CS 450: Numerical Anlaysis

Lecture 21

Chapter 7 Numerical Integration and Differentiation

Basic Numerical Quadrature Methods

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April 6, 2018

Integrability and Sensitivity

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

  Seek to compute $I(f) = \int_a^b f(x)dx$*, define* $||f||_\infty = \max_{x\in[a,b]} |f(x)|$

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

  Suppose the input function is perturbed $\hat{f} = f + \delta f$*, then*

$$\begin{aligned} \delta I &= |I(\hat{f}) - I(f)| \\ &\leq |I(\delta f)| \\ &\leq (b-a)||\delta f||_\infty \end{aligned}$$

  Note that this result does not depend on the magnitude of f *or its derivatives, which means integration is generally very well-conditioned, which makes sense since integration corresponds to averaging.*

Quadrature Rules

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

$$Q_n(f) = \sum_{i=1}^{n} w_i f(x_i)$$

  - $\{x_i\}_{i=1}^n$ *are quadrature nodes or abscissas*, $\{w_i\}_{i=1}^n$ *are quadrature weights.*
  - *Quadrature rule is closed if* $x_1 = a, x_n = b$ *and open otherwise.*
  - *Rule is progressive if nodes of* Q_n *are a subset of those of* Q_{n+1}.
- For a fixed set of n nodes, unique quadrature weights give exact $(n-1)$*-degree quadrature rule*:

  The rule is exact for all $(n-1)$*-degree polynomials. Express the unique* $(n-1)$*-degree polynomial interpolant in the Lagrange basis* $p(x) = \sum_{i=1}^n \phi_i(x) f(x_i)$. *The quadrature rule is defined by*

$$Q_n(f) = I(p(x)) = \sum_{i=1}^{n} \underbrace{I(\phi_i)}_{w_i} f(x_i).$$

Quadrature Rules and Error

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

$$\boldsymbol{V}(\boldsymbol{x}, \{\phi_i\}_{i=1}^n)\boldsymbol{w} = \boldsymbol{y}(\{\phi_i\}_{i=1}^n), \quad \textit{where} \quad y_i = I(\phi_i)$$

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

$$\begin{aligned} |I(f) - Q_n(f)| &= |I(f - p_{n-1}(x))| \\ &\leq (b-a)||f - p_{n-1}||_\infty \\ &\leq \frac{b-a}{4n} h^n ||f^{(n)}||_\infty \end{aligned}$$

where $h = \max_i(x_{i+1} - x_i)$

Newton-Cotes Quadrature

- *Newton-Cotes* quadrature rules are defined by equispaced nodes on $[a, b]$: *open:* $x_i = a + i(b-a)/(n+1)$, *closed:* $x_i = a + (i-1)(b-a)/(n-1)$.
- The *midpoint rule* is the $n = 1$ open Newton-Cotes rule:

$$M(f) = (b-a)f\left(\frac{a+b}{2}\right)$$

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

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

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

$$S(f) = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$

Error in Newton-Cotes Quadrature

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

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

Integrating the Taylor approximation of f, we note that the odd terms drop,

$$I(f) = \underbrace{f(m)(b-a)}_{M(f)} + \underbrace{\frac{f''(m)}{24}(b-a)^3}_{E(f)} + O((b-a)^5)$$

  - *The midpoint rule is third-order accurate (first degree).*
  - *The trapezoid rule is also first degree, despite using higher-degree polynomial interpolant approximation.*
  - *Error can be conveniently approximated by difference of two rules,*

$$T(f) - M(f) \approx 3E(f).$$

Conditioning of Newton-Cotes Quadrature

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

$$\begin{aligned} |Q_n(\hat{f}) - Q_n(f)| &= |Q_n(\delta f)| \\ &= \sum_{i=1}^{n} w_i \delta f(x_i) \\ &\leq ||\boldsymbol{w}||_1 ||\delta f||_\infty. \end{aligned}$$

  Note that we always have $\sum_i w_i = b - a$, since the quadrature rule must be correct for a constant function. So if $\boldsymbol{w}$ is positive $||\boldsymbol{w}||_1 = b - a$, the quadrature rule is stable, i.e. it matches the conditioning of the problem.

- Newton-Cotes quadrature rules have at least one negative weight for any $n \geq 11$: *More generally, $||\boldsymbol{w}||_1 \to \infty$ as $n \to \infty$ for fixed $b - a$. This means that the Newton-Cotes rules can be ill-conditioned.*

Clenshaw-Curtis Quadrature

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

  Chebyshev quadrature nodes ensure that interpolant polynomial has bounded coefficients so long as f is bounded, since the Vandermonde system defining its coefficients is well-conditioned. Formally, it can be shown that $w_i > 0$ for Chebyshev-node (Clenshaw-Curtis) quadrature.