Numerical Analysis Hilary Term 2018
Lecture 13: Gaussian quadrature

Suppose that w is a weight function, defined, positive and integrable on the open interval (a, b) of $\mathbb{R}$.

Lemma. Let $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ be orthogonal polynomials for the inner product $\langle f, g\rangle = \int_a^b w(x)f(x)g(x)\,\mathrm{d}x$. Then, for each $k = 0, 1, \ldots,$ ϕ_k has k distinct roots in the interval (a, b).

Proof. Since $\phi_0(x) \equiv$ const. $\neq 0$, the result is trivially true for $k = 0$. Suppose that $k \geq 1$: $\langle \phi_k, \phi_0\rangle = \int_a^b w(x)\phi_k(x)\phi_0(x)\,\mathrm{d}x = 0$ with ϕ_0 constant implies that $\int_a^b w(x)\phi_k(x)\,\mathrm{d}x = 0$ with $w(x) > 0$, $x \in (a, b)$. Thus $\phi_k(x)$ must change sign in (a, b), i.e., ϕ_k has at least one root in (a, b).

Suppose that there are ℓ points $a < r_1 < r_2 < \cdots < r_\ell < b$ where ϕ_k changes sign for some $1 \leq \ell \leq k$. Then

$$q(x) = \prod_{j=1}^{\ell}(x - r_j) \times \text{ the sign of } \phi_k \text{ on } (r_\ell, b)$$

has the same sign as ϕ_k on (a, b). Hence

$$\langle \phi_k, q\rangle = \int_a^b w(x)\phi_k(x)q(x)\,\mathrm{d}x > 0,$$

and thus it follows from the previous lemma (cf. Lecture 12) that q, (which is of degree ℓ) must be of degree $\geq k$, i.e., $\ell \geq k$. However, ϕ_k is of exact degree k, and therefore the number of its distinct roots, ℓ, must be $\leq k$. Hence $\ell = k$, and ϕ_k has k distinct roots in (a, b). □

Quadrature revisited. The above lemma leads to very efficient quadrature rules since it answers the question: how should we choose the quadrature points $x_0, x_1, \ldots, x_n$ in the quadrature rule

$$\int_a^b w(x)f(x)\,\mathrm{d}x \approx \sum_{j=0}^{n} w_j f(x_j) \tag{1}$$

so that the rule is exact for polynomials of degree as high as possible? (The case $w(x) \equiv 1$ is the most common.)

Recall: the Lagrange interpolating polynomial

$$p_n = \sum_{j=0}^{n} f(x_j)L_{n,j} \in \Pi_n$$

is unique, so $f \in \Pi_n \implies p_n \equiv f$ whatever interpolation points are used, and moreover

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

exactly, where

$$w_j = \int_a^b w(x) L_{n,j}(x)\,\mathrm{d}x. \tag{2}$$

Theorem. Suppose that $x_0 < x_1 < \cdots < x_n$ are the roots of the $n+1$-st degree orthogonal polynomial ϕ_{n+1} with respect to the inner product

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

Then, the quadrature formula (1) with weights (2) is exact whenever $f \in \Pi_{2n+1}$.

Proof. Let $p \in \Pi_{2n+1}$. Then by the Division Algorithm $p(x) = q(x)\phi_{n+1}(x) + r(x)$ with $q, r \in \Pi_n$. So

$$\int_a^b w(x)p(x)\,\mathrm{d}x = \int_a^b w(x)q(x)\phi_{n+1}(x)\,\mathrm{d}x + \int_a^b w(x)r(x)\,\mathrm{d}x = \sum_{j=0}^{n} w_j r(x_j) \tag{3}$$

since the integral involving $q \in \Pi_n$ is zero by the lemma above and the other is integrated exactly since $r \in \Pi_n$. Finally $p(x_j) = q(x_j)\phi_{n+1}(x_j) + r(x_j) = r(x_j)$ for $j = 0, 1, \ldots, n$ as the x_j are the roots of ϕ_{n+1}. So (3) gives

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

where w_j is given by (2) whenever $p \in \Pi_{2n+1}$. □

These quadrature rules are called **Gaussian quadratures**.

- $w(x) \equiv 1$, $(a, b) = (-1, 1)$: Gauss–Legendre quadrature.
- $w(x) = (1 - x^2)^{-1/2}$ and $(a, b) = (-1, 1)$: Gauss–Chebyshev quadrature.
- $w(x) = \mathrm{e}^{-x}$ and $(a, b) = (0, \infty)$: Gauss–Laguerre quadrature.
- $w(x) = \mathrm{e}^{-x^2}$ and $(a, b) = (-\infty, \infty)$: Gauss–Hermite quadrature.

