AMS526: Numerical Analysis I (Numerical Linear Algebra for Computational and Data Sciences)

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Announcement: Final Exam

- Final exam will be accumulative, covering all the material from the semester
- About 50–60% will be on material after Test 2 (i.e., eigenvalue problems and iterative methods, which are closely connected with earlier materials, especially QR and SVD)
- As usual, you can have a single-sided, one-page, letter-size (8.5inx11in) cheat sheet

Topics Covered in The Course

- Fundamental concepts: norms, orthogonality, conditioning, stability
- Least squares problems using direct methods (QR factorization)
- Singular value decomposition, properties, and relationship with eigenvalue problems
- Eigenvalue problems, properties, and algorithms (QR algorithm and Lanczos iterations)
- Solving linear systems using direct (Gaussian elimination) and iterative (Krylov subspace) methods
- Conditioning of problems, stability and backward stability of algorithms
- Efficiency of algorithms, convergence rate of iterative methods

Matrix Properties and Transformations

Properties

- Hermitian (symmetric), skew symmetry, positive definite
- unitary (orthogonal), normal, (orthogonal and oblique) projection matrix
- singular/nonsingular, defective/nondefective
- triangular, Hessenberg, tridiagonal, diagonal, Jordan-form, sparse

Transformations

- orthogonalization (Gram-Schmidt)
- triangularization (Gaussian elimination, Cholesky factorization, Householder QR)
- reduction to Hessenberg or tridiagonal form
- similarity transformation and unitary similarity transformation (Schur factorization)
- congruence transformation (preserves symmetry and inertia)

Fundamental Algorithms

- QR factorization using classical and modified Gram-Schmidt
- QR factorization using Householder triangularization
- Gaussian elimination with partial pivoting and Cholesky factorization
- Reduction to Hessenberg/tridiagonal form for eigenvalue problems
- QR algorithm with or without shifts for eigenvalue problems
- Lanczos iterations and conjugate gradients
- Do not need to memorize the details of the algorithms
- Understand when they work, how they work, why they work, and how well they work
- Understand relationships among each other: how one transforms into another, and to make an intelligent choice

Eigenvalue Problem

- Eigenvalue problem of $m \times m$ matrix A is $Ax = \lambda x$
- Characteristic polynomial is $det(A \lambda I)$
- Eigenvalue decomposition of A is $A = X \Lambda X^{-1}$ (does not always exist)
- Geometric multiplicity of λ is dim(null($A \lambda I$)), and algebraic multiplicity of λ is its multiplicity as a root of p_A , where algebraic multiplicity \geq geometric multiplicity
- Similar matrices have the same eigenvalues, and algebraic and geometric multiplicities
- Schur decomposition $A = QTQ^*$ uses unitary similarity transformations

Eigenvalue Algorithms

- Underlying concepts: power iterations, Rayleigh quotient, inverse iterations, convergence rate
- Schur decomposition is typically done in two steps
 - Reduction to Hessenberg form for nonhermitian matrices or reduction to tridiagonal form for hermitian matrices by unitary similarity transformation
 - Finding eigenvalues of Hessenberg or tridiagonal form
- Finding eigenvalue of tridiagonal forms
 - QR algorithm with shifts, and their interpretations as (inverse) simultaneous iterations
 - Others: Bisection and divide-and-conquer
- Alternative method is Jacobi method for symmetric matrices using Jacobi rotations

Relationship between SVD and Eigenvalue Decomposition

- SVD works for all matrices (even rectangular matrices), but eigenvalue decomposition (i.e., diagonalization) works only for nondefective square matrices
- Singular vectors are always orthonormal and singular values are always real, while eigenvectors may not be orthogonal and eigenvalues may be complex numbers
- For normal matrices, singular values and eigenvalues are particularly closely related, which make them particularly powerful analytical tools

Iterative Methods

- Advantages and disadvantages of iterative methods vs. direct methods
- We focus on Krylov subspace methods for symmetric matrices
- Given A and b, Krylov subspace is $\{b, Ab, A^2b, \cdots A^kb\}$
- Key observation: QR factorization of leading vectors of Krylov subspace leads to Hessenberg form for nonsymmetric matrices and tridiagonal form for symmetric matrices
- Lanczos iterations take advantage of the tridiagonal form to get three-term recurrence version of Arnoldi iterations
- Conjugate gradient methods for solving SPD linear systems: solution as quadratic optimization problem, finite-termination properties with exact arithmetic, and convergence with floating-point arithmetic
- GMRES, Bi-CG, Bi-CGSTAB for nonsymmetric matrices
- Concepts of preconditioners, and multigrid method

