Math 225
Scientific Computing II

Outline of Lectures

Spring Semester 2003

I. Interpolating polynomials

Lagrange formulation of interpolating polynomial

Uniqueness of interpolating polynomial of degree n

Error formula for interpolating polynomial, with proof

Computing values of an interpolating polynomial by Neville's method

Newton divided differences formulation for interpolating polynomial

Hermite interpolation (brief treatment)

Osculating polynomial (brief mention)

II. Splines

Continuous piecewise linear spline

C^2 piecewise cubic spline, with derivation (natural and clamped)

Solving tridiagonal system to obtain C^2 piecewise cubic spline

Error for cubic splines (statement only)

Other splines, briefly (quintic splines, Hermite splines, and B-splines)

III. Trigonometric polynomial interpolation and DFT

Trigonometric polynomial

Discrete Fourier Transform (DFT), Danielson-Lanczos Lemma, Fast Fourier Transform (FFT), and Power Spectral Density (PSD)

DFT applications to time-series analysis and to numerical PDE (brief mention)

IV. Approximating functions by means of orthogonal polynomials

General least squares problem

Gram-Schmidt algorithm for generating orthogonal polynomials

Proof that orthogonal polynomials can be used to solve the least squares problem and to approximate to specified accuracy

V. Numerical integration

Preliminaries: weighted mean value theorem; differentiating Newton divided differences

Trapezoidal rule with error (derived)

Key concepts: error, asymptotic error, degree of precision, order of convergence, Aitkin extrapolation and error detection

Simpson's rule with error (derived)

Midpoint rule with error (stated)

Newton-Cotes formulas, with error (stated)

Richardson extrapolation and detailed error for trapezoidal rule

Romberg integration

Adaptive quadrature

Gaussian quadrature (generally); Gauss-Legendre quadrature and comparison of error with Newton-Cotes error

VI. Numerical differentiation

Uses: approximate derivatives from data; obtain formulas for numerical ODE and PDE

First-order left- and right-hand difference formulas, with errors

Second-order symmetric difference formula, with error

Second-order difference formulas for right and left endpoints, with errors

Richardson extrapolation for high-order symmetric difference formulas

Second-order symmetric difference formula for second derivative, with error

Error in data: effect on numerical derivatives

VII. Numerical ordinary differential equations

Introduction

Definition of IVP; comparison of numerical solution to "true" solution

Reduction of high-order ODE to first-order system

Non-IVP examples: boundary value problems and delay ODEs

Forward Euler and backward Euler formulas for IVP and their relation to slope fields for autonomous and non-autonomous IVP

Sources of error (geometric, informal treatment): accumulated error, local truncation error, finite-place arithmetic

Numerical failures when existence or uniqueness of true solution is not assured

Existence and uniqueness theorem for IVP (stated); emphasis on Lipschitz condition

Continuous dependence and its relationship to a "stable" numerical method

Multistep methods and Runge-Kutta methods (brief characterization, methods compared)

Fundamental concepts in numerical ODE (brief and intuitive): consistency, stability, convergence, local truncation error, global truncation error

Multistep methods

Definition of consistency and example (forward Euler); order of a method

General theorem for consistency and order (stated)

Convergence for forward Euler (theorem and proof)

Stability for forward Euler (proof)

Example of a method that is not stable (Atkinson, p. 396)

Effect of rounding error on forward Euler

Asymptotic error for forward Euler

The midpoint method: stated, derived, order

The trapezoidal method: stated, derived, order

Adams-Bashforth and Adams-Moulton methods: how derived (informal), error comparison

Formal definitions of stability and convergence for multistep methods

Key result stated: A consistent, multistep method is a convergent method if and only if it is a stable method.

Runge-Kutta methods

Advantages and disadvantages

Conceptual precursor: Taylor methods

Second-order Runge-Kutta methods: modified Euler (Heun's method No. 1), Midpoint method, Heun's method (No. 2)

General Runge-Kutta methods: how derived

Derivation of second-order Runge-Kutta methods for autonomous IVP

Fourth-order Runge-Kutta method (stated)

Consistency, convergence, order, and stability for Runge-Kutta methods (defined and asserted)

Stability and convergence of multistep methods

The model problem

Examples: weak stability of midpoint method; A-stability of trapezoidal method

Informal reasoning about model problem: locally it approximates most problems

The characteristic equation and its roots; the root condition

Key theorem: Given a consistent, multistep method, the following are equivalent: (1) The root condition is satisfied; (2) The method is stable; (3) The method is convergent. (Proof summarized.)

Characterization of relative stability, strong root condition, and weak stability

Venn diagram:
methods meeting strong root condition
$\subset$ relatively stable methods
$\subset$ methods that are convergent and stable
$\subset$ methods that are consistent
$\subset$ all potential methods

Stability examples: Adams methods and midpoint method (revisit)

Stability regions

Idea of stability regions; example, forward Euler

Region of absolute stability (definition)

Examples of regions of absolute stability (overhead transparencies): Adams and Runge-Kutta methods

A-stable multistep methods: backward Euler and trapezoidal methods, only

Implicit Runge-Kutta methods; there exist A-stable implicit Runge-Kutta methods of all orders

Miscellany

Predictor-corrector methods: introduction based on midpoint-trapezoidal method

Runge-Kutta-Fehlberg methods (brief mention)

Stiff ODEs: basic concepts, quantitative comparison of backward Euler and trapezoidal method, recommendation of implicit Runge-Kutta methods and backward difference formulas (idea for derivation of backward difference formulas)

Boundary value problems

Finite difference methods

Shooting methods

Solving a time-dependent problem that has the boundary value problem as its steady state