MA5233 Computational Mathematics

Lecture 15: Quadrature

Simon Etter

National University of Singapore

2019/2020

Quadrature

Def: Quadrature

Computing an approximation $Q \approx \int_a^b f\, dx$ given a finite number of point-values $f(x_k)$.

Def: Quadrature rule (quadrule)

Formula for computing Q as a linear function of the point values $f(x_k)$,

$$Q := \sum_{k=1}^{n} w_k\, f(x_k)$$

- x_k are called *quadrature points/nodes*.
- w_k are called *quadrature weights*.

Quadrature

Discussion

Given n, we of course want to choose x_k, w_k such that the error

$$E(f,n) := \left| \int_a^b f(x)\,dx - \sum_{k=1}^{n} w_k\, f(x_k) \right|$$

becomes as small as possible.

However, this is not a reasonable question:

- For any f, there exists an exact $n = 1$ quadrule, namely

$$w_1 = \tfrac{1}{f(x_1)} \int_a^b f(x)\,dx.$$

- For any quadrule, there exists a sequence f_k such that

$$\lim_{k\to\infty} E(f_k, n) = \infty.$$

Alternative: choose a finite-dimensional space of functions V and demand that quadrule is exact for all $f \in V$.

In practice, we almost always choose $V = \mathcal{P}_d$ for some d.

Quadrature

Def: Polynomial degree of exactness

A quadrule $(x_k, w_k)_{k=1}^n$ is said to be exact on $\mathcal{P}_d$ if for all $p \in \mathcal{P}_d$ it holds

$$\sum_{k=1}^n w_k\, p(x_k) = \int_a^b p(x)\, dx.$$

Thm: Quadrules exact on $\mathcal{P}_{n-1}$

Given distinct points $(x_k)_{k=1}^n$, there exist weights $(w_k)_{k=1}^n$ such that the resulting quadrature rule is exact on $\mathcal{P}_{n-1}$.

Proof. Recall Lagrange polynomials $\ell_k(x) = \prod_{j \neq k} \frac{x - x_j}{x_k - x_j}$ from lecture on polynomial approximation. We observe that

$$\int_a^b p(x)\, dx = \int_a^b \sum_{k=1}^n \ell_k(x)\, p(x_k)\, dx = \sum_{k=1}^n w_k\, p(x_k)$$

if we set

$$w_k := \int_a^b \ell_k(x)\, dx.$$

Quadrature

Thm: Quadrature error estimate

Assume the quadrature rule $(x_k, w_k)_{k=1}^n$ is exact on $\mathcal{P}_{n-1}$.
Denote by $p \in \mathcal{P}_{n-1}$ the polynomial interpolant to f on x_k. Then,

$$\left| \int_a^b f(x)\,dx - \sum_{k=1}^n w_k\, f(x_k) \right| \leq (b-a)\, \|f-p\|_{[a,b]}.$$

Proof.

$$\begin{aligned}\left| \int_a^b f(x)\,dx - \sum_{k=1}^n w_k\, f(x_k) \right| &= \left| \int_a^b f(x)\,dx - \int_a^b p(x)\,dx \right| \\ &\leq \int_a^b \left| f(x) - p(x) \right| dx \leq \|f-p\|_{[a,b]} \int_a^b 1\,dx.\end{aligned}$$

Corollary

Convergence theory for quadrature follows immediately from theory for polynomial interpolation.

Quadrature

Special quadrature rules

- Newton-Cotes rules: choose x_k as equispaced points.
- Clenshaw-Curtis rules: choose x_k as Chebyshev points.

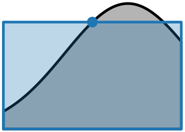
Recall from lecture on polynomial approximation that interpolation in equispaced points is ill-conditioned and may diverge for $n \to \infty$.

Hence Newton-Cotes rules are bad for large n, but they are fine for $n \lesssim 5$.

Special Newton-Cotes rules ($m := \frac{a+b}{2}$)

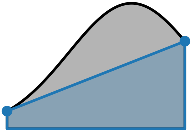
Midpoint

$\frac{b-a}{2}\, f(m)$



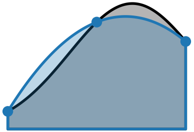
Trapezoidal

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



Simpson

$\frac{b-a}{6}\, \big(f(a) + 4\, f(m) + f(b)\big)$



Quadrature

Discussion

We have seen that for every set of distinct points $(x_k)_{k=1}^n$, there exist weights $(w_k)_{k=1}^n$ such that the resulting quadrature rule is exact on $\mathcal{P}_{n-1}$.

