Numerical Programming 1 (CSE)

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Contents

1 What can't be ignored

1.1 Floating point numbers (26.10.) [QSG, Ch. 1.2]

motivation and definition of floating point numbers, the IEEE standard double precision, floating point numbers are not equally spaced, definition of machine epsilon, rounding, the relative rounding error is bounded by half the machine epsilon, overflow and underflow, motivation of the standard model of floating point arithmetic, floating point addition need not be associative

1.2 Matrices (28.10.) [QSG, Ch. 1.4]

definition of matrices, row vectors and column vectors, matrix sums, scalar multiples of matrices, matrix products, the identity matrix, invertible matrices, diagonal matrices, invertible diagonal matrices, the product of diagonal matrices is diagonal, triangular matrices, invertible triangular matrices, the product of triangular matrices is triangular, the transpose of a matrix, symmetric matrices

1.3 Vectors (2.11.) [QSG, Ch. 1.4.1]

definition of linear independence for a finite set of vectors in $\mathbb{R}^n$, definition of a basis for $\mathbb{R}^n$, the canonical basis in $\mathbb{R}^n$, the scalar product and the euclidean norm in $\mathbb{R}^n$, proof of the Cauchy-Schwarz inequality, the p-norm and the maximum norm in $\mathbb{R}^n$ with the corresponding unit balls in $\mathbb{R}^2$, definition of eigenvector and eigenvalue for complex matrices

1.4 Functions (4.11.) [QSG, Ch. 1.5]

polynomials with real and complex coefficients, reminder of the fundamental theorem of algebra and Abel's impossibility theorem, definition of continuity and differentiability, reminder of the mean value theorem for derivatives and integrals, Rolle's theorem, Taylor's formula, and the fundamental theorem of calculus

1.5 Conditioning (9.11.) [TB, Lect. 12]

examples for cancellation and an ill-conditioned matrix, definition of absolute and relative condition numbers, if f is differentiable in x, then the condition numbers depend on the size of the derivative of f in x (derivation from Taylor's formula for scalar and vectorial functions), examples: $x \mapsto \frac{1}{2}x$, $x \mapsto \sqrt{x}$, $(x_1, x_2) \mapsto x_1 - x_2$, polynomial root finding

1.6 Condition of matrices (11.11.) [TB, Lect. 12]

all norms on $\mathbb{R}^n$ are equivalent, condition of matrix-vector-multiplication, especially for invertible matrices, definition of the condition number of an invertible matrix, formulation and discussion of the diagonalisation of self-adjoint matrices, the condition number of an invertible, self-adjoint matrix is the quotient of the $|\cdot|$-maximal over the $|\cdot|$-minimal eigenvalue

1.7 Stability (18.11.) [TB, Lect. 14 & 15]

example: loss of four digits when computing a well-conditioned polynomial root, definition of (forward) stability, product formula for the stability indicator implies that a stable algorithm should be built on well-conditioned subproblems which are solved with stable algorithms, definition of backward stability

1.8 More on stability (23.11.) [TB, Lect. 14 & 15]

recapitulation of stability and backward stability, proof, that backward stability implies stability, product formula for the backward stability indicator implies that a backward stable algorithm should have starting steps with well-conditioned inverse mapping, $g(x) = x+1$ as an example with badly conditioned inverse for small $|x|$, floating point subtraction is stable, remark, that the four basic floating point operations are backward stable, inner products are backward stable, outer products are stable, but not backward stable

2 Nonlinear equations

2.1 Newton's method (25.11.) [QSG, Ch. 2.3]

motivation of Newton's method for approximating zeros of functions $f : \mathbb{R} \to \mathbb{R}$, if Newton's method converges in the case of a non-degenerate zero, then it converges quadratically, Newton's method as a special fixed point iteration, linear convergence of fixed point iterations with $\phi' < 1$, Newton's method need not converge for any initial datum, discussion of a stopping criterium

2.2 Extrapolation (30.11) [QSG, Ch. 2.3 & 2.5]

Newton's method for approximating zeros of functions $f : \mathbb{R}^n \to \mathbb{R}^n$, motivation of Aitken's method for accelerating convergence of a linearly convergent fixed point method, Aitken's method as a fixed point method, numerical examples in one and two dimensions

3 Interpolation

3.1 Polynomial interpolation (7.12.) [QSG, Ch. 3.1],[BT]

existence and uniqueness for an interpolating polynomial of degree $\leq n$ through $n+1$ points, derivation of the first barycentric interpolation formula, the first barycentric interpolating formula allows a backward stable computation of the interpolating polynomial, the Lebesgue constant Λ_n is the absolute condition number of polynomial interpolation, regardless of the nodes $\Lambda_n \to \infty$ as $n \to \infty$, for equispaced nodes Λ_n grows exponentially, while for the Chebyshev nodes it grows only logarithmically in n

3.2 Trigonometric interpolation (9.12) [QSG, Ch. 3.3.4]

derivation of an explicit formula for the coefficients of the trigonometric interpolant on n equidistant nodes in $[0, 2\pi)$, computation of the coefficients by a matrix-vector-product, factorization of the Fourier matrix for $n = 2^m$ yields to a Fast Fourier Transform (FFT), the relation of trigonometric interpolants to Fourier series, example for aliasing

