Part IB — Numerical Analysis
Theorems

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These notes are not endorsed by the lecturers, and I have modified them (often significantly) after lectures. They are nowhere near accurate representations of what was actually lectured, and in particular, all errors are almost surely mine.

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]

Contents

0 Introduction

1 Polynomial interpolation

1.1 The interpolation problem

1.2 The Lagrange formula

Theorem. The interpolation problem has exactly one solution.

1.3 The Newton formula

Theorem (Recurrence relation for Newton divided differences)**.** For $0 \leq j < k \leq n$, we have

$$f[x_j, \cdots, x_k] = \frac{f[x_{j+1}, \cdots, x_k] - f[x_j, \cdots, x_{k-1}]}{x_k - x_j}.$$

1.4 A useful property of divided differences

Lemma. Let $g \in C^m[a, b]$ have a continuous mth derivative. Suppose g is zero at $m + \ell$ distinct points. Then $g^{(m)}$ has at least ℓ distinct zeros in $[a, b]$.

Theorem. Let $\{x_i\}_{i=0}^n \in [a, b]$ and $f \in C^n[a, b]$. Then there exists some $\xi \in (a, b)$ such that

$$f[x_0, \cdots, x_n] = \frac{1}{n!} f^{(n)}(\xi).$$

1.5 Error bounds for polynomial interpolation

Theorem. Assume $\{x_i\}_{i=0}^n \subseteq [a, b]$ and $f \in C[a, b]$. Let $\bar{x} \in [a, b]$ be a non-interpolation point. Then

$$e_n(\bar{x}) = f[x_0, x_1, \cdots, x_n, \bar{x}]\omega(\bar{x}),$$

where

$$\omega(x) = \prod_{i=0}^n (x - x_i).$$

Theorem. If in addition $f \in C^{n+1}[a, b]$, then for each $x \in [a, b]$, we can find $\xi_x \in (a, b)$ such that

$$e_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x)\omega(x)$$

Corollary. For all $x \in [a, b]$, we have

$$|f(x) - p_n(x)| \leq \frac{1}{(n+1)!} \|f^{(n+1)}\|_\infty |\omega(x)|$$

Lemma (3-term recurrence relation)**.** The Chebyshev polynomials satisfy the recurrence relations

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

with initial conditions

$$T_0(x) = 1, \quad T_1(x) = x.$$

Theorem (Minimal property for $n \geq 1$)**.** On $[-1, 1]$, among all polynomials $p \in P_n[x]$ with leading coefficient 1, $\frac{1}{2^{n-1}}\|T_n\|$ minimizes $\|p\|_\infty$. Thus, the minimum value is $\frac{1}{2^{n-1}}$.

Corollary. Consider

$$w_\Delta = \prod_{i=0}^{n}(x - x_i) \in P_{n+1}[x]$$

for any distinct points $\Delta = \{x_i\}_{i=0}^n \subseteq [-1, 1]$. Then

$$\min_\Delta \|\omega_\Delta\|_\infty = \frac{1}{2^n}.$$

This minimum is achieved by picking the interpolation points to be the zeros of T_{n+1}, namely

$$x_k = \cos\left(\frac{2k+1}{2n+2}\pi\right), \quad k = 0, \cdots, n.$$

Theorem. For $f \in C^{n+1}[-1, 1]$, the Chebyshev choice of interpolation points gives

$$\|f - p_n\|_\infty \leq \frac{1}{2^n}\frac{1}{(n+1)!}\|f^{(n+1)}\|_\infty.$$

2 Orthogonal polynomials

2.1 Scalar product

2.2 Orthogonal polynomials

Theorem. Given a vector space V of functions and an inner product $\langle \cdot, \cdot \rangle$, there exists a unique monic orthogonal polynomial for each degree $n \geq 0$. In addition, $\{p_k\}_{k=0}^n$ form a basis for $P_n[x]$.

2.3 Three-term recurrence relation

Theorem. Monic orthogonal polynomials are generated by

$$p_{k+1}(x) = (x - \alpha_k)p_k(x) - \beta_k p_{k-1}(x)$$

with initial conditions

$$p_0 = 1, \quad p_1(x) = (x - \alpha_0)p_0,$$

where

$$\alpha_k = \frac{\langle xp_k, p_k \rangle}{\langle p_k, p_k \rangle}, \quad \beta_k = \frac{\langle p_k, p_k \rangle}{\langle p_{k-1}, p_{k-1} \rangle}.$$

2.4 Examples

2.5 Least-squares polynomial approximation

Theorem. If $\{p_n\}_{k=0}^n$ are orthogonal polynomials with respect to $\langle \cdot, \cdot \rangle$, then the choice of c_k such that

$$p = \sum_{k=0}^n c_k p_k$$

minimizes $\|f - p\|^2$ is given by

$$c_k = \frac{\langle f, p_k \rangle}{\|p_k\|^2},$$

and the formula for the error is

$$\|f - p\|^2 = \|f\|^2 - \sum_{k=0}^n \frac{\langle f, p_k \rangle^2}{\|p_k\|^2}.$$

3 Approximation of linear functionals

3.1 Linear functionals

3.2 Gaussian quadrature

Proposition. There is no choice of ν weights and nodes such that the approximation of $\int_a^b w(x)f(x)\ \mathrm{d}x$ is exact for all $f \in P_{2\nu}[x]$.

Theorem (Ordinary quadrature)**.** For any distinct $\{c_k\}_{k=1}^\nu \subseteq [a, b]$, let $\{\ell_k\}_{k=1}^\nu$ be the Lagrange cardinal polynomials with respect to $\{c_k\}_{k=1}^\nu$. Then by choosing

$$b_k = \int_a^b w(x)\ell_k(x)\ \mathrm{d}x,$$

the approximation

$$L(f) = \int_a^b w(x)f(x)\ \mathrm{d}x \approx \sum_{k=1}^\nu b_k f(c_k)$$

is exact for $f \in P_{\nu-1}[x]$.

We call this method ordinary quadrature.

Theorem. For $\nu \geq 1$, the zeros of the orthogonal polynomial p_ν are real, distinct and lie in (a, b).

Theorem. In the ordinary quadrature, if we pick $\{c_k\}_{k=1}^\nu$ to be the roots of $p_\nu(x)$, then get we exactness for $f \in P_{2\nu-1}[x]$. In addition, $\{b_n\}_{k=1}^\nu$ are all positive.

4 Expressing errors in terms of derivatives

Theorem (Peano kernel theorem)**.** If λ annihilates polynomials of degree k or less, then

$$\lambda(f) = \frac{1}{k!}\int_a^b K(\theta) f^{(k+1)}(\theta)\;\mathrm{d}\theta$$

for all $f \in C^{k+1}[a, b]$, where

5 Ordinary differential equations

5.1 Introduction

5.2 One-step methods

Theorem (Convergence of Euler's method)**.**

(i) For all $t \in [0, T]$, we have

$$\lim_{\substack{h \to 0 \\ nh \to t}} \mathbf{y}_n - \mathbf{y}(t) = 0.$$

(ii) Let λ be the Lipschitz constant of f. Then there exists a $c \geq 0$ such that

$$\|\mathbf{e}_n\| \leq ch \frac{e^{\lambda T} - 1}{\lambda}$$

for all $0 \leq n \leq [T/h]$, where $\mathbf{e}_n = \mathbf{y}_n - \mathbf{y}(t_n)$.

5.3 Multi-step methods

Theorem. An s-step method has order p ($p \geq 1$) if and only if

$$\sum_{\ell=0}^{s} \rho_\ell = 0$$

and

$$\sum_{\ell=0}^{s} \rho_\ell \ell^k = k \sum_{\ell=0}^{s} \sigma_\ell \ell^{k-1}$$

for $k = 1, \cdots, p$, where $0^0 = 1$.

Theorem. A multi-step method has order p (with $p \geq 1$) if and only if

$$\rho(e^x) - x\sigma(e^x) = O(x^{p+1})$$

as $x \to 0$.

Theorem (Dahlquist equivalence theorem)**.** A multi-step method is convergent if and only if

(i) The order p is at least 1; and

(ii) The root condition holds.

