Numerical Analysis Hilary Term 2023
Lecture 11: Gauss quadrature

Terminology: Quadrature $\equiv$ numerical integration

Goal: given a (continuous) function $f : [a, b] \to \mathbb{R}$, find its integral $I = \int_a^b f(x)dx$, as accurately as possible.

Idea: Approximate and Integrate. Find a polynomial p_n from data $\{(x_k, f(x_k))\}_{k=0}^n$ by Lagrange interpolation (lecture 1), and integrate $\int_{x_0}^{x_n} p_n(x)\,\mathrm{d}x =: I_n$. Ideally, $I_n = I$ or at least $I_n \approx I$. Is this true?

If we choose x_k to be equispaced points in $[a, b]$, the resulting I_n is known as the Newton-Cotes quadrature. This method is actually quite unstable and inaccurate, and a much more accurate and elegant quadrature rule exists: Gauss quadrature. In this lecture we cover this beautiful result involving orthogonal polynomials.

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

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

Proof. Since $\phi_0(x) \equiv \text{const.} \neq 0$, the result is trivially true for $k = 0$. Suppose that $k \geq 1$: $\langle \phi_k, \phi_0\rangle = \displaystyle\int_a^b w(x)\phi_k(x)\phi_0(x)\,\mathrm{d}x = 0$ with ϕ_0 constant implies that $\displaystyle\int_a^b w(x)\phi_k(x)\,\mathrm{d}x = 0$ 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). $\square$

Application to quadrature. The above lemma leads to very efficient quadrature rules since it answers the question: how should we choose the quadrature points $x_0, x_1, \dots, x_n$ 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 $p \in \Pi_{2n+1}$. $\square$

These quadrature rules are called **Gauss 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 Gauss 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 Gauss quadrature is exact for polynomials of this degree and the second by interpolation. Thus

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

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

Remark: the "direct" approach of finding Gauss 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

$$2 = \int_{-1}^1 1\,\mathrm{d}x = w_0 + w_1 \tag{4}$$
$$0 = \int_{-1}^1 x\,\mathrm{d}x = w_0x_0 + w_1x_1 \tag{5}$$
$$\tfrac{2}{3} = \int_{-1}^1 x^2\,\mathrm{d}x = w_0x_0^2 + w_1x_1^2 \tag{6}$$
$$0 = \int_{-1}^1 x^3\,\mathrm{d}x = w_0x_0^3 + w_1x_1^3. \tag{7}$$

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

$$x_0x_1^3 - x_1x_0^3 = 0$$

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

$$x_0x_1(x_1 - x_0)(x_1 + x_0) = 0.$$

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

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

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

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

Convergence: Gauss quadrature converges astonishingly fast. It can be shown that if f is analytic on $[a, b]$, the convergence is geometric (exponential) in the number of samples. This is in contrast to other (more straightforward) quadrature rules:

- Newton-Cotes: Find interpolant in n equispaced points, and integrate interpolant. Convergence: (often) Divergent!
- (Composite) trapezium rule: Find piecewise-linear interpolant in n equispaced points, and integrate interpolant. Convergence: $O(1/n^2)$ (assumes f'' exists)
- (Composite) Simpson's rule: Find piecewise-quadratic interpolant in n equispaced points (each subinterval containing three points), and integrate interpolant. Convergence: $O(1/n^4)$ (assumes f'''' exists)

The figure below illustrates the performance on integrating the Runge function.

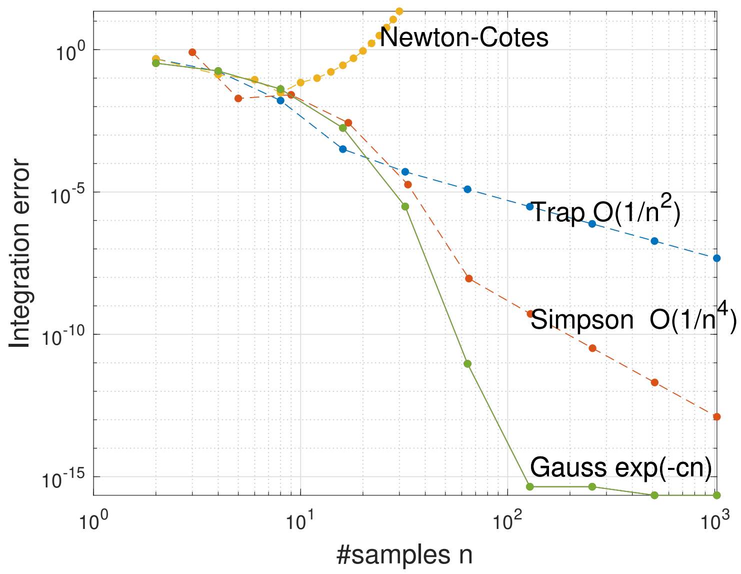
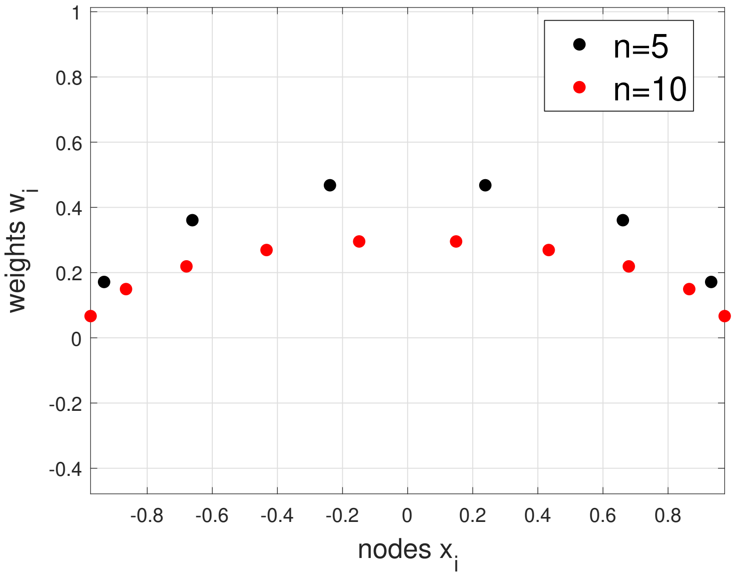


Figure 1: Convergence of quadrature rules for $\int_{-1}^{1} \frac{1}{25x^2+1} dx$ (Runge function)

Nodes and weights for Gauss(-Legendre) quadrature The figure below shows the nodes (interpolation points) and the corrsponding weights with the standard Gauss-Legendre quadrature rule, i.e., when $w(x) = 1$ and $[a, b] = [-1, 1]$. In Chebfun these are computed conveniently by `[x,w] = legpts(n+1)`



Note that the nodes/interpolation points cluster near endpoints (and sparser in the middle); this is a general phenomenon, and very analogous to the Chebyshev interpolation points mentioned in the least-squares lecture (Gauss and Chebyshev points have asymptotically the same distribution of points). Note also that the weights are all positive and shrink as n grows; they have to because they sum to 2 (why?).