CS 450: Numerical Anlaysis[1]

Numerical Integration and Differentiation

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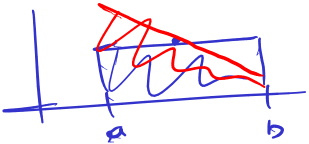
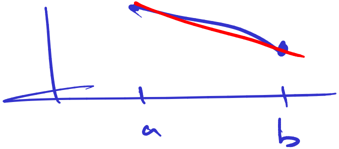
[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

$$\int_a^b f(x)\,dx \approx \langle w, y \rangle$$

uniformly spaced nodes

Newton-Cotes are exact for polynomials of degree $n-1$, when using n nodes





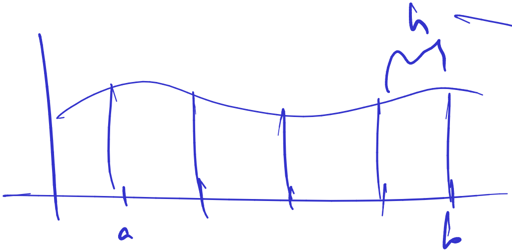
ill-conditioned for large n

↳ Chebyshev nodes (Clenshaw-Curtis quad.)

Gaussian Quadrature (select both nodes & weights)

↳ degree $2n-1$

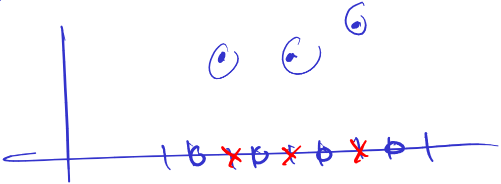
piecewise interpolation → composite quadrature rules



errors scales as

$O(h^n)$

progressive quadrature (rule for 2n nodes includes nodes used in rule for n nodes)



Integrability and Sensitivity

- Seek to compute $\mathcal{I}(f) = \int_a^b f(x)dx$:

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

Quadrature Rules

- Approximate the integral $\mathcal{I}(f)$ by a weighted sum of function values:

- For a fixed set of n nodes, polynomial interpolation followed by integration give $(n-1)$*-degree quadrature rule*:

Determining Weights for Quadrature Rules

- A quadrature rule provides $\boldsymbol{x}$ and $\boldsymbol{w}$ so as to approximate

- *Method of undetermined coefficients* obtains $\boldsymbol{y}$ from *moment equations*, which insure the quadrature rule is exact for all monomials of degree $n-1$:

Newton-Cotes Quadrature

Demo: *Newton-Cotes weight finder*

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

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

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

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

Error in Newton-Cotes Quadrature

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

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

Error Estimation

- The trapezoid rule is also first degree, despite using higher-degree polynomial interpolant approximation, since

- The above derivation allows us to obtain an error approximation via a difference of midpoint and trapezoidal rules:

Error in Polynomial Quadrature Rules

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

Conditioning of Newton-Cotes Quadrature

- We can ascertain stability of quadrature rules, by considering the amplification of a perturbation $\hat{f} = f + \delta f$:
- Newton-Cotes quadrature rules have at least one negative weight for any $n \geq 11$:

Clenshaw-Curtis Quadrature

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

Demo: Gaussian quadrature weight finder

Gaussian Quadrature

- So far, we have only considered quadrature rules based on a fixed set of nodes, but we may also be able to choose nodes to maximize accuracy:

- The *unique* n-point *Gaussian quadrature rule* is defined by the solution of the nonlinear form of the moment equations in terms of *both* x and w:

Using Gaussian Quadrature Rules

- Gaussian quadrature rules are hard to compute, but can be enumerated for a fixed interval, e.g. $a = 0, b = 1$, so it suffices to transform the integral to $[0, 1]$

- Gaussian quadrature rules are accurate and stable but not progressive (nodes cannot be reused to obtain higher-degree approximation):

