Ma221 Lecture 9
Eigenvalue Problems

Goals:

- Canonical Forms (recall Jordan, why Schur form better)
- Variations on eigenvalue problems (not just one matrix...)
- Perturbation theory (can I trust the answer?)
- Algorithms (for a single nonsymmetric matrix)

Recommended on webpage:
Templates for Solution of Algebraic Eigenvalue Problems

Recall definitions for $n \times n$ A

Def: $p(\lambda) = \det(A - \lambda I)$ is characteristic polynomial, n roots are eigenvalues

Def: If λ eigenvalue, a nonzero null vector x : $(A - \lambda I)x = 0$ must exist, ie. $Ax = \lambda x$, x is a right e-vector
Analagously $\exists\ y^H (A - \lambda I) = 0$ or $y^H A = \lambda y^H$
y^H is left e-vector

Def: S nonsingular and $B = SAS^{-1}$
S is a similarity transform
A and B are similar

Lemma: A and B similar $\Rightarrow$ have same e-vals, e-vecs are related by multiplying by S

proof $Ax = \lambda x$ iff $\underbrace{SAS^{-1}}_{B} Sx = \lambda Sx$

or $B(Sx) = \lambda(Sx)$

$y^H A = \lambda y^H$ iff $y^H S^{-1} S A S^{-1} = \lambda y^H S^{-1}$

or $(y^H S^{-1}) B = \lambda (y^H S^{-1})$

Goal: Transform A to a simpler similar B, whose evals and e-vecs are "easy"

Simplest: B diagonal, then e-vals are $B(i,i)$ and e-vecs $= \begin{array}{c|} \\ \\ \\ \end{array}\begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} i$

Lemma: if $Ax_i = \lambda_i x_i$ for $i = 1$ to n and $S = [x_1, \ldots, x_n]$ is nonsingular, i.e. $\exists$ n linearly independent e-vecs. Then $A = S \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} S^{-1}$.

Conversely if $A = S \Lambda S^{-1}$ where Λ diagonal, then columns of S are e-vecs, $\lambda_i = \Lambda(i,i)$ are e-vals.

proof: $A = S\Lambda S^{-1}$ iff

$AS = S\Lambda$ iff

$AS[:,i] = S[:,i]\lambda_i$ for all i

But we can't always "diagonalize" A, for 2 reasons:

may be mathematically impossible (recall Jordan form)

may be numerically unstable (even if it exists)

Recall Jordan: For any A there is a similar $J = SAS^{-1}$ such that $J = \mathrm{diag}(J_1, \dots, J_k)$ where each J_i is a Jordan Block

$$J_i = \begin{bmatrix} \lambda & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & \lambda \end{bmatrix}$$

Up to permuting order of J_i, unique

Different J_i can have same λ

eg $A = I$, Only one right (left) e-vec

per Jordan Block:

$$\begin{bmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

So a matrix has n independent e-vecs iff has n 1×1 Jordan Blocks, called diagonalizable, otherwise defective. The number of times λ appears is called its multiplicity

Why not Compute Jordan Form? Consider slightly perturbed 2×2 identity matrix:

(1) $\begin{bmatrix} 1 & 0 \\ 0 & 1+e \end{bmatrix}$: $\left(1, \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right)$ and $\left(1+e, \begin{bmatrix} 1 \\ e \end{bmatrix}\right)$

(2) $\begin{bmatrix} 1 & e \\ e & 1 \end{bmatrix}$: $\left(1+e, \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right)$ and $\left(1-e, \begin{bmatrix} 1 \\ -1 \end{bmatrix}\right)$

evecs rotated 45°

(3) $\begin{bmatrix} 1 & e \\ 0 & 1+e^2 \end{bmatrix}$: $\left(1, \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right)$ and $\left(1+e^2, \begin{bmatrix} 1 \\ e \end{bmatrix}\right)$

evecs nearly parallel

(4) $\begin{bmatrix} 1 & e \\ 0 & 1 \end{bmatrix}$: $\left(1, \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right)$

only one evec

(5) $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$: (1, anything) and (1, anything)

When e-vals are nearly multiple Jordan form very ill-conditioned

Best we can hope for is backward stability: Getting exact e-vals and e-vecs for a slightly perturbed $A+E$, $\|E\| = O(\varepsilon)\|A\|$

