Lecture 5. Quadrature Nick Trefethen, 4 Oct. 2017

1. Quadrature formulas

[Ref: chap. 19 of *ATAP*]

$I_n = \sum_{k=1}^{n} w_k f(x_k)$. Given *nodes* x_k, the *weights* w_k are chosen to integrate certain interpolants exactly.

Nonperiodic f: the interpolant is usually a polynomial.
Equispaced points: *Newton-Cotes* (1714). Diverges in general as $n \to \infty$ (Runge phenomenon, Pólya 1933).
Legendre points: *Gauss* (1814). Chebyshev points: *Clenshaw-Curtis* (1960). Both converge as $n \to \infty$ for all continuous f.

Periodic f: the obvious choice is equispaced points and a trigonometric interpolant ($I_n \approx$ zeroth Fourier series coefficient). This is equivalent to the (much more elementary) *trapezoidal rule*.

It follows from approximation theory and the positivity of the weights (except for N-C) that if f has a few derivatives, all these formulas (except N-C) converge at a corresponding algebraic rate as $n \to \infty$, and if f is analytic, they converge geometrically. [Periodic trapezoidal rule: T & Weideman, *SIAM Review*, 2014]

If the nodes are perturbed but not too far, the convergence properties persist. [Austin & T, *SINUM* 2017]

Periodic integrals with analytic integrands arise all the time in $\mathbb{C}$: Cauchy integrals over smooth contours.

2. Computing Gauss nodes and weights

Golub & Welsch (1969) formulated an elegant eigenvalue problem. Work $O(n^2)$ in principle, $O(n^3)$ in easy Matlab.

More recently an unexpected speedup to $O(n)$ with a very small constant: Glaser-Liu-Rokhlin 2007, Bogaert-Michiels-Fostier 2012, Hale-Townsend 2013, Bogaert 2014. Key idea: an inexact asymptotic formula for $n \to \infty$ may give 16 digits of accuracy when n is not too small. In Chebfun: **`[s,w] = legpts(n)`**.

3. Quadrature formula = rational approximation to log((z+1)/(z−1))

[Gauss 1814, Takahasi-Mori 1971, T-Weideman-Schmelzer 2003]

$I_n = \sum_{k=1}^{n} w_k f(x_k)$ is given by a contour integral: $I_n = \frac{1}{2\pi i}\oint f(z)\, r(z) dz,\ r(z) = \sum_{k=1}^{n} \frac{w_k}{z-x_k}$.

Note that the poles and residues of r are the nodes and weights of the quadrature formula.

$I = \int_{-1}^{1} f(x)dx$ is also given by a contour integral: $I = \frac{1}{2\pi i}\oint f(z)\, \varphi(z) dz,\ \varphi(z) = \log\frac{z+1}{z-1}$.

Proof: $f(x) = \frac{1}{2\pi i}\oint \frac{f(z)dz}{z-x},\ \int_{-1}^{1}\frac{dx}{z-x} = \log\frac{z+1}{z-1}$.

Subtracting shows that if $r \approx \varphi$ in a region of the z-plane where f is analytic, then $I_n \approx I$.

4. Contour integrals for matrix problems $f(A)$ and eigs(A)

For a scalar function $f(a)$, the Cauchy integral formula is $f(a) = \frac{1}{2\pi i}\oint (z-a)^{-1} f(z) dz$.

For a matrix function $f(A)$, we analogously have $f(A) = \frac{1}{2\pi i}\oint (zI-A)^{-1} f(z) dz$. If this is discretized by the periodic trapezoidal rule in, say, 16 points, then evaluating $f(A)$ is reduced to 16 linear solves.
[T-Weideman-Schmelzer 2006, Hale-Higham-T 2008]

Other contour integrals find poles of $(zI-A)^{-1}$, i.e., eigenvalues of A.
[Sakurai-Sugiura 2003, Polizzi 2008 "FEAST", Austin-Kravanja-T 2015]

5. Three ways in which polynomial degrees suggest misleading conclusions for quadrature

(a) Nonzero polynomial coefficients may be negligible → *Clenshaw-Curtis is as accurate as Gauss for nonanalytic f.*
[T, *SIREV* 2008]

(b) Polynomial approximability is a skewed measure of accuracy → *Gauss quadrature is not optimal*.
[Hale and T, *SINUM* 2008]

(c) Polynomials of a given total degree underresolve along diagonals of the hypercube
→ *"Euclidean degree" should be used instead*. [T, *SIREV* 2017]

These three affect work estimates by factors of *(a)* 2, *(b)* $\pi/2$, *(c)* $\approx d^{d/2}$ (d = dimension). [T, "Six myths…"]