Question: can we increase degree of exactness by choosing x_k cleverly?

The answer is yes, but seeing how requires some preparation.

Inner product for functions

The function

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

is an inner product on the space of all functions $f, g : [a, b] \to \mathbb{R}$ for which the integral exists.

Proof. Check that $\langle f, g\rangle$ satisfies all the properties of an inner product.

Quadrature

Legendre polynomials

Sequence of polynomials $(L_k \in \mathcal{P}_k)_{k=0}^{\infty}$ such that $L_k(1) = 1$ and

$$k' \neq k \iff \langle L_{k'}, L_k \rangle = \int_{-1}^{1} L_{k'}(x)\, L_k(x)\, dx = 0.$$

Determining the Legendre polynomials

Main challenge is to establish orthogonality: once $\tilde{L}_k(x)$ such that $\langle \tilde{L}_{k'}, \tilde{L}_k \rangle = 0$ have been determined, the correct scaling can be achieved by setting $L_k(x) := \tilde{L}_k(x)/\tilde{L}_k(1)$.

Bad way of determining $\tilde{L}_k(x)$

Apply Gram-Schmidt to the sequence $1, x, x^2, x^3, \ldots$, i.e.

$$\tilde{L}_0(x) = 1, \quad \tilde{L}_1(x) = x - \tfrac{\langle 1,x \rangle}{\langle 1,1 \rangle}\, 1, \quad \tilde{L}_2(x) = x^2 - \tfrac{\langle 1,x^2 \rangle}{\langle 1,1 \rangle}\, 1 - \tfrac{\langle x,x^2 \rangle}{\langle x,x \rangle}\, x, \quad \ldots$$

This is numerically unstable and unnecessarily costly.
See next slide for better algorithm.

Quadrature

Good way of determining $\tilde{L}_k(x)$

Use Arnoldi with "matrix" $(Af)(x) := x\, f(x)$ and "vector" $b(x) = 1$, i.e.

$$\tilde{L}_0(x) = 1, \quad \tilde{L}_1(x) = x\,\tilde{L}_0(x) - \tfrac{\langle \tilde{L}_0, x\tilde{L}_0(x)\rangle}{\langle \tilde{L}_0, \tilde{L}_0\rangle}\,\tilde{L}_0(x),$$
$$\tilde{L}_2(x) = x\,\tilde{L}_1(x) - \tfrac{\langle \tilde{L}_0, x\tilde{L}_1(x)\rangle}{\langle \tilde{L}_0, \tilde{L}_0\rangle}\,\tilde{L}_0(x) - \tfrac{\langle \tilde{L}_1, x\tilde{L}_1(x)\rangle}{\langle \tilde{L}_1, \tilde{L}_1\rangle}\,\tilde{L}_1(x), \quad \dots$$

This approach is numerically stable. Furthermore, Arnoldi simplifies to Lanczos iteration since the "matrix" A is symmetric with respect to the inner product $\langle f, g\rangle$,

$$\langle f, Ag\rangle = \int_{-1}^{1} f(x)\,\big(x\,g(x)\big)\,dx = \int_{-1}^{1} \big(x\,f(x)\big)\,g(x)\,dx = \langle Af, g\rangle$$

Lanczos iter. can be adapted to directly produce $L_k(x)$ rather than $\tilde{L}_k(x)$. This leads to the three-term recurrence relation

$$L_0(x) = 1, \quad L_1(x) = x,$$
$$(k+1)\,L_{k+1}(x) = (2k+1)\,x\,L_k(x) - k\,L_{k-1}(x).$$

Quadrature

Thm: Gauss quadrature

A quadrature rule $(x_k, w_k)_{k=1}^n$ exact on $\mathcal{P}_{2n-1}$ is obtained if we choose

- x_k as the roots of the Legendre polynomial $L_n(x)$, and
- w_k such that (x_k, w_k) is exact on $\mathcal{P}_{n-1}$.