Ma221 Lecture 9 Segment 2

Backward Stable approach to computing e-vals and e-vecs

Chap 3: Multiplying by orthogonal matrices is backward stable

$$fl(Q_k(Q_{k-1}(\cdots(Q_1 A))\cdots) = Q(A+E)$$
where $QQ^T = I$, $\|E\| = O(\varepsilon)\|A\|$

Apply to computing orthogonal similarity

$$fl(Q_k(\cdots(Q_2(Q_1 A Q_1^T)Q_2^T)\cdots Q_k^T)$$
$$= Q(A+E)Q^T \qquad QQ^T = I$$
$$\|E\| = O(\varepsilon)\|A\|$$

If we restrict to orthog (unitary) similarities, how close to Jordan form can we get?

Thm (Schur Canonical Form):
Given any $n \times n$ A there is a unitary Q s.t. $Q^H \cdot A \cdot Q = T$ upper triangular with evals are $T(i,i)$, which can appear in any order

Computing e-vecs of T: just triangular solve:

$$\begin{array}{c|c} & \begin{array}{ccc} i-1 & 1 & n-i \end{array} \\ \begin{array}{c} i-1 \\ 1 \\ n-i \end{array} & \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ & T(i,i) & T_{23} \\ & & T_{33} \end{bmatrix} \end{array} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = T(i,i) \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$T_{11} \cdot x_1 + T_{12} x_2 + T_{13} x_3 = T(i,i) x_1$$
$$T(i,i) x_2 + T_{23} x_3 = T(i,i) x_2$$
$$T_{33} \; x_3 = T(i,i) x_3$$

If one $T(i,i)$ on diagonal, then only x_3 that satisfies $T_{33} x_3 = T(i,i) x_3$ is $x_3 = 0$

$\Rightarrow \; T(i,i) x_2 = T(i,i) x_2$

choose $x_2 = 1$

$\Rightarrow \; T_{11} x_1 + T_{12} = T(i,i) x_1$

$(T_{11} - T(i,i) I) x_1 = -T_{12}$

if $T(i,i)$ only appears once, nonsingular triangular system, else singular, as expected

What does LAPACK (Matlab) do if

there are multiple eigenvalues: always returns something, try eig($\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$) see what happens.

proof of Schur form: Induction

let x be unit right evec $Ax = \lambda x$, $\|x\|_2 = 1$

Let $Q = [x, Q']$ be unitary matrix

$$Q^H A Q = \begin{bmatrix} x^H \\ Q'^H \end{bmatrix} A \begin{bmatrix} x, Q' \end{bmatrix}$$

$$= \begin{bmatrix} x^H A x & x^H A Q' \\ Q'^H A x & Q'^H A Q' \end{bmatrix}$$

$$= \begin{bmatrix} \lambda x^H x & x^H A Q' \\ \lambda Q'^H x & Q'^H A Q' \end{bmatrix}$$

$$= \begin{bmatrix} \lambda & x^H A Q' \\ 0 & Q'^H A Q' \end{bmatrix}$$

apply induction to $Q'^H A Q' = U^H T U$

T upper triangular, U unitary

$$Q^H A Q = \begin{bmatrix} \lambda & x^H A Q' \\ 0 & U^H T U \end{bmatrix}$$

$$= \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & U^H \end{array}\right] \left[\begin{array}{c|c} \lambda & x^H A Q' U^H \\ \hline & T \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & U \end{array}\right]$$

$$\underbrace{\left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & U \end{array}\right] Q^H}_{\text{unitary}} A \underbrace{Q \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & U^H \end{array}\right]}_{\text{inverse}} = \underbrace{\left[\begin{array}{c|c} \lambda & x^H A Q' U^H \\ \hline 0 & T \end{array}\right]}_{\text{upper triangular as desired}}$$

what about real matrices with complex evals?

Ma221 Lecture 9 Segment 3

Schur Form for Real Matrices

Real A can have complex evals (unless, say, $A = A^T$, see Chap 5) so Schur form could be complex.