Lemma. An s-step backward differentiation method of order s is obtained by choosing

$$\rho(w) = \sigma_s \sum_{\ell=1}^{s} \frac{1}{\ell} w^{s-\ell}(w-1)^\ell,$$

with σ_s chosen such that $\rho_s = 1$, namely

$$\sigma_s = \left(\sum_{\ell=1}^{s} \frac{1}{\ell}\right)^{-1}.$$

5.4 Runge-Kutta methods

6 Stiff equations

6.1 Introduction

6.2 Linear stability

Theorem (Maximum principle)**.** Let g be analytic and non-constant in an open set $\Omega \subseteq \mathbb{C}$. Then $|g|$ has no maximum in Ω.

7 Implementation of ODE methods

7.1 Local error estimation

7.2 Solving for implicit methods

8 Numerical linear algebra

8.1 Triangular matrices

8.2 LU factorization

8.3 $A = LU$ for special A

Theorem. A sufficient condition for the existence for both the existence and uniqueness of $A = LU$ is that $\det(A_k) \neq 0$ for $k = 1, \cdots, n-1$.

Theorem. If $\det(A_k) \neq 0$ for all $k = 1, \cdots, n$, then $A \in R^{n\times n}$ has a unique factorization of the form

$$A = LD\hat{U},$$

where D is non-singular diagonal matrix, and both L and $\hat{U}$ are unit triangular.

Theorem. Let $A \in \mathbb{R}^{n\times n}$ be non-singular and $\det(A_k) \neq 0$ for all $k = 1, \cdots, n$. Then there is a unique "symmetric" factorization

$$A = LDL^T,$$

with L unit lower triangular and D diagonal and non-singular.

Theorem. Let $A \in \mathbb{R}^{n\times n}$ be a positive-definite matrix. Then $\det(A_k) \neq 0$ for all $k = 1, \cdots, n$.

Theorem. A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is *positive-definite* iff we can factor it as

$$A = LDL^T,$$

where L is unit lower triangular, D is diagonal and $D_{kk} > 0$.

Proposition. If a band matrix A has band width r and an LU factorization $A = LU$, then L and U are both band matrices of width r.

9 Linear least squares

Theorem. A vector $\mathbf{x}^* \in \mathbb{R}^n$ minimizes $\|A\mathbf{x} - \mathbf{b}\|^2$ if and only if

$$A^T(A\mathbf{x}^* - \mathbf{b}) = 0.$$

Corollary. If $A \in \mathbb{R}^{m\times n}$ is a full-rank matrix, then there is a unique solution to the least squares problem.

Proposition. A matrix $A \in \mathbb{R}^{m\times n}$ can be transformed into upper-triangular form by applying n Householder reflections, namely

$$H_n \cdots H_1 A = R,$$

where each H_n introduces zero into column k and leaves the other zeroes alone.

Lemma. Let $\mathbf{a}, \mathbf{b} \in \mathbb{R}^m$, with $\mathbf{a} \neq \mathbf{b}$, but $\|\mathbf{a}\| = \|\mathbf{b}\|$. Then if we pick $\mathbf{u} = \mathbf{a} - \mathbf{b}$, then

$$H_{\mathbf{u}}\mathbf{a} = \mathbf{b}.$$

Lemma. If the first $k-1$ components of $\mathbf{u}$ are zero, then

(i) For every $\mathbf{x} \in \mathbb{R}^m$, $H_{\mathbf{u}}\mathbf{x}$ does not alter the first $k-1$ components of $\mathbf{x}$.

(ii) If the last $(m-k+1)$ components of $\mathbf{y} \in \mathbb{R}^m$ are zero, then $H_{\mathbf{u}}\mathbf{y} = \mathbf{y}$.

Lemma. Let $\mathbf{a}, \mathbf{b} \in \mathbb{R}^m$, with

$$\begin{pmatrix} a_k \\ \vdots \\ a_m \end{pmatrix} \neq \begin{pmatrix} b_k \\ \vdots \\ b_m \end{pmatrix},$$

but

$$\sum_{j=k}^m a_j^2 = \sum_{j=k}^m b_j^2.$$

Suppose we pick

$$\mathbf{u} = (0, 0, \cdots, 0, a_k - b_k, \cdots, a_m - b_m)^T.$$

Then we have

$$H_{\mathbf{u}}\mathbf{a} = (a_1, \cdots, a_{k-1}b_k, \cdots, b_m).$$