated quadrature weights using

$$w_k = \int_a^b \ell_k(x) w(x) dx \tag{9}$$

where ℓ_k is the kth Lagrange basis polynomial.

Now consider integrating a polynomial f of degree at most $2n+1$. The key observation is that by using long division, f can always be written as

$$f(x) = p(x) u_{n+1}(x) + r(x) \tag{10}$$

where p and r are polynomials of degree at most n. The exact integral of f is given by

$$I[f] = \int_a^b f(x) w(x) dx = \int_a^b \left(p(x) u_{n+1}(x) + r(x) \right) w(x) dx = \int_a^b r(x) w(x) dx \tag{11}$$

where the orthogonality relation of Eq. 8 has been used to eliminate the term involving p. Applying the quadrature scheme to f yields

$$Q[f] = \sum_{k=0}^{n} w_k f(x_k) = \sum_{k=0}^{n} w_k \left(p(x_k) u_{n+1}(x_k) + r(x_k) \right) = \sum_{k=0}^{n} w_k r(x_k). \tag{12}$$

Here, the terms involving p vanish because the points x_k are chosen to be at the roots of u_{n+1}. Since r is a polynomial of degree at most n, it follows that

$$Q[f] = \sum_{k=0}^{n} w_k r(x_k) = \int_a^b r(x) w(x) dx = I[f], \tag{13}$$

so the quadrature scheme is exact for $f \in \mathbb{P}_{2n+1}$.

The result for Gaussian quadrature is therefore established by considering the special case when $w(x) = 1$, where the orthogonal polynomials are the Legendre polynomials (*i.e.* $u_k = P_k$). However, the same principles can be used to derive other practical quadrature schemes. If $w(x) = (1-x^2)^{-1/2}$, then the orthogonal polynomials become the Chebyshev polynomials, $u_k = T_k$. The roots of the Chebyshev polynomials are clustered more tightly toward the interval endpoints, reflective of the fact that the choice of $w(x)$ adds more weight to those regions.