But if A real, prefer all real computations:

- reduce # flops
- less memory
- make sure complex evals, evecs

appear in complex
conjugate pairs

Instead of triangular T,
use block triangular T:

$$T = \begin{bmatrix} T_{11} & T_{12} & \cdots & T_{1k} \\ & T_{22} & \cdots & T_{2k} \\ & & \ddots & \vdots \\ & & & T_{kk} \end{bmatrix}$$

evals of T are the union of evals of all T_{ii} (HW 4.1). Show any real matrix orthogonally similar to block triangular T where each diagonal block either 1×1 (real eval) or 2×2 (2 complex conjugate evals)

Thm (Real Schur Canonical Form) Given real $n \times n$ A, $\exists$ real orthog Q such that QAQ^T is block upper triangular with 1×1 and 2×2 blocks

Generalize evec to "invariant subspace"

Def: $V = \text{span}\{x_1, \ldots, x_m\} = \text{span}(X)$, $X = [x_1, \ldots, x_m]$
be a subspace of $\mathbb{R}^n$. It is invariant
if $A \cdot V = \text{span}(AX) \subseteq V$

Ex: $V = \text{span}\{x\} = \{\alpha x$ for all scalars $\alpha\}$
where $Ax = \lambda x$
$A \cdot V = \{A(\alpha x) \ \forall \alpha\}$
$= \{\alpha \lambda x \ \ \forall \alpha\} \subseteq V$
($= V$ unless $\lambda = 0$)

Ex $V = \text{span}\{x_1, \ldots, x_k\} = \{\sum_{i=1}^{k} \alpha_i x_i \ \forall \alpha_i\}$
where $A x_i = \lambda_i x_i$
$A V = \{A \sum_{i=1}^{k} \alpha_i x_i \ \ \forall \alpha_i\}$
$= \{\sum_{i=1}^{k} \alpha_i \lambda_i x_i \ \ \forall \alpha_i\}$
$\subseteq V$

Lemma: $V = \text{span}\{x_1, \ldots, x_m\} = \text{span}(X)$ where
$\text{dimension}(V) = m$. Then there is
an $m \times m$ B such that $A \cdot X = X \cdot B$
The evals of B are evals of A.
pf: existence of B follows from def:
$A x_i$ in $V \Rightarrow \exists$ scalars $B(1,i) \ldots B(m,i)$

such that $A x_i = \sum_{j=1}^{m} x_j B(j,i)$ i.e. $AX = XB$

$By = \lambda y \qquad A(Xy) = XBy = \lambda(Xy)$

i.e. Xy evec of A, eval λ

Lemma: Let $V = \mathrm{span}(X)$ be m-dimensional invariant subspace of A as above,

$AX = XB$. $X = QR$, Let $[\overset{m}{Q}, \overset{n-m}{Q'}]$

be square and orthog

$$[Q, Q']^T \cdot A \cdot [Q, Q'] = \begin{array}{c} \\ m \\ \\ \end{array} \begin{array}{cc} m & \\ \left[\begin{array}{c} A_{11} \\ 0 \end{array}\right. & \left.\begin{array}{c} A_{12} \\ A_{22} \end{array}\right] \end{array}$$

$A_{11} = R \cdot B \cdot R^{-1}$ has same evals as B

proof: $[Q, Q']^T A [Q, Q']$

$$= \begin{bmatrix} Q^T A Q & Q^T A Q' \\ Q'^T A Q & Q'^T A Q' \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

$$AQ = AXR^{-1} = XBR^{-1} = Q\,RBR^{-1}$$

so $A_{11} = Q^T A Q = Q^T Q R B R^{-1} = RBR^{-1}$

$A_{21} = \underbrace{Q'^T Q}_{0} RBR^{-1} = 0$

Proof of Real Schur Form:

Induction: if $Ax = \lambda x$, where x, λ are real, reduce to $n-1 \times n-1$ problem as in proof of Schur form (all arith real)

If x, λ complex: look at real and imaginary parts of $Ax = \lambda x$

$$X = [re(x), im(x)], \quad B = \begin{bmatrix} re(\lambda) & im(\lambda) \\ -im(\lambda) & re(\lambda) \end{bmatrix}$$

