Gauss quadrature

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May 2, 2016

These notes derive Gauss quadrature using Hermite interpolation.

We would like to approximate the integral

$$I[f] = \int_a^b f(x)\,dx,$$

of a real function $f : [a, b] \to \mathbb{R}$ by an n-point rule of the form

$$I_n[f] = \sum_{i=1}^{n} w_i f(x_i), \tag{1}$$

for certain points $a \le x_1 < x_2 < \cdots < x_n \le b$ and weights $w_i \in \mathbb{R}$.

We say that I_n has degree of precision d if it is exact for polynomials of degree $\le d$, i.e., for polynomials in π_d.

For any choice of points x_i we can find weights w_i for which I_n has degree of precision $\ge n - 1$. We do this by integrating the Lagrange interpolant $p \in \pi_{n-1}$ to f at these points. Since

$$p(x) = \sum_{i=1}^{n} L_i(x) f(x_i),$$

where

$$L_i(x) = \prod_{j \ne i} \frac{x - x_j}{x_i - x_j},$$

we have

$$I[p] = \sum_{i=1}^{n} w_i f(x_i),$$

where $w_i = I[L_i]$. This gives us the rule

$$I_n[f] = I[p], \tag{2}$$

and it has degree of precision at least $n-1$ because if $f \in \pi_{n-1}$ then $p = f$.

The idea of Gauss quadrature is to choose the n points x_i in the rule (2) in such a way as to raise its degree of precision to $2n-1$. We note that there is no hope of raising its degree of precision to $2n$ or higher because for any points x_i if

$$s(x) = (x - x_1)(x - x_2) \cdots (x - x_n), \tag{3}$$

then $s^2 \in \pi_{2n}$ but

$$I_n[s^2] = 0, \qquad I[s^2] > 0.$$

One way to derive the Gauss rule is to integrate the Hermite interpolant q to f, the polynomial $q \in \pi_{2n-1}$ such that

$$q(x_i) = f(x_i), \quad q'(x_i) = f'(x_i), \qquad i = 1, \ldots, n.$$

If we set

$$I_n[f] = I[q]$$

then I_n clearly has degree of precision $2n-1$, which is what we want. At the same time, it turns out that it is possible to choose the x_i in such a way that the integral of q is independent of the derivatives $f'(x_i)$. To see this define the inner product of two functions f and g on $[a, b]$ by

$$\langle f, g \rangle = \int_a^b f(x) g(x) \, dx.$$

Theorem 1 *If s in (3) is orthogonal to π_{n-1} then*

$$I[q] = I[p].$$

Proof. Since $q - p$ is a polynomial in π_{2n-1} which is zero at x_i, $i = 1, \ldots, n$, there must be some polynomial $r \in \pi_{n-1}$ such that

$$q = p + sr.$$

Therefore,

$$I[q] = I[p] + \langle s, r \rangle,$$

and since r is orthogonal to s, the inner product on the right is zero. $\square$

Thus if $x_1, \ldots, x_n$ are the roots of a polynomial in π_n that is orthogonal to π_{n-1} the rule (2) has degree of precision $2n-1$, and this is what we call the n-point Gauss quadrature rule. Fortunately there is a solution. We have shown earlier that we can construct a sequence of polynomials ϕ_k, $k = 0, 1, 2, \ldots$ such that $\phi_k \in \pi_k$ and $\langle \phi_j, \phi_k \rangle = 0$ for $j \neq k$ and $\langle \phi_k, \phi_k \rangle \neq 0$. These are known as Legendre polynomials.

Theorem 2 *The Legendre polynomial ϕ_n has real, distinct roots and they are all in (a, b).*

Proof. Let $a < x_1 < x_2 < \cdots < x_m < b$ be the m sign-changes of ϕ_n in (a, b), $m \leq n$, and let $q(x) = (x - x_1) \cdots (x - x_m)$. Then the product $q\phi_n$ is a function of one sign in $[a, b]$, and so $\langle q, \phi_n \rangle \neq 0$, and thus ϕ_n is not orthogonal to q. Therefore, the degree of q must be at least n, i.e., $m = n$. □

If ϕ_n is normalized to have leading coefficient 1, we can thus set $s = \phi_n$, so that $x_1, \ldots, x_n$ are the roots of ϕ_n. In addition to its high degree of precision, Gauss quadrature also has positive weights which gives it numerical stability.

Theorem 3 *The weights in the Gauss rule are positive because $w_i = I[L_i^2]$.*

Proof. By definition, $w_i = I[L_i]$. Therefore,

$$w_i = I[L_i^2] + I[L_i(1 - L_i)].$$

Since $L_i(1 - L_i)$ has degree $2n - 2$ and zeros $x_1, \ldots, x_n$, there is some polynomial $r_i \in \pi_{n-2}$ such that

$$L_i(1 - L_i) = s r_i,$$

and since $\langle s, r_i \rangle = 0$,

$$I[L_i(1 - L_i)] = 0.$$

□

We also obtain the error in the Gauss rule from the Newton form of q.

Theorem 4 *If $f \in C^{2n}[a,b]$ then there is some $\xi \in (a,b)$ such that*

$$I[f] - I_n[f] = \frac{f^{(2n)}(\xi)}{(2n)!} I[s^2].$$

Proof. The Newton error formula for Hermite interpolation gives

$$f(x) - q(x) = s^2(x)[x_1, \ldots, x_n, x_1, \ldots, x_n, x]f,$$

and integrating this equation over $[a,b]$ gives

$$I[f] - I_n[f] = \int_a^b s^2(x)[x_1, \ldots, x_n, x_1, \ldots, x_n, x]f \, dx,$$

and since s^2 is a function of one sign in $[a,b]$ and

$$[x_1, \ldots, x_n, x_1, \ldots, x_n, x]f$$

is a continuous function of x, the mean value theorem for integrals implies there is some $\eta \in [a,b]$ such that

$$I[f] - I_n[f] = [x_1, \ldots, x_n, x_1, \ldots, x_n, \eta]f \int_a^b s^2(x) \, dx,$$

which gives the result. □

Example 1. I_1 is the midpoint rule, $I_1[f] = 2f(0)$.
Example 2. To derive I_2 recall that $\phi_2(x) = x^2 - 1/3$, and so $x_1 = -1/\sqrt{3}$ and $x_2 = 1/\sqrt{3}$. Then

$$L_1(x) = (1 - \sqrt{3}x)/2, \qquad L_2(x) = (1 + \sqrt{3}x)/2,$$

and $I[L_1] = I[L_2] = 1$, and so

$$I_2[f] = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right).$$