Reading course on Numerical Solution of Eigenvalue Problems

Lecture 1

Introduction: Definitions, Hermitian Matrices, Perturbation theory, Basic Algorithms

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1 Definitions

Consider

$$Ax = \lambda x, \quad x \neq 0, \quad A \in \mathbb{C}^{n,n}, \quad x \in \mathbb{C}^n, \quad , \lambda \in \mathbb{C}. \tag{1}$$

Definition 1.1. *λ is an eigenvalue of A if (1) holds. The vector $x \neq 0$ is called an eigenvector. Here precisely x is a right eigenvector for λ. If $x^*A = \lambda x^*$ then x is a left eigenvector.*

$E_\lambda(A) = Ker(A - \lambda I) = \{x \in \mathbb{C}^n, |(A - \lambda I)x = 0\}$ is called eigenspace of A belonging to λ

If $det(A - \lambda I) = (\lambda - \lambda_j)^{a(\lambda_j)} q(\lambda)$ with $q(\lambda) \in \mathcal{P}_{n-a(\lambda_j)}$ and $q(\lambda_j) \neq 0$ then $a(\lambda_j))$ is called the algebraic multiplicity of λ_j. The geometric multiplicity is given by $g(\lambda_j) = dim E_{\lambda_j}(A)$. Usually $g(\lambda_j) \leq (\lambda_j)$.

An eigenvector defines a one-dimensional subspace, that is invariant under premultiplication by A. Eigenvectors are the simplest invariant subspace.

Definition 1.2. *$\mathcal{S} \in \mathbb{C}^n$ is called invariant subspace of A if $A\mathcal{S} \subset \mathcal{S}$, i.e. $s \in \mathcal{S} \Rightarrow As \in \mathcal{S}$*

Note that if $\exists X \in \mathbb{C}^{n,k}$, $B \in \mathbb{C}^{k,k}$, rank$(X) = k$ and $AX = XB$, then $\mathcal{S} =$ Im(X) is an A-invariant subspace.

Furthermore from $By = \lambda y \Rightarrow A(Xy) = XBy = \lambda(Xy)$ follows that, if X has full rank then $AX = XB$ implies $\Lambda(B) \subset \Lambda(A)$.

If X is square and nonsingular rank$(X) = k = n$ then $\Lambda(B) = \Lambda(A)$ and we say that A and $B = X^{-1}AX$ are similar and X is a similarity transform.

2 Similarity Transforms

Theorem 2.1 (Jordan Canonical Form)**.** *Let $A \in \mathbb{C}^{n,n}$. Then there exists a nonsingular $X \in \mathbb{C}^{n,n}$ such that*

$$X^{-1}AX = \begin{bmatrix} J_1(\lambda_1) & & \\ & \ddots & \\ & & J_r(\lambda_r) \end{bmatrix}$$

where $\lambda_1 \neq \lambda_2 \neq \ldots \neq \lambda_r$ and

$$J_j(\lambda_j) = \begin{bmatrix} J_{j,1} & & \\ & \ddots & \\ & & J_{j,g(\lambda_j)} \end{bmatrix} \in \mathbb{C}^{a(\lambda_j), a(\lambda_j)},$$

and

$$J_{jk} = \begin{bmatrix} \lambda_j & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_j \end{bmatrix} \in \mathbb{C}^{m_{jk},m_{jk}},$$

where m_{jk} are partial multiplicities of λ_j.

Note that the Jordan Canonical Form is expensive to calculate and it is *very* sensitive to small perturbations.

Hence, we need to find $\hat{A} = Y^{-1}AY$ such that $\Lambda(\hat{A})$ is easy to calculate *and* $\kappa(Y) \approx 1$ (i.e. no error amplification).

Therefore unitary transforms must be used in order to achieve numerical stability.