Proof. Consider $p \in \mathcal{P}_{2n-1}$. By polynomial division with remainder, there exist $p_1, p_2 \in \mathcal{P}_{n-1}$ such that $p(x) = p_1(x)\, L_n(x) + p_2(x)$.

Using orthogonality of $L_n(x)$ and choice of x_k for the first integral and exactness on $\mathcal{P}_{n-1}$ for second integral, we obtain

$$\begin{aligned}
\int_{-1}^{1} p(x)\, dx &= \int_{-1}^{1} p_1(x)\, L_n(x)\, dx + \int_{-1}^{1} p_2(x)\, dx \\
&= \qquad\qquad 0 \qquad\qquad + \sum_{k=1}^{n} w_k\, p_2(x_k) \\
&= \sum_{k=1}^{n} w_k\, p_1(x_k)\, L_n(x) + \sum_{k=1}^{n} w_k\, p_2(x_k) = \sum_{k=1}^{n} w_k\, p(x_k).
\end{aligned}$$

Quadrature

Remarks on Gauss quadrature

One can show:

- $L_n(x)$ has n distinct roots in $[-1, 1]$. (Gauss quadrature is well defined.)
- Gauss quadrature rules are unique.

Thm: Gauss quadrature error estimate

Let $(x_k, w_k)_{k=1}^n$ be a Gauss quadrule.

Denote by $p \in \mathcal{P}_{2n-1}$ the polynomial interpolant to f on x_k plus $n-1$ arbitrary additional interpolation points. Then,

$$\left| \int_a^b f(x)\,dx - \sum_{k=1}^n w_k\, f(x_k) \right| \leq (b-a)\, \|f - p\|_{[a,b]}.$$

Proof. Analogous to previous result.

Discussion

One can show that the interpolation error described above behaves similarly as the error for interpolation in $2n-1$ Chebyshev points.

Conclusion: Gauss converges twice as fast as Clenshaw-Curtis.

At least in theory. In practice, CC often performs better than theoretical upper bound.

Quadrature

Thm: Optimality of Gauss quadrature

No quadrature rule $(x_k, w_k)_{k=1}^n$ is exact on $\mathcal{P}_{2n}$.

Proof. By contradiction. Assume $(x_k, w_k)_{k=1}^n$ is exact on $\mathcal{P}_{2n}$, and consider $p(x) := \prod_{k=1}^n (x - x_k)^2 \in \mathcal{P}_{2n}$. Then,

$$\int_a^b p(x)\,dx > 0 \text{ since } p(x) \geq 0, \qquad \text{but} \qquad \sum_{k=1}^n w_k\, p(x_k) = 0.$$

Remark

Heuristic for degree of exactness of Gauss quadrules:
$(x_k, w_k)_{k=1}^n$ introduces $2n$ "unknowns", $\mathcal{P}_{2n-1}$ is $2n$ dimensional.

Gauss quadrature in practice

Quite a bit of code is required for computing the Gauss quadrature points, i.e. the roots of the Legendre polynomials.

Advice: use package to compute Gauss quadrules whenever possible.

In Julia, use `FastGaussQuadrature.jl`.

Quadrature

Mapping of integrals

Recall integration by substitution:

$$\int_a^b f(x)\,dx = \int_{\varphi^{-1}(a)}^{\varphi^{-1}(b)} f\big(\varphi(\hat{x})\big)\,\varphi'(\hat{x})\,d\hat{x}.$$

In the context of quadrature, this formula has (at least) two applications:

- Assume we have a quadrule $(\hat{x}_k, \hat{w}_k)_{k=1}^n$ for integration on $[0, 1]$. We can then approximate integrals on arbitrary intervals $[a, b]$ using

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_0^1 f\big(a + (b-a)\,\hat{x}\big)\,(b-a)\,d\hat{x} \\ &\approx \sum_{k=1}^n (b-a)\,\hat{w}_k\,f\big(a + (b-a)\,\hat{x}_k\big).\end{aligned}$$

Quadrature

Mapping of integrals

Recall integration by substitution:

$$\int_a^b f(x)\,dx = \int_{\varphi^{-1}(a)}^{\varphi^{-1}(b)} f\big(\varphi(\hat{x})\big)\,\varphi'(\hat{x})\,d\hat{x}.$$

In the context of quadrature, this formula has (at least) two applications:

- Consider the substitution $x = \sin(\theta)$ applied to

$$\int_{-1}^{1} \sqrt{1-x^2}\,dx = \int_{-\pi/2}^{\pi/2} \sqrt{1-\sin(\theta)^2}\,\cos(x)\,d\theta = \int_{-\pi/2}^{\pi/2} \cos(\theta)^2\,d\theta.$$

  Derivative of original integrand blows up at $x = 1$, which leads to algebraic convergence of quadrature. Integrand on the right is analytic everywhere, hence quadrature converges superexponentially.