They give better accuracy than Newton–Cotes quadrature for the same number of function evaluations.

Note when using quadrature on unbounded intervals, the integral should be of the form $\int_0^\infty \mathrm{e}^{-x} f(x)\,\mathrm{d}x$ and only f is sampled at the nodes.

Note that by the linear change of variable $t = (2x - a - b)/(b - a)$, which maps $[a, b] \to [-1, 1]$, we can evaluate for example

$$\int_a^b f(x)\,\mathrm{d}x = \int_{-1}^{1} f\left(\frac{(b-a)t + b + a}{2}\right)\frac{b-a}{2}\,\mathrm{d}t \simeq \frac{b-a}{2}\sum_{j=0}^{n} w_j f\left(\frac{b-a}{2}t_j + \frac{b+a}{2}\right),$$

where $\simeq$ denotes "quadrature" and the t_j, $j = 0, 1, \ldots, n$, are the roots of the $n+1$-st degree Legendre polynomial.

Example. 2-point Gauss–Legendre quadrature: $\phi_2(t) = t^2 - \frac{1}{3} \implies t_0 = -\frac{1}{\sqrt{3}}$, $t_1 = \frac{1}{\sqrt{3}}$ and

$$w_0 = \int_{-1}^{1} \frac{t - \frac{1}{\sqrt{3}}}{-\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}} \,\mathrm{d}t = -\int_{-1}^{1} \left(\tfrac{\sqrt{3}}{2}t - \tfrac{1}{2}\right) \mathrm{d}t = 1,$$

with $w_1 = 1$, similarly. So e.g., changing variables $x = (t+3)/2$,

$$\int_1^2 \frac{1}{x} \,\mathrm{d}x = \frac{1}{2}\int_{-1}^{1} \frac{2}{t+3} \,\mathrm{d}t \simeq \frac{1}{3+\frac{1}{\sqrt{3}}} + \frac{1}{3-\frac{1}{\sqrt{3}}} = 0.6923077\ldots\ .$$

Note that the trapezium rule (also two evaluations of the integrand) gives

$$\int_1^2 \frac{1}{x} \,\mathrm{d}x \simeq \frac{1}{2}\left[\frac{1}{2} + 1\right] = 0.75,$$

whereas $\displaystyle\int_1^2 \frac{1}{x} \,\mathrm{d}x = \ln 2 = 0.6931472\ldots\ .$

Theorem. Error in Gaussian quadrature: suppose that $f^{(2n+2)}$ is continuous on (a,b). Then

$$\int_a^b w(x) f(x) \,\mathrm{d}x = \sum_{j=0}^{n} w_j f(x_j) + \frac{f^{(2n+2)}(\eta)}{(2n+2)!} \int_a^b w(x) \prod_{j=0}^{n} (x - x_j)^2 \,\mathrm{d}x,$$

for some $\eta \in (a,b)$.

Proof. The proof is based on the Hermite interpolating polynomial H_{2n+1} to f on $x_0, x_1, \ldots, x_n$. [Recall that $H_{2n+1}(x_j) = f(x_j)$ and $H'_{2n+1}(x_j) = f'(x_j)$ for $j = 0, 1, \ldots, n$.] The error in Hermite interpolation is

$$f(x) - H_{2n+1}(x) = \frac{1}{(2n+2)!} f^{(2n+2)}(\eta(x)) \prod_{j=0}^{n} (x - x_j)^2$$

for some $\eta = \eta(x) \in (a,b)$. Now $H_{2n+1} \in \Pi_{2n+1}$, so

$$\int_a^b w(x) H_{2n+1}(x) \,\mathrm{d}x = \sum_{j=0}^{n} w_j H_{2n+1}(x_j) = \sum_{j=0}^{n} w_j f(x_j),$$

the first identity because Gaussian quadrature is exact for polynomials of this degree and the second by interpolation. Thus

$$\begin{aligned}\int_a^b w(x) f(x) \,\mathrm{d}x - \sum_{j=0}^{n} w_j f(x_j) &= \int_a^b w(x)[f(x) - H_{2n+1}(x)] \,\mathrm{d}x \\ &= \frac{1}{(2n+2)!} \int_a^b f^{(2n+2)}(\eta(x)) w(x) \prod_{j=0}^{n} (x - x_j)^2 \,\mathrm{d}x,\end{aligned}$$

and hence the required result follows from the integral mean value theorem as $w(x)\prod_{j=0}^{n}(x-x_j)^2 \geq 0$. $\square$

