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).*

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 $n-1$:

Demo: *Newton-Cotes weight finder*

Newton-Cotes Quadrature

- *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

- By our analysis of polynomial quadrature, Newton-cotes rules are exact for polynomials of degree $n-1$, however (1) some, notably the midpoint and Simpson's rule are exact also for degree n, and (2) we also want to understand the error scaling with respect to $b-a$
- 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 just degree 1, since via the prior expansion, $f(m) = f(x) - f'(m)(x - m) - \ldots$, so using $x = a, b$, we get

- 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 applying our error analysis of interpolation,

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:

Gaussian Quadrature

Demo: *Gaussian quadrature weight finder*

- 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 $w_1, \ldots, w_n$ and nodes $t_1, \ldots, t_n$ obtain

Demo: *Taking Derivatives with Vandermonde Matrices*

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:

- *Centered differencing* provides second-order accuracy.

Extrapolation Techniques

- Given a sequence of approximations to the result of a smooth function, a more accurate approximation may be obtained by *extrapolating* this series.

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

High-Order Extrapolation

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

- Extrapolation can be used within an iterative procedure at each step:
  For example, Steffensen's method for finding roots of nonlinear equations,
  $$x_{n+1} = x_n + \frac{f(x_n)}{1 - f(x_n + f(x_n))/f(x_n)},$$
  derived from Aitken's delta-squared extrapolation process: