Part IB — Numerical Analysis
Definitions

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Polynomial approximation
Interpolation by polynomials. Divided differences of functions and relations to derivatives. Orthogonal polynomials and their recurrence relations. Least squares approximation by polynomials. Gaussian quadrature formulae. Peano kernel theorem and applications. [6]

Computation of ordinary differential equations
Euler's method and proof of convergence. Multistep methods, including order, the root condition and the concept of convergence. Runge-Kutta schemes. Stiff equations and A-stability. [5]

Systems of equations and least squares calculations
LU triangular factorization of matrices. Relation to Gaussian elimination. Column pivoting. Factorizations of symmetric and band matrices. The Newton-Raphson method for systems of non-linear algebraic equations. QR factorization of rectangular matrices by Gram-Schmidt, Givens and Householder techniques. Application to linear least squares calculations. [5]

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0 Introduction

1 Polynomial interpolation

Notation. We write $P_n[x]$ for the real linear vector space of polynomials (with real coefficients) having degree n or less.

1.1 The interpolation problem

1.2 The Lagrange formula

Definition (Lagrange cardinal polynomials)**.** The *Lagrange cardinal polynomials* with respect to the interpolation points $\{x_i\}_{i=0}^n$ are, for $k = 0, \cdots, n$,

$$\ell_k(x) = \prod_{i=0, i\neq k}^{n} \frac{x - x_i}{x_k - x_i}.$$

1.3 The Newton formula

1.4 A useful property of divided differences

1.5 Error bounds for polynomial interpolation

Definition (Chebyshev polynomial)**.** The *Chebyshev polynomial* of degree n on $[-1, 1]$ is defined by

$$T_n(x) = \cos(n\theta),$$

where $x = \cos\theta$ with $\theta \in [0, \pi]$.

2 Orthogonal polynomials

2.1 Scalar product

Definition (Orthogonalilty)**.** Given a vector space V and an inner product $\langle \cdot\,, \cdot \rangle$, two vectors $f, g \in V$ are *orthogonal* if $\langle f, g\rangle = 0$.

2.2 Orthogonal polynomials

Definition (Orthogonal polynomial)**.** Given a vector space V of polynomials and inner product $\langle \cdot\,, \cdot \rangle$, we say $p_n \in P_n[x]$ is the *nth orthogonal polynomial* if

$$\langle p_n, q\rangle = 0 \text{ for all } q \in P_{n-1}[x].$$

In particular, $\langle p_n, p_m\rangle = 0$ for $n \neq m$.

Definition (Monic polynomial)**.** A polynomial $p \in P_n[x]$ is *monic* if the coefficient of x^n is 1.

2.3 Three-term recurrence relation

2.4 Examples

2.5 Least-squares polynomial approximation

3 Approximation of linear functionals

3.1 Linear functionals

Definition (Linear functional)**.** A *linear functional* is a linear mapping $L : V \to \mathbb{R}$, where V is a real vector space of functions.

3.2 Gaussian quadrature

4 Expressing errors in terms of derivatives

Definition (Sharp error bound)**.** The constant c_L is said to be *sharp* if for any $\varepsilon > 0$, there is some $f_\varepsilon \in C^{k+1}[a, b]$ such that

$$|e_L(f)| \geq (c_L - \varepsilon)\|f_\varepsilon^{(k+1)}\|_\infty.$$

Definition (Peano kernel)**.** The *Peano kernel* is

$$K(\theta) = \lambda((x - \theta)_+^k).$$

5 Ordinary differential equations

5.1 Introduction

Definition (Lipschitz function)**.** A function $\mathbf{f} : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$ is *Lipschitz with Lipschitz constant* $\lambda \geq 0$ if

$$\|\mathbf{f}(t, \mathbf{x}) - \mathbf{f}(t, \hat{\mathbf{x}})\| \leq \lambda \|\mathbf{x} - \hat{\mathbf{x}}\|$$

for all $t \in [0, T]$ and $\mathbf{x}, \hat{\mathbf{x}} \in \mathbb{R}^N$.

A function is *Lipschitz* if it is Lipschitz with Lipschitz constant λ for some λ.

5.2 One-step methods

Definition ((Explicit) one-step method)**.** A numerical method is *(explicit) one-step* if $\mathbf{y}_{n+1}$ depends only on t_n and $\mathbf{y}_n$, i.e.

$$\mathbf{y}_{n+1} = \boldsymbol{\phi}_h(t_n, \mathbf{y}_n)$$

for some function $\boldsymbol{\phi}_h : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$.

Definition (Euler's method)**.** *Euler's method* uses the formula

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n).$$

Definition (Convergence of numerical method)**.** For each $h > 0$, we can produce a sequence of discrete values $\mathbf{y}_n$ for $n = 0, \cdots, [T/h]$, where $[T/h]$ is the integer part of T/h. A method *converges* if, as $h \to 0$ and $nh \to t$ (hence $n \to \infty$), we get

$$\mathbf{y}_n \to \mathbf{y}(t),$$

where $\mathbf{y}$ is the true solution to the differential equation. Moreover, we require the convergence to be uniform in t.

Definition (Local truncation error)**.** For a general (multi-step) numerical method

$$\mathbf{y}_{n+1} = \boldsymbol{\phi}(t_n, \mathbf{y}_0, \mathbf{y}_1, \cdots, \mathbf{y}_n),$$

the *local truncation error* is

$$\boldsymbol{\eta}_{n+1} = \mathbf{y}(t_{n+1}) - \boldsymbol{\phi}_n(t_n, \mathbf{y}(t_0), \mathbf{y}(t_1), \cdots, \mathbf{y}(t_n)).$$

Definition (Order)**.** The order of a numerical method is the largest $p \geq 1$ such that $\boldsymbol{\eta}_{n+1} = O(h^{p+1})$.

Definition (θ-method)**.** For $\theta \in [0, 1]$, the *θ-method* is

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\Big(\theta \mathbf{f}(t_n, \mathbf{y}_n) + (1 - \theta)\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1})\Big).$$

5.3 Multi-step methods

Definition (2-step Adams-Bashforth method). The *2-step Adams-Bashforth (AB2) method* has

$$\mathbf{y}_{n+2} = \mathbf{y}_{n+1} + \frac{1}{2}h\left(3\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) - \mathbf{f}(t_n, \mathbf{y}_n)\right).$$

Definition (Multi-step method). A *s-step numerical method* is given by

$$\sum_{\ell=0}^{s} \rho_\ell \mathbf{y}_{n+\ell} = h\sum_{\ell=0}^{s} \sigma_\ell \mathbf{f}(t_{n+\ell}, \mathbf{y}_{n+\ell}).$$

This formula is used to find the value of $\mathbf{y}_{n+s}$ given the others.

Definition (Root condition). We say $\rho(w)$ satisfies the *root condition* if all its zeros are bounded by 1 in size, i.e. all roots w satisfy $|w| \leq 1$. Moreover any zero with $|w| = 1$ must be simple.

Definition (Adams method). An *Adams method* is a multi-step numerical method with $\rho(w) = w^{s-1}(w-1)$.

Definition (Adams-Bashforth method). An *Adams-Bashforth* method is an explicit Adams method.

Definition (Adams-Moulton method). An *Adams-Moulton* method is an implicit Adams method.

Definition (Backward differentiation method). A *backward differentiation method* has $\sigma(w) = \sigma_s w^s$, i.e.

$$\sum_{\ell=0}^{s} \rho_\ell \mathbf{y}_{n+\ell} = \sigma_s \mathbf{f}(t_{n+s}, \mathbf{y}_{n+s}).$$

5.4 Runge-Kutta methods

Definition (Runge-Kutta method). General (implicit) ν-stage *Runge-Kutta (RK) methods* have the form

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{\ell=1}^{\nu} b_\ell \mathbf{k}_\ell,$$

where

$$\mathbf{k}_\ell = \mathbf{f}\left(t_n + c_n h, \mathbf{y}_n + h\sum_{j=1}^{\nu} a_{\ell j}\mathbf{k}_j\right)$$

for $\ell = 1, \cdots, \nu$.