Theorem 2.2. *If $A \in \mathbb{C}^{n,n}$, $B \in \mathbb{C}^{k,k}$, and $X \in \mathbb{C}^{n,k}$ satisfy*

$$AX = XB, \quad rank(X) = k,$$

then there exists a unitary $Q \in \mathbb{C}^{n,n}$ such that

$$Q^*AQ = T = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix}$$

where $\Lambda(T_{11}) = \Lambda(A) \cap \Lambda(B)$.

Proof. See Golub/van Loan. □

We see that a matrix can be reduced to block triangular form using unitary similarity transformations if we know one of its invariant subspaces.

Theorem 2.3 (Schur Decomposition)**.** *If $A \in \mathbb{C}^{n,n}$ then there exists a unitary $Q \in \mathbb{C}^{n,n}$ such that*

$$Q^*AQ = T = D + N$$

where $D = diag(\lambda_1, \ldots, \lambda_n)$ and $N \in \mathbb{C}^{n,n}$ is strictly upper triangular. Q can be chosen so that the eigenvalues λ_i appear in any order along the diagonal.

Proof. See Golub/van Loan. □

Definition 2.1. *$A \in \mathbb{C}^{n,n}$ is* normal *if and only if $A^*A = AA^*$.*

Corollary 2.1. *$A \in \mathbb{C}^{n,n}$ is normal if and only if there exists a unitary transform $Q \in \mathbb{C}^{n,n}$ such that $Q^*AQ = D$.*

Proof. Exercise. □

It is easy to see that Hermitian matrices $A = A^*$ are normal. From now on we want to consider Hermitian matrices (or, as they are called in the real case, symmetric matrices). We mention some of their properties and numerical eigenvalue algorithms.

3 Hermitian Matrices and Properties

Theorem 3.1 (Spectral Theorem)**.** *All eigenvalues of Hermitian matrices are real. If* $\lambda_j \neq \lambda_k$ *then* $(x_j, x_k) = x_k^* x_j = 0$ *and*

$$A = X^* \Lambda X = \sum_{i=1}^{n} \lambda_i x_i x_i^*, \quad I = X X^* = \sum_{i=1}^{n} x_i x_i^*.$$

Hence $X = [x_1, \ldots, x_n]$ is the matrix of orthonormal eigenvectors of A. Any invariant subspace is just the span of an approximate subset of eigenvectors.

Consider the *generalized Hermitian eigenproblem*

$$Ax = \lambda M x, \tag{2}$$

where $A, M \in \mathbb{C}^{n,n}$ Hermitian and M positive definite. Then all eigenvectors may be chosen to be M-orthogonal, i.e. $x_i^* M x_j = 0$, $i \neq j$.

The generalised HEP can be transformed into a Hermitian eigenproblem as follows. First factor $M = LL^*$ where L is nonsingular (Cholesky factorisation), then solve HEP $\hat{A} = L^{-1} A L^{-*}$. The eigenvalues of $\hat{A}$ and $Ax = \lambda M x$ are identical, the eigenvectors are $x = L^{-*}\hat{x}$.

Also let Λ and X be eigenvalue and eigenvector matrix of $AX = MX\Lambda$. Then $X^* A X = X^* M X \Lambda$. Since x_i are unit vectors orthogonal w.r.t. the inner product induced by M we see that $X^* M X = \Lambda_M$ and hence $\Lambda_A = X^* A X = \Lambda_M \Lambda$ is diagonal, too.

4 Quadratic Forms and the Rayleigh Quotient

Self-adjoint (Hermitian) matrices arise in the study of quadratic forms

$$\Psi(x) = x^* A x = \sum_{i=1}^{n} \sum_{i=1}^{n} a_{ij} \bar{x}_i x_j,$$

usually this represents some form of energy. A linear change of variable, $x \to y = F^{-1}x$ forces a change in the form,

$$\Psi(x) = \hat{\Psi}(y) = y^* \hat{A} y, \text{ for all } x$$

only if $\hat{A} = F^* A F$. This mapping $A \to F^* A F$ is called *congruence transform.* Unlike similarity transform it does not preserve the eigenvalues, but the signs of the eigenvalues.