3.3 Spline interpolation (14.12.) [QSG, Ch. 3.4]

piecewise linear interpolation with error estimate for $f \in C^2[a, b]$, definition of splines of degree k, cubic splines and complete, natural, perdiodic boundary conditions or the not-a-knot-condition, the construction of natural cubic splines leads to tridiagional, strictly row-dominant linear systems

4 Quadrature

4.1 Basics (16.12.) [QSG, Ch. 4.3]

condition numbers for integration and quadrature, integration and quadrature of highly oscillatory functions may be ill-conditioned, if the quadrature formula integrates constants exactly, then positive quadrature weights keep the absolute condition numbers of integration and qudrature equal, discussion and error estimate of the simple midpoint formula, the midpoint formula integrates linear functions exactly

4.2 More on quadrature (11.1.) [QSG, Ch. 4.3]

motivation and error estimate for the simple trapezoidal formula, the trapezoidal formula integrates linear functions exactly, discussion of Simpson's formula, Simpson's formula integrates cubic polynomials exactly, composite quadrature rules, discussion of a composite midpoint formula, error estimate via the discrete mean-value theorem, discussion and error estimate for a composite trapezoidal formula

4.3 Monte Carlo quadrature (13.1.) [DR, Ch. 5.6–5.9]

motivation of product rules in two dimensions, products of functions, which are integrated exactly by the one-dimensional rules, are integrated exactly by the product rule, discussion of the computational effort for d-dimensional product rules, the curse of dimensionality, motivation of Monte Carlo quadrature by the Law of Large Numbers, definition of the variance of a function, the Central Limit Theorem implies the convergence rate $O(n^{-1/2})$ for n sampling points for any dimension

5 Linear systems

5.1 LU factorization (18.1.) [TB, Lect. 20 & 21]

Gaussian elimination solves the linear system $Ax = b$ by transforming A to upper triangular form, this is achieved by left multiplication with lower triangular matrices $L_k = I - l_k e_k^T$, in this case $A = LU$ with L lower unit triangular and U upper triangular, this requires $\sim 2/3n^3$ floating point operations, well-conditioned matrices might have ill-conditioned L and U factors, for every invertible $A \in \mathbb{R}^{n\times n}$ there exist permutation matrices $P_1, \ldots, P_{n-1}$ and lower unit triangular matrices $L_1, \ldots, L_{n-1}$ such that $L_{n-1}P_{n-1} \cdots L_1 P_1 A$ is upper triangular.

5.2 Pivoting & Stability (20.1.) [TB, Lect. 21 & 22], [ST]

partial pivoting exchanges rows to use an entry below the diagonal which has maximal modulus as the pivot element, for every invertible $A \in \mathbb{R}^{n\times n}$ there exists a permutation matrix P, a lower unit triangular L with $|L(i,j)| \leq 1$ and an upper triangular matrix U such that $PA = LU$, backward error estimate for Gaussian elimination with partial pivoting, discussion of the worst case example with $\|U\|_\infty/\|A\|_\infty = 2^{n-1}/n$, indication how smoothed analysis explains and improves growth factors

5.3 Least-squares-method (25.1.) [TB, Lect. 11]

approaching an overdetermined linear system $Ax = b$ with $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$, $m > n$, by the least squares method, that is, by mimizing $\|b - Ax\|_2$, polynomial fitting by interpolation or least squares approximation, derivation of the normal equations $A^T Ax = A^T b$, existence and uniqueness of solutions if A has maximal rank, definition of the condition number of a rectangular matrix via the singular value decomposition, example of ill-conditioned normal equations

5.4 Iterative methods (27.1.) [K, Ch. 1]

recapitulation of the singular value decomposition and its applicability for least squares problems, motivation of the Richardson iteration as a stationary iterative method, proof, that stationary iterative methods with $\|M\| < 1$ converge for all initial iterates x_0, convergence of the (preconditioned) Richardson iteration, motivation of matrix splitting, discussion of the Jacobi iteration

6 Eigenvalue problems

6.1 Power method (1.2) [QSS, Ch. 5.2& 5.3]

convergence of the Jacobi iteration for matrices, which are strictly diagonal dominant by row, discussion of the forward Gauss-Seidel iteration, the condition numbers for simple eigenvalues an their eigenvectors, motivation of the power method for diagonalizable matrizes with a simple dominant eigenvalue, convergence of the power method

6.2 Inverse iteration (3.2.) [QSG, Ch. 6.4 & 6.5]

discussion of the Rayleigh quotient, within the power method the Rayleigh quotient converges to the dominant eigenvalue λ_1, the convergence rate is $O(|\lambda_2/\lambda_1|^k)$ and even $O(|\lambda_2/\lambda_1|^{2k})$ for hermitian matrices, discussion of the inverse iteration with shift

6.3 QR algorithm (8.2.) [S, Lect. 15]

motivation of QR factorization, reduced and full QR factorization of rectangular matrices, application to least squares problems, motivation and discussion of the simple QR algorithm for reducing a matrix to Schur form (unitary transformations to upper triangular form)

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