6 Stiff equations

6.1 Introduction

6.2 Linear stability

Definition (Linear stability domain)**.** If we apply a numerical method to

$$y'(t) = \lambda y(t)$$

with $y(0) = 1$, $\lambda \in \mathbb{C}$, then its linear stability domain is

$$D = \left\{ z = h\lambda : \lim_{n\to\infty} y_n = 0 \right\}.$$

Definition (A-stability)**.** A numerical method is *A-stable* if

$$\mathbb{C}^- = \{z \in \mathbb{C} : \mathrm{Re}(z) < 0\} \subseteq D.$$

7 Implementation of ODE methods

7.1 Local error estimation

7.2 Solving for implicit methods

8 Numerical linear algebra

8.1 Triangular matrices

Definition (Triangular matrix)**.** A matrix A is *upper triangular* if $A_{ij} = 0$ whenever $i > j$. It is *lower triangular* if $A_{ij} = 0$ whenever $i < j$. We usually denote upper triangular matrices as U and lower triangular matrices as L.

8.2 LU factorization

Definition (LU factorization)**.** $A = LU$ is an *LU factorization* if U is upper triangular and L is *unit* lower triangular (i.e. the diagonals of L are all 1).

8.3 $A = LU$ for special A

Definition (Leading principal submatrix)**.** The *leading principal submatrices* $A_k \in \mathbb{R}^{k\times k}$ for $k = 1, \cdots, n$ of $A \in \mathbb{R}^{n\times n}$ are

$$(A_k)_{ij} = A_{ij}, \quad i, j = 1, \cdots, k.$$

In other words, we take the first k rows and columns of A.

Definition (Positive definite matrix)**.** A matrix $A \in R^{n\times n}$ is *positive-definite* if

$$\mathbf{x}^T A\mathbf{x} > 0$$

for $\mathbf{x} \neq \mathbf{0} \in \mathbb{R}^n$.

Definition (Cholesky factorization)**.** The *Cholesky factorization* of a symmetric positive-definite matrix A is a factorization of the form

$$A = LDL^T,$$

with L unit lower triangular and D a positive-definite diagonal matrix.

Definition (Band matrix)**.** A *band matrix* of *band width* r is a matrix A such that $A_{ij} \neq 0$ implies $|i - j| \leq r$.

9 Linear least squares

Definition (Orthogonal matrix)**.** A square matrix $Q \in \mathbb{R}^{n\times n}$ is orthogonal if $Q^T Q = I$.

Definition (QR factorization)**.** A *QR factorization* of an $m \times n$ matrix A is a factorization of the form

$$A = QR,$$

where $Q \in \mathbb{R}^{m\times m}$ is an orthogonal matrix, and $R \in \mathbb{R}^{m\times n}$ is "upper triangular" matrix, where "upper triangular" means

$$R = \begin{pmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{22} & \cdots & R_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{mm} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

Definition (Givens rotation)**.** In $\mathbb{R}^m$, where $m > 2$, we define the *Givens rotation* on 3 parameters $1 \leq p < q \leq m, \theta \in [-\pi, \pi]$ by

$$\Omega_\theta^{[p,q]} = \begin{pmatrix} 1 \\ & \ddots \\ & & 1 \\ & & & \cos\theta & & & & \sin\theta \\ & & & & 1 \\ & & & & & \ddots \\ & & & & & & 1 \\ & & & -\sin\theta & & & & \cos\theta \\ & & & & & & & & 1 \\ & & & & & & & & & \ddots \\ & & & & & & & & & & 1 \end{pmatrix} \in \mathbb{R}^{m\times m},$$

where the sin and cos appear at the p, qth rows and columns.

Definition (Householder reflection)**.** For $\mathbf{u} \neq \mathbf{0} \in \mathbb{R}^m$, we define the *Householder reflection* by

$$H_{\mathbf{u}} = I - 2\frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}} \in \mathbb{R}^{m\times m}.$$