$AX = BX$: first col is real$(Ax = \lambda x)$

second col is imag$(Ax = \lambda x)$

X invariant subspace

evals of B are λ and $\bar{\lambda}$

so use lemma 2 to do orthog similarity to get $\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}$

evals of A_{11} are λ and $\bar{\lambda}$

Ma221 Lecture 9 Segment 4

Review other eigenproblems that can arise. In Lecture 1, showed that ODEs can give rise to more general eigenproblems:

(1) ODE: $x'(t) = Kx(t) \rightarrow$

If $K \cdot x(0) = \lambda \cdot x(0)$ then $x(t) = e^{\lambda t} x(0)$, similar if $x(0)$ is linear comb. of evecs

(2) When $M x''(t) + Kx(t) = 0$ and $\lambda^2 M x(0) + Kx(0) = 0$ then

$x(t) = e^{\lambda t} x(0)$

"generalized eigenproblem" for (M, K) with eval λ^2 and evec $x(0)$. Usual def of eval becomes $\det(\lambda' M + K) = 0$, $\lambda' = \lambda^2$

(3) $Mx''(t) + Dx'(t) + Kx(t) = 0$

$\Rightarrow$ "nonlinear eigenproblem"

$$\lambda^2 M x(0) + \lambda D x(0) + K x(0) = 0$$

can be reduced linear problem of twice the size

(4) $x'(t) = A x(t) + B u(t)$

"linear control system"

how to choose $u(t)$ to "control" $x(t)$ turns into singular eigenproblem for rectangular

$$[B, A] \text{ and } [0, I]$$

All ideas of Chap 4 (eval, evecs, Jordan form, Schur form, algorithms) generalize to these cases, see Chap 4.5 for details; continue discussion for 1 matrix

Perturbation Theory: how can I trust my answer

Goal: Backward Stability:
right answer (evals) for a slightly wrong problem $A+E$, $\|E\| = O(\varepsilon)\|A\|$

Last time: showed if evals are close evecs very sensitive (disappear, be nonunique, for $A=I$)

To describe perturbations in evals:

Def: Epsilon pseudospectrum of A is set of all evals of all matrices within distance ε of A:

$$\Lambda_\varepsilon(A) = \{\lambda : (A+E)x = \lambda x \text{ for some } x \neq 0 \text{ and } \|E\|_2 \leq \varepsilon\}$$

Ideal case: $\Lambda_\varepsilon(A)$ = union of disks of radius ε around evals of A (attained by adding $\varepsilon \cdot I$ to A)
true for $A = A^H$ (Chap 5)

Worst case: (Trefethen + Reichel)

Given any simply connected $R \subseteq \mathbb{C}$,

any $x \in R$

any $\varepsilon > 0$

there exists A

with one eval at x

$\Lambda_\varepsilon(A)$ nearly fills out R

i.e. evals can be very sensitive

proof: use Riemann Mapping Thm

Ex: Perturb $n \times n$ Jordan Block, $\lambda = 0$ with $J(n,1) = \varepsilon$

$$\begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ \varepsilon & & & 0 \end{bmatrix}$$

$p(\lambda) = \lambda^n - \varepsilon = 0 \Rightarrow$

$\lambda = \sqrt[n]{\varepsilon}$ uniformly spaced on circle of radius $\sqrt[n]{\varepsilon}$

$\varepsilon = 10^{-16}$ $n = 16$ radius $= .1$

(1) evals are not always differentiable functions of A (slope of $\varepsilon^{1/n}$ is ∞ at $\varepsilon = 0$)

(2) expect sensitive evals when (nearly) multiple, as was case for evecs

Condition number of simple (nonmultiple) eval:

Thm: λ simple eval of A

$$Ax = \lambda x \quad y^H A = \lambda y^H, \quad \|x\|_2 = \|y\|_2 = 1$$

If we perturb A to $A+E$, then

λ perturbed to $\lambda + \delta\lambda$

$$\delta\lambda = \frac{y^H E x}{y^H x} + O(\|E\|^2)$$

$$|\delta\lambda| \le \frac{\|E\|_2}{|y^H x|} + O(\|E\|^2)$$

$$= \sec(\theta)\,\|E\|_2 + O(\|E\|^2)$$

where θ = angle between x and y

i.e. $\sec(\theta)$ is condition number

proof: Subtract $Ax = \lambda x$ from

$$(A+E)(x+\delta x) = (\lambda + \delta\lambda)(x + \delta x)$$

$$\underline{Ax} + A\delta x + Ex + E\delta x = \underline{\lambda x} + \lambda\delta x + \delta\lambda x + \delta\lambda\delta x$$

cancel

ignore second order terms: $E\delta x$, $\delta\lambda\delta x$

$$A \cdot \delta x + Ex = \lambda\delta x + \delta\lambda x$$

multiply by y^H

$$\underline{y^H A \delta x} + y^H E x = \underline{\lambda y^H \delta x} + \delta\lambda\, y^H x$$

cancel

$$\delta\lambda = \frac{y^H E x}{y^H x}$$

Note: $y^H x = 0$ for Jordan Block!

$$x = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad y = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

Special case: A real symmetric / Hermitian or normal $(AA^H = A^H A)$: all evecs are orthonormal

Cor: If A normal, perturbing A to $A+E$

$\Rightarrow |\delta\lambda| \le \|E\| + O(\|E\|^2)$, ie. condition number $= 1$

Proof: $A = Q \Lambda Q^H$ is eigendecomp

Q unitary, $AQ = Q\Lambda$

$\Rightarrow$ right evecs are cols of Q

$Q^H A = \Lambda Q^H \Rightarrow$ left evecs also columns of Q

Later, Chap 5, for Hermitian A, if $A+E$, E also Hermitian

$|\delta\lambda| \le \|E\|_2$ (no $O(\|E\|^2)$ term)

Extend to eliminate $O(\|E\|^2)$ in general

Thm (Bauer-Fike) A has all simple evals, call them λ_i, with evecs x_i, y_i with $\|x_i\|_2 = \|y_i\|_2 = 1$. Then for any E the evals of $A+E$ lie in the union of disks D_i, with centers λ_i and radius $n \cdot \|E\|_2 / |y_i^H x_i|$

Note: bound n times larger than asymptotic result. If 2 disks overlap, only guarantee is that 2 evals lie in union $D_i \cup D_j$ (analogous if multiple disks overlap) (see proof in book)

Ma221 Lecture 9 Segment 5

Algorithms for Nonsymmetric Eigenproblem

Ultimate Algorithm: Hessenberg QR
takes nonsymmetric A, computes
Schur form $A = QTQ^*$ in $O(n^3)$ flops.
Build up to it via simpler algorithms
that are also used, eg to find just
a few evals/evecs of large sparse
matrices. Hessenberg QR also building
block, because we "approximate" large
sparse matrix by small dense matrix,
on which we use Hessenberg QR (Chap 7)

Plan:

Power Method: Just repeated
multiplication of x by A, converges
to evec for eval of largest magnitude

Inverse Iteration: Apply power
method to $B = (A - \sigma I)^{-1}$ which has
same evecs as A, largest eval in
magnitude corresponds to eval of A

closest to σ ("shift"). So by choosing σ appropriately, can converge to any eval/evec

Orthogonal Iteration: Extends power method from one evec to whole invariant subspace

QR Iteration: Combine Inverse Iteration and Orthogonal Iteration

lots of other techniques, to get complexity down to $O(n^3)$, real Schur form, reduce movement, discuss later

Power Method:

$i = 0$
repeat
  $y_{i+1} = A x_i$
  $x_{i+1} = y_{i+1} / \|y_{i+1}\|_2$ ... approx evec
  $\lambda'_{i+1} = x_{i+1}^T A x_{i+1}$ ... approx eval
  $i = i+1$
until convergence

Consider $A = diag(\lambda_1, \ldots, \lambda_n)$
where $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \ldots$, generalize later

$$x_i = A^i x_0 / \|A^i x_0\|_2$$
$$= [\lambda_1^i x_0(1), \lambda_2^i x_0(2), \ldots] / \| " \|_2$$
$$= \lambda_1^i \left[x_0(1), \left(\frac{\lambda_2}{\lambda_1}\right)^i x_0(2), \left(\frac{\lambda_3}{\lambda_1}\right)^i x_0(3) \ldots \right] / \|\cdot\|_2$$

all < 1

as i grows converges to $[1, 0, \ldots 0]$
as desired, evec for λ_1

error is $O\left(\left(\frac{\lambda_2}{\lambda_1}\right)^i\right)$, assuming $x_0(1) \neq 0$