Theorem 4.1 (Sylvester's inertia theorem)**.** *Each A is congruent to a matrix $diag(I_\pi, I_\nu, 0_\zeta)$, where the number triple (π, ν, ζ) depends only on A and is called A's inertia. Moreover π, ν and ζ are the number of positive, negative and zero eigenvalues of A.*

Proof. See Golub/van Loan. □

This theorem leads to a method about *slicing the spectrum* of a generalised Hermitian eigenproblem. There is an elegant way to determine the number of A's eigenvalues that are less than any given real number σ.

Theorem 4.2. *Suppose that $A - \sigma M$ permits triangular factorisation $A - \sigma M = L_\sigma \Delta_\sigma L_\sigma^*$, where Δ_σ is diagonal, and suppose that the pair (A, M) has a full set of real eigenvectors. Then*

$$\nu(\Lambda - \sigma I) = \nu(A - \sigma M) = \nu(\Delta_\sigma),$$

where $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$ and λ_i is an eigenvalue of the pair (A, M)

Proof. Since L_σ is unit lower triangular it is invertible and so $A - \sigma M$ is congruent to Δ_σ. By simultaneous reduction of two quadratic forms there is an invertible matrix F such that

$$F^*(A - \sigma M)F = \Lambda - \sigma I,$$

whence $A - \sigma M$ is congruent to $\Lambda - \sigma I$ The result follows from Silvester's inertia theorem applied to the congruent diagonal matrices $\Lambda - \sigma I$ and Δ_σ. □

On the one hand $\nu(\Delta_\sigma)$ is simply the number of negative elements on Δ_σ's diagonal. On the other hand $\nu(\Lambda - \sigma I)$ is the number of eigenvalues of the pencil (A, M) which are less than σ.

Now we restrict the quadratic form to its values on the unit sphere and get the so called *Rayleigh quotient*:

$$\rho(u) = \rho(u; A) = \frac{u^* A u}{u^* u}, \quad u \neq 0.$$

Theorem 4.3. *The RQ enjoys the following basic properties:*

- Homogeneity*: $\rho(\alpha u) = \rho(u), \quad \alpha \neq 0$*
- Boundedness*: $\rho(u)$ ranges over the interval $[\lambda_1, \lambda_n]$ as u ranges over all nonzero n-vectors*
- Stationarity*: $\rho(u)$ is stationary (i.e. the gradient of ρ is 0 at and only at the eigenvectors of A.*

Proof. Exercise. □

It is worth mentioning one particular property here. Define the special residual vector $r(u)$

$$r(u) = (A - \rho(u))u$$

Proposition 4.1 (Minimum residual property)**.** *For each $u \in \mathbb{C}^n$ we have*

$$\|(A - \rho(u))u\| \leq \|(A - \mu)u\|, \quad \forall \mu \in \mathbb{C}.$$

Proof. Proof by illustration. □

Note that the Rayleigh quotient for generalized HEP (2) is given by

$$\rho(u) = \rho(u; A, M) = \frac{u^* A u}{u^* M u}.$$

An important theorem related to the Rayleigh quotient is the following

Theorem 4.4 (Courant-Fischer minimax theorem)**.** *If $A \in \mathbb{R}^{n,n}$ is symmetric then*

$$\lambda_k(A) = \max_{dim(S)=k} \min_{0 \neq y \in S} \frac{y^T A y}{y^T y},$$

for $k = 1, \ldots, n$ where $S \subset \mathbb{R}^n$ is some subspace.

Proof. See Golub/van Loan. □

From this minimax property we get

$$\begin{aligned} \lambda_1 &= \max_{x \neq 0} \frac{x^T A x}{x^T x} \\ \lambda_n &= \min_{x \neq 0} \frac{x^T A x}{x^T x} \end{aligned}$$

and

$$\max_{x \neq 0} |\rho(u, A)| = \max\{|\lambda_1|, |\lambda_n|\} = \|A\|_2.$$

5 Some Perturbation Theory

Since we determine eigenvalues iteratively, we need an informative perturbation theory that tells us, how to think about approximate eigenvalues and invariant subspaces.