Progressive Gaussian-like Quadrature Rules

- *Kronod* quadrature rules construct $(2n+1)$-point $(3n+1)$-degree quadrature K_{2n+1} that is progressive with respect to Gaussian quadrature rule G_n:

- *Patterson* quadrature rules use $2n+2$ more points to extend $(2n+1)$-point Kronod rule to degree $6n+4$, while reusing all $2n+1$ points.
- Gaussian quadrature rules are in general open, but *Gauss-Radau* and *Gauss-Lobatto* rules permit including end-points:

Composite and Adaptive Quadrature

- *Composite quadrature rules* are obtained by integrating a piecewise interpolant of f:

- Composite quadrature can be done with adaptive refinement:

More Complicated Integration Problems

- To handle improper integrals can either transform integral to get rid of infinite limit or use appropriate open quadrature rules.
- Double integrals can simply be computed by successive 1-D integration.
- High-dimensional integration is often effectively done by *Monte Carlo*:

Integral Equations

- Rather than evaluating an integral, in solving an *integral equation* we seek to compute the integrand. A typical linear integral equation has the form

$$\int_a^b K(s,t)u(t)dt = f(s), \quad \text{where} \quad K \quad \text{and} \quad f \quad \text{are known.}$$

- Using a quadrature rule with weights $w_1, \dots, w_n$ and nodes $t_1, \dots, t_n$ obtain

Numerical Differentiation

- Automatic (symbolic) differentiation is a surprisingly viable option:

- Numerical differentiation can be done by interpolation or finite differencing:

Accuracy of Finite Differences

Demo: *Finite Differences vs Noise*
Demo: *Floating point vs Finite Differences*

- *Forward and backward differencing* provide first-order accuracy:

$$f(x \pm h) = f(x) \pm h f'(x) + \frac{h^2}{2} f''(x) + \dots$$

$$f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{Forward difference}} - \boxed{\frac{h}{2} f''(x)} + \dots$$

- *Centered differencing* provides second-order accuracy.

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

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \boxed{\frac{h}{2} f''(x)} + \dots$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Extrapolation Techniques

***Demo:** Richardson with Finite Differences*
***Activity:** Richardson Extrapolation*

- Given a series of approximate solutions produced by an iterative procedure, a more accurate approximation may be obtained by *extrapolating* this series.

$$F(h) = a_0 + a_1 h^p + O(h^r)$$

true solution

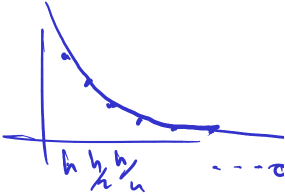
goal to compute $F(0) = a_0$

- In particular, given two guesses, *Richardson extrapolation* eliminates the leading order error term.

$a_1 h^p$ we use $F(h)$ and $F(h/2)$

$$F(h) = a_0 + a_1 h^p + O(h^r)$$

$$F(h/2) = a_0 + \frac{a_1 h^p}{2^p} + O(h^r)$$



$$a_0 = F(h) - \frac{F(h) - F(h/2)}{1 - 1/2^p} + O(h^r)$$

$$= \frac{\overbrace{\left(1 - \left(1 - 1/2^p\right)\right)}^{1/2^p} \cdot F(h)}{1 - 1/2^p} + \frac{F(h/2)}{1 - 1/2^p} + O(h^r)$$

High-Order Extrapolation

- Given a series of k approximations, *Romberg integration* applies $(k-1)$-levels of Richardson extrapolation.

Richardson extrap.

h	$I_h(f)$			
$h/2$	$I_{h/2}(f)$	X		
$h/4$	$I_{h/4}(f)$	X	X	
$h/8$	$I_{h/8}(f)$	X	X	X

- Extrapolation can be used within an iterative procedure at each step:

Steffensen's method for nonlinear solve (alternative to Newton and Secant!)

$$x_{n+1} = x_n + \frac{f(x_n)}{1 - (f(x_n + f(x_n)))/f(x_n)}$$

quadratic convergence