Now suppose A diagonalizable $A = S \Lambda S^{-1}$

$$A^i = S \Lambda^i S^{-1} = S \cdot diag(\lambda_1^i, \lambda_2^i \ldots \lambda_n^i) S^{-1}$$

$z = S^{-1} x_0$

$$A^i x_0 = S[\lambda_1^i z_1, \lambda_2^i z_2 \ldots]$$
$$= \lambda_1^i S\left[z_1, \left(\frac{\lambda_2}{\lambda_1}\right)^i z_2 \ldots\right]$$
$$\rightarrow \lambda_1^i S[z_1, 0 \ldots 0]$$
$= z_1 \lambda_1^i S(:,1)$, multiple of evec for λ_1

For this to converge at good rate,
need (1) $\left|\frac{\lambda_2}{\lambda_1}\right| < 1$, smaller the better

can't count on this, eg
if A orthogonal, then
all $|\lambda_i| = 1$, no convergence

(2) z_1 nonzero, pick x_0 randomly
chance z_1 tiny very small

How to achieve $|\lambda_1| \gg |\lambda_2|$?

Inverse Iteration: power method
on $B = (A - \sigma I)^{-1}$

$i = 0$
repeat
$\quad y_{i+1} = (A - \sigma I)^{-1} x_i$
$\quad x_{i+1} = y_{i+1} / \|y_{i+1}\|_2$ ... approx evec
$\quad \lambda'_{i+1} = x_{i+1}^T A x_{i+1}$ ... approx eval
$\quad i = i+1$
until convergence

evecs of B same as for A
evals of B are $\frac{1}{\lambda_i - \sigma}$,

Suppose σ closest to λ_k

Do same analysis as above with vector

$$\begin{bmatrix} [(\lambda_k-\sigma)/(\lambda_1-\sigma)]^i \cdot \frac{z_1}{z_k} \\ [(\lambda_k-\sigma)/(\lambda_2-\sigma)]^i \frac{z_2}{z_k} \\ \vdots \\ 1 \\ [(\lambda_k-\sigma)/(\lambda_n-\lambda)]^i \frac{z_n}{z_k} \end{bmatrix} \begin{matrix} \\ \\ \\ k^{th} \text{ component} \\ \\ \end{matrix}$$

If we can make σ much closer to λ_k than any other λ_i, can converge as fast as we want. Where do we get σ? Algorithm computes estimate of λ_k. This makes convergence quadratic, even cubic in some cases.

Ma 221 Lecture 9 Segment 6

Last time: power method and inverse iteration; extend power method from one vector to multiple vectors.

Orthogonal Iteration:

given Z_0, $n \times p$ orthog matrix

$i = 0$
repeat
$Y_{i+1} = A Z_i$
factor $Y_{i+1} = Z_{i+1} R_{i+1}$ ... QR decomp
... Z_{i+1} spans an approximate invariant subspace
$i = i+1$
until convergence

$p = 1$, same as power method

Similar to some randomized algs. when Z_0 chosen randomly.

Informal Analysis:

$A = S \Lambda S^{-1}$ diagonalizable

$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_p| > |\lambda_{p+1}| \geq \cdots$

↑ needed for convergence

$\text{span}(Z_{i+1}) = \text{span}(Y_{i+1}) = \text{span}(A Z_i)$

... $\text{span}(A^i Z_0)$ by induction

$= \text{span}(S \Lambda^i S^{-1} Z_0)$

$S \Lambda^i S^{-1} Z_0$

$= S \cdot \lambda_p^i \, \mathrm{diag}\Big(\underbrace{\left(\tfrac{\lambda_1}{\lambda_p}\right)^i, \left(\tfrac{\lambda_2}{\lambda_p}\right)^i \cdots}_{\geq 1}, \underset{p}{1}, \underbrace{\left(\tfrac{\lambda_{p+1}}{\lambda_p}\right)^i, \cdots}_{<1} \Big) S^{-1} Z_0$

$= S \cdot \lambda_p^i \begin