AMS526: Numerical Analysis I (Numerical Linear Algebra)

Lecture 16: Linear Algebra Software; Overview of Eigenvalue Problems

Xiangmin Jiao

SUNY Stony Brook

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Outline

Software for Linear Algebra

- LAPACK: Linear Algebra PACKage (`www.netlib.org/lapack/lug`)
  - Standard library for solving linear systems and eigenvalue problems
  - Successor of LINPACK (`www.netlib.org/linpack`) and EISPACK (`www.netlib.org/eispack`)
  - Depends on BLAS (Basic Linear Algebra Subprograms)
  - Parallel extensions include ScaLAPACK and PLAPACK
  - Note: Uses Fortran conventions for matrix arrangements
- MATLAB
  - Factorization $\boldsymbol{A}$: lu(A) and chol(A)
  - Solve $\boldsymbol{Ax} = \boldsymbol{b}$: $x = A \backslash b$
    - Uses back/forward substitution for triangular matrices
    - Uses Cholesky factorization for positive-definite matrices
    - Uses LU factorization with column pivoting for nonsymmetric matrices
    - Uses Householder QR for least squares problems
    - Uses some special routines for matrices with special sparsity patterns
  - Uses LAPACK and other packages internally
- Serial and parallel solvers for sparse matrices (e.g., SuperLU, TAUCS)

Some Commonly Used Functions

Example BLAS routines: Matrix-vector multip.: dgemv; Matrix-matrix multip: dgemm

	LU Factorization		Solve linear system		Est. cond
	General	Symmetric	General	Symmetric	
LAPACK	dgetrf	dpotrf/dsytrf	**dgesv**	**dposv/dposvx**	dgecon
LINPACK	dgefa	dpofa/dsifa	dgesl	dposl/dsisl	dgeco
MATLAB	lu	chol	\	\	rcond

	Linear least squares			Eigenvalue/vector		SVD
	QR	Solve	Rank-deficient	General	Sym.	
LAPACK	dgeqrf	**dgels**	**dgelsy/s/d**	**dgeev**	**dsyev**	**dgesvd**
LINPACK	dqrdc	dqrsl	dqrst	-	-	dsvdc
MATLAB	qr	\	\	eig	eig	svd

For BLAS, LINPACK, and LAPACK, first letter s stands for single-precision real, d for double-precision real, c for single-precision complex, and z for double-precision complex. Boldface LAPACK routines are **driver** routines; others are **computational** routines.

Using LAPACK Routines in C Programs

- LAPACK was written in Fortran 77. Special attention is required when calling from C.
- Key differences between C and Fortran
  1. Storage of matrices: column major (Fortran) versus row major (C/C++)
  2. Argument passing for subroutines in C and Fortran: pass by reference (Fortran) and pass by value (C/C++)
- Smple example C code, example.c, for solving linear system using sgesv.
  - See class website for sample code.
  - To compile, issue command "cc -o example example.c -llapack -lblas"
- Hint: To find a function name, refer to LAPACK Users' Guide.
- To find out arguments for a given function, search on netlib.org

Outline

Eigenvalue Decomposition

- *Eigenvalue problem* of $m \times m$ matrix $\boldsymbol{A}$ is

$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$$

  with eigenvalues λ and eigenvectors $\boldsymbol{x}$ (nonzero)

- *Eigenvalue decomposition* of $\boldsymbol{A}$ is

$$\boldsymbol{A} = \boldsymbol{X}\boldsymbol{\Lambda}\boldsymbol{X}^{-1} \text{ or } \boldsymbol{A}\boldsymbol{X} = \boldsymbol{X}\boldsymbol{\Lambda}$$

  with eigenvectors as columns of $\boldsymbol{X}$ and eigenvalues along diagonal of $\boldsymbol{\Lambda}$

- Eigenvalue decomposition is change of basis to "eigenvector coordinates"

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \quad \rightarrow \quad (\boldsymbol{X}^{-1}\boldsymbol{b}) = \boldsymbol{\Lambda}(\boldsymbol{X}^{-1}\boldsymbol{x})$$

- Question: How does eigenvalue decomposition differ from SVD?

Multiplicity

- Eigenvectors corresponding to a single eigenvalue λ form an *eigenspace* $E_\lambda \subseteq \mathbb{C}^{m\times m}$
- *Geometric multiplicity* of λ is dimension of E_λ, i.e., $\dim(\text{null}(\boldsymbol{A} - \lambda \boldsymbol{I}))$
- The *characteristic polynomial* of $\boldsymbol{A}$ is

$$p_{\boldsymbol{A}}(z) = \det(z\boldsymbol{I} - \boldsymbol{A}) = (z - \lambda_1)(z - \lambda_2)\cdots(z - \lambda_m)$$

- λ is eigenvalue of $\boldsymbol{A}$ iff $p_{\boldsymbol{A}}(\lambda) = 0$
  - If λ is eigenvalue, then by definition, $\lambda\boldsymbol{x} - \boldsymbol{A}\boldsymbol{x} = (\lambda\boldsymbol{I} - \boldsymbol{A})\boldsymbol{x} = 0$, so $(\lambda\boldsymbol{I} - \boldsymbol{A})$ is singular and its determinant is 0
  - If $(\lambda\boldsymbol{I} - \boldsymbol{A})$ is singular, then for $\boldsymbol{x} \in \text{null}(\lambda\boldsymbol{I} - \boldsymbol{A})$ we have $\lambda\boldsymbol{x} - \boldsymbol{A}\boldsymbol{x} = 0$
- *Algebraic multiplicity* of λ is its multiplicity as a root of $p_{\boldsymbol{A}}$
- Any matrix $\boldsymbol{A}$ has m eigenvalues, counted with algebraic multiplicity
- Question: What are the eigenvalues of a triangular matrix?

Similarity Transformations

- The map $\boldsymbol{A} \to \boldsymbol{Y}^{-1}\boldsymbol{A}\boldsymbol{Y}$ is a *similarity transformation* of $\boldsymbol{A}$ for any nonsingular $\boldsymbol{Y} \in \mathbb{C}^{m \times m}$
- $\boldsymbol{A}$ and $\boldsymbol{B}$ are *similar* if there is a similarity transformation $\boldsymbol{B} = \boldsymbol{Y}^{-1}\boldsymbol{A}\boldsymbol{Y}$

Theorem

If $\boldsymbol{Y}$ is nonsingular, then $\boldsymbol{A}$ and $\boldsymbol{Y}^{-1}\boldsymbol{A}\boldsymbol{Y}$ have the same characteristic polynomials, eigenvalues, and algebraic and geometric multiplicities.

1. For characteristic polynomial:

$$\det(z\boldsymbol{I} - \boldsymbol{Y}^{-1}\boldsymbol{A}\boldsymbol{Y}) = \det(\boldsymbol{Y}^{-1}(z\boldsymbol{I} - \boldsymbol{A})\boldsymbol{Y}) = \det(z\boldsymbol{I} - \boldsymbol{A})$$

   so algebraic multiplicities remain the same

2. If $\boldsymbol{x} \in E_\lambda$ for $\boldsymbol{A}$, then $\boldsymbol{Y}^{-1}\boldsymbol{x}$ is in eigenspace of $\boldsymbol{Y}^{-1}\boldsymbol{A}\boldsymbol{Y}$ corresponding to λ, and vice versa, so geometric multiplicities remain the same

Algebraic Multiplicity $\geq$ Geometric Multiplicity

- Let n be be geometric multiplicity of λ for $\boldsymbol{A}$. Let $\hat{\boldsymbol{V}} \in \mathbb{C}^{m\times n}$ constitute of orthonormal basis of the E_λ
- Extend $\hat{\boldsymbol{V}}$ to unitary $\boldsymbol{V} \equiv [\hat{\boldsymbol{V}}, \tilde{\boldsymbol{V}}] \in \mathbb{C}^{m\times m}$ and form

$$\boldsymbol{B} = \boldsymbol{V}^*\boldsymbol{A}\boldsymbol{V} = \begin{bmatrix} \hat{\boldsymbol{V}}^*\boldsymbol{A}\hat{\boldsymbol{V}} & \hat{\boldsymbol{V}}^*\boldsymbol{A}\tilde{\boldsymbol{V}} \\ \tilde{\boldsymbol{V}}^*\boldsymbol{A}\hat{\boldsymbol{V}} & \tilde{\boldsymbol{V}}^*\boldsymbol{A}\tilde{\boldsymbol{V}} \end{bmatrix} = \begin{bmatrix} \lambda\boldsymbol{I} & \boldsymbol{C} \\ 0 & \boldsymbol{D} \end{bmatrix}$$

- $\det(z\boldsymbol{I} - \boldsymbol{B}) = \det(z\boldsymbol{I} - \lambda\boldsymbol{I})\det(z\boldsymbol{I} - \lambda\boldsymbol{D}) = (z-\lambda)^n\det(z\boldsymbol{I} - \lambda\boldsymbol{D})$, so the algebraic multiplicity of λ as an eigenvalue of $\boldsymbol{B}$ is $\geq n$
- $\boldsymbol{A}$ and $\boldsymbol{B}$ are similar, so the algebraic multiplicity of λ as an eigenvalue of $\boldsymbol{A}$ is at least $\geq n$
- Examples:

$$\boldsymbol{A} = \begin{bmatrix} 2 & & \\ & 2 & \\ & & 2 \end{bmatrix}, \qquad \boldsymbol{B} = \begin{bmatrix} 2 & 1 & \\ & 2 & 1 \\ & & 2 \end{bmatrix}$$

Their characteristic polynomial is $(z-2)^3$, so algebraic multiplicity of $\lambda = 2$ is 3. But geometric multiplicity of $\boldsymbol{A}$ is 3 and that of $\boldsymbol{B}$ is 1.

Defective and Diagonalizable Matrices

- An eigenvalue of a matrix is *defective* if its algebraic multiplicity $>$ its geometric multiplicity
- A matrix is *defective* if it has a defective eigenvalue. Otherwise, it is called *nondefective*.

Theorem

An $m \times m$ matrix $\boldsymbol{A}$ is nondefective iff it has an eigenvalue decomposition $\boldsymbol{A} = \boldsymbol{X}\boldsymbol{\Lambda}\boldsymbol{X}^{-1}$.

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- $(\Leftarrow)$ Λ is nondefective, and $\boldsymbol{A}$ is similar to Λ, so $\boldsymbol{A}$ is nondefective.
- $(\Rightarrow)$ A nondefective matrix has m linearly independent eigenvectors. Take them as columns of $\boldsymbol{X}$ to obtain $\boldsymbol{A} = \boldsymbol{X}\boldsymbol{\Lambda}\boldsymbol{X}^{-1}$.
- Nondefective matrices are therefore also said to be *diagonalizable*.