Theorem 5.1 (Bauer-Fike). *If μ is an eigenvalue of $A+E \in \mathbb{C}^{n,n}$ and $X^{-1}AX = D = diag(\lambda_1, \ldots, \lambda_n)$, then*

$$\min_{\lambda \in \Lambda(A)} |\lambda - \mu| \leq \kappa_p(X)\|E\|_p \tag{3}$$

where $\|\cdot\|_p$ denotes any of the p-norms.

Proof. We only need to consider $\mu \notin \Lambda(A)$. Then $D - \mu I$ is invertible, and $X^{-1}(A+E-\mu I)X = D - \mu I + X^{-1}EX$ is singular. So is $I + (D-\mu I)^{-1}X^{-1}EX$. Hence

$$\begin{aligned} 1 &\leq \|(D-\mu I)^{-1}X^{-1}EX\|_p & (4)\\ &\leq \|(D-\mu I)^{-1}\|_p\|X^{-1}\|_p\|E\|_p\|X\|_p & (5)\\ &= \max_{j=1,\ldots,n} \frac{1}{|\lambda_j - \mu|}\kappa_p(X)\|E\|_p. & (6) \end{aligned}$$

□

Note that for Hermitian matrices $X = Q$ becomes unitary, and hence (3) becomes

$$\exists \lambda_j \, |\mu - \lambda_j| \leq \|E\|_2.$$

We can step up this estimate by the theorem of Weyl:

Theorem 5.2 (Weyl). *If $(\mu_1, \ldots, \mu_n)$ are the eigenvalues of $A + E \in \mathbb{C}^{n,n}$ and $(\lambda_1, \ldots, \lambda_n)$ are the eigenvalues of $A \in \mathbb{C}^{n,n}$. Then*

$$|\mu_j - \lambda_j| \leq \|E\|_2.$$

Proof. This can be proved using Courant Fischer's minimax theorem. Exercise. □

There are also several theorem's on approximate invariant subspaces, which we will not consider here.

Theorem 5.3 (Gershgorin). *Suppose $A \in \mathbb{R}^{n,n}$ is symmetric and that $Q \in \mathbb{R}^{n,n}$ is orthogonal. If $Q^TAQ = D + F$ where $D = diag(d_1, \ldots, d_n)$ and F has zero diagonal entries, then*

$$\lambda(A) \subseteq \bigcup_{i=1}^{n} [d_i - r_i, d_i + r_i],$$

where $r_i = \sum_{i=1}^{n} |f_{ij}|$ for $i = 1, \ldots, n$.

Proof. See Golub/van Loan. □

6 Basic Algorithms for Hermitian Problems

There are several algorithms available for computing the eigenvalues and eigenvectors of Hermitian Matrices. Their efficiency and cost depend on whether one is looking only for a small number of eigenvalues or all eigenvalues and whether one also wants to compute the eigenvectors. Of course, some algorithms are also applicable to Non-Hermitian eigenproblems.

For all algorithms below, except Rayleigh quotient iteration and Jacobi's method, assume the matrix has first been reduced to tridiagonal form (Householder reflections). This is an initial cost of $(4/3)n^3$ flops, $(8/3)n^3$ if eigenvectors are also required

- Power iteration, Inverse iteration, Rayleigh quotient iteration
- (Tridiagonal) QR iteration (finds all eigenvalues and optionally all eigenvectors) currently the fastest practical method to find all the eigenvalues of a symmetric tridiagonal matrix.
- Divide-and-conquer method: currently the fastest method to find all the eigenvalues and eigenvectors of symmetric tridiagonal matrices larger than $n = 25$
- Bisection method
- Jacobi's method
- Lanczos method
- Jacobi-Davidson method