Remark: the "direct" approach of finding Gaussian quadrature formulae sometimes works for small n, but more sophisticated algorithms are used for large n.[1]

Example. To find the two-point Gauss–Legendre rule $w_0 f(x_0) + w_1 f(x_1)$ on $(-1,1)$ with weight function $w(x) \equiv 1$, we need to be able to integrate any cubic polynomial exactly, so

$$2 = \int_{-1}^{1} 1\,\mathrm{d}x = w_0 + w_1 \tag{4}$$

$$0 = \int_{-1}^{1} x\,\mathrm{d}x = w_0 x_0 + w_1 x_1 \tag{5}$$

$$\tfrac{2}{3} = \int_{-1}^{1} x^2\,\mathrm{d}x = w_0 x_0^2 + w_1 x_1^2 \tag{6}$$

$$0 = \int_{-1}^{1} x^3\,\mathrm{d}x = w_0 x_0^3 + w_1 x_1^3. \tag{7}$$

These are four nonlinear equations in four unknowns w_0, w_1, x_0 and x_1. Equations (5) and (7) give

$$\begin{bmatrix} x_0 & x_1 \\ x_0^3 & x_1^3 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

which implies that

$$x_0 x_1^3 - x_1 x_0^3 = 0$$

for w_0, $w_1 \neq 0$, i.e.,

$$x_0 x_1 (x_1 - x_0)(x_1 + x_0) = 0.$$

If $x_0 = 0$, this implies $w_1 = 0$ or $x_1 = 0$ by (5), either of which contradicts (6). Thus $x_0 \neq 0$, and similarly $x_1 \neq 0$. If $x_1 = x_0$, (5) implies $w_1 = -w_0$, which contradicts (4). So $x_1 = -x_0$, and hence (5) implies $w_1 = w_0$. But then (4) implies that $w_0 = w_1 = 1$ and (6) gives

$$x_0 = -\tfrac{1}{\sqrt{3}} \qquad \text{and} \qquad x_1 = \tfrac{1}{\sqrt{3}},$$

which are the roots of the Legendre polynomial $x^2 - \frac{1}{3}$.

[1] See e.g., the research paper by Hale and Townsend, "Fast and accurate computation of Guass–Legendre and Gauss–Jacobi quadrature nodes and weights" SIAM J. Sci. Comput. 2013.

Table 1: Abscissas x_j (zeros of Legendre polynomials) and weight factors w_j for Gaussian quadrature: $\int_{-1}^{1} f(x)\,\mathrm{d}x \simeq \sum_{j=0}^{n} w_j f(x_j)$ for $n = 0$ to 6.

	x_j	w_j
$n=0$	0.000000000000000e+0	2.000000000000000e+0
$n=1$	5.773502691896258e−1	1.000000000000000e+0
	−5.773502691896258e−1	1.000000000000000e+0
	7.745966692414834e−1	5.555555555555556e−1
$n=2$	0.000000000000000e+0	8.888888888888889e−1
	−7.745966692414834e−1	5.555555555555556e−1
	8.611363115940526e−1	3.478548451374539e−1
$n=3$	3.399810435848563e−1	6.521451548625461e−1
	−3.399810435848563e−1	6.521451548625461e−1
	−8.611363115940526e−1	3.478548451374539e−1
	9.061798459386640e−1	2.369268850561891e−1
	5.384693101056831e−1	4.786286704993665e−1
$n=4$	0.000000000000000e+0	5.688888888888889e−1
	−5.384693101056831e−1	4.786286704993665e−1
	−9.061798459386640e−1	2.369268850561891e−1
	9.324695142031520e−1	1.713244923791703e−1
	6.612093864662645e−1	3.607615730481386e−1
$n=5$	2.386191860831969e−1	4.679139345726910e−1
	−2.386191860831969e−1	4.679139345726910e−1
	−6.612093864662645e−1	3.607615730481386e−1
	−9.324695142031520e−1	1.713244923791703e−1
	9.491079123427585e−1	1.294849661688697e−1
	7.415311855993944e−1	2.797053914892767e−1
	4.058451513773972e−1	3.818300505051189e−1
$n=6$	0.000000000000000e+0	4.179591836734694e−1
	−4.058451513773972e−1	3.818300505051189e−1
	−7.415311855993944e−1	2.797053914892767e−1
	−9.491079123427585e−1	1.294849661688697e−1