CS 450: Numerical Anlaysis

Lecture 21
Chapter 7 Numerical Integration and Differentiation
Basic Numerical Quadrature Methods

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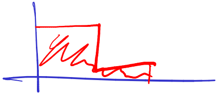
Integrability and Sensitivity

- Function f is integrable if continuous and bounded, in practice a finite number of discontinuities is also ok:



$$I(f) = \int_a^b f(x)\,dx, \quad \|f\|_\infty = \max_{x\in[a,b]} |f(x)|$$

- The condition number of integration is bounded by the distance $b-a$:

$$\hat{f} = f + \delta f, \quad \|\hat{f} - f\|_\infty \leq \|\delta f\|_\infty$$

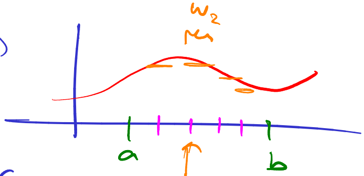
$$|I(\hat{f}) - I(f)| = |I(\hat{f} - f)| = |I(\delta f)|$$

$$\leq (b-a)\|\delta f\|_\infty$$

Quadrature Rules

- To approximate the integral $I(f)$, compute a weighted sum of points:

$$I(f) \approx \underset{\text{n-points}}{Q_n}(f) = \sum_{i=1}^{n} w_i f(x_i)$$



w_i - quadrature weights

x_i - ... nodes

so if Q_n uses x_2 a subset of nodes of Q_{n+1}, rule is progressive

- For a fixed set of n nodes, unique quadrature weights give exact $(n-1)$*-degree quadrature rule*:

polynomial interpolant of degree n-1 is unique, and so its integral is unique.

If $y_i = f(x_i)$, $p_{n-1}(x) = \sum_{i=1}^{n} y_i \ell_i(x)$, so $Q_n(f) = \sum_{i=1}^{n} y_i \int_a^b \ell_i(x)\,dx$

ℓ_i: ith Lagrange basis function

Quadrature Rules and Error

- Quadrature weights can be alternatively determined for a rule by solving the moment equations:

$$\begin{bmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_n) \\ \vdots & & \\ \varphi_n(x_1) & \cdots & \varphi_n(x_n) \end{bmatrix} \begin{bmatrix} \\ w \\ \\ \end{bmatrix} = \begin{bmatrix} I(\varphi_1) \\ \vdots \\ I(\varphi_n) \end{bmatrix}$$

- We can approximate the error bound for a polynomial quadrature rule by

$$|I(f) - Q_n(f)| = |I(f - p_{n-1})|$$

$$= |I(\alpha_1 x^n + \alpha_2 x^{n+1} \ldots)|$$

$$= \frac{(b-a)}{4n!} \|f^{(n)}\|_\infty \cdot h^n, \quad h = \max_i (x_{i+1} - x_i)$$

Newton-Cotes Quadrature

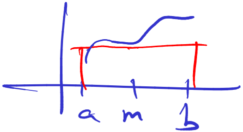
- *Newton-Cotes* quadrature rules are defined by equispaced nodes on $[a, b]$:

closed if including a, b: $x_i = a + \frac{(i-1)(b-a)}{n-1}$

open otherwise $\quad x_i = a + \frac{i(b-a)}{n+1}$

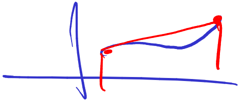
- The *midpoint rule* is the $n = 1$ open Newton-Cotes rule:

$x_1 = a + \frac{(b-a)}{2} = a/2 + b/2$, $\quad f((a+b)/2)$



- The *trapezoid rule* is the $n = 2$ closed Newton-Cotes rule:

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



- *Simpson's rule* is the $n = 3$ closed Newton-Cotes rule:

quadratic interpolant

Error in Newton-Cotes Quadrature

- Consider the Taylor expansion of f about the midpoint of the integration interval $m = (a+b)/2$:

$$f(x) = f(m) + f'(m)(x-m) + \frac{f''(m)}{2}(x-m)^2 + \dots$$

$$I(f) = \underbrace{(b-a)f(m)}_{M(f)} + 0 + \underbrace{\frac{f''(m)}{24}(b-a)^3}_{E(f)} + \dots$$

Error of Midpoint rule

is $E(f) + O((b-a)^5)$

Trapezoid rule has nearly same bound

$$M(f) - T(f) = \underline{3E(f)} + O((b-a)^5)$$

Conditioning of Newton-Cotes Quadrature

- We can ascertain stability of quadrature rules, by considering the amplification of a perturbation $\hat{f} = f + \delta f$:

$$|Q_n(\hat{f}) - Q_n(f)| = |Q_n(\delta f)|$$
$$= \left|\sum_{i=1}^{n} w_i \, \delta f(x_i)\right|$$
$$\leq \|w\|_1 \|\delta f\|_\infty$$

$$\boxed{\sum_{i=1}^{n} w_i = 1}$$

- Newton-Cotes quadrature rules have at least one negative weight for any $n \geq 11$:

as $n \to \infty$

$\|w\|_1 \to \infty$ despite $\sum_{i=1}^{n} w_i = 1$

Clenshaw-Curtis Quadrature

- To obtain a more stable quadrature rule, we need to ensure the integrated interpolant is well-behaved as n increases:

Chebyshev nodes for quadrature
rules defined e.g. by integrate Lagrange

good stability
also efficient by use of cos-transform