Quadrature

Def: Composite quadrature rules

Consider interval $[a, b]$ with partition $a = y_0 < y_2 < \ldots < y_m = b$.

Composite quadrules compute $\int_a^b f(x)\,dx$ by writing

$$\int_a^b f(x)\,dx) = \sum_{\ell=1}^{m} \int_{y_{\ell-1}}^{y_\ell} f(x)\,dx$$

and applying a *nested* quadrule to each of the terms on the right.

Examples

- Composite midpoint rule:

$$\int_a^b f(x)\,dx \approx \sum_{\ell=1}^{m} (y_\ell - y_{\ell-1})\, f\left(\tfrac{y_{\ell-1}+y_\ell}{2}\right).$$

- Composite trapezoidal rule:

$$\int_a^b f(x)\,dx \approx \sum_{\ell=1}^{m} \tfrac{y_\ell - y_{\ell-1}}{2} \left(f(y_{\ell-1}) + f(y_\ell)\right).$$

Quadrature

Reasons for considering composite quadrules

- Function is defined piecewise (cf. finite element method).
- Quadrules for large n are tedious to construct.
- Adaptive quadrature: refine partition in regions where integrand lacks smoothness.

Error estimate for composite quadrules

Assume

- equispaced partition $y_\ell := a\,(1 - \frac{\ell}{m}) + b\,\frac{\ell}{m}$ with $\ell \in \{0, \dots, m\}$,
- local quadrule is exact on $\mathcal{P}_d$, and
- $f : [a, b] \to \mathbb{R}$ has $d + 1$ continuous derivatives.

Then, the composite quadrature error e_m satisfies

$$e_m = \mathcal{O}\big(m^{-d-1}\big) \qquad \text{for } m \to \infty.$$

Proof on next slide.

Quadrature

Proof. We have seen that local quadrule exact on $\mathcal{P}_d$ implies that the local quadrature error is bounded by

$$\left| \int_{y_{\ell-1}}^{y_\ell} f(x)\, dx - Q_\ell \right| \leq (y_\ell - y_{\ell-1})\, \|f - p\|_{[y_{\ell-1}, y_\ell]}$$

where p is the interpolant to f in $d+1$ distinct points $x_k \in [y_{\ell-1}, y_\ell]$. Recall from previous lecture the interpolation error estimate

$$f(x) - p(x) = \frac{f^{(d+1)}(\xi)}{(d+1)!} \prod_{k=0}^{d} (x - x_k).$$

Since $x, x_k \in [y_{\ell-1}, y_\ell]$, we have $|x - x_k| \leq y_\ell - y_{\ell-1}$ and hence

$$\left| \int_{y_{\ell-1}}^{y_\ell} f(x)\, dx - Q_\ell \right| \leq C\, (y_\ell - y_{\ell-1})^{(d+2)} = \mathcal{O}\big(m^{-d-2}\big).$$

Global error estimate follows by summing local error estimate over m intervals.

Quadrature

Error estimates for special quadrature rules

- Midpoint ($n = 1$): $e_m = \mathcal{O}\left(m^{-2}\right)$.
- Trapezoidal ($n = 2$): $e_m = \mathcal{O}\left(m^{-2}\right)$.
- Simpson ($n = 3$): $e_m = \mathcal{O}\left(m^{-4}\right)$.

Note that midpoint and Simpson rules (and in general any Newton-Cotes rule with odd n) achieve $e_m = \mathcal{O}\left(m^{-n-1}\right)$ rather than $e_m = \mathcal{O}\left(m^{-n}\right)$ because they are exact on $\mathcal{P}_n$ rather than $\mathcal{P}_{n-1}$.

References and further reading

- E. Suli and D. F. Mayers. *An Introduction to Numerical Analysis.* Cambridge University Press (2003), `doi:10.1017/CBO9780511801181`
  Can be accessed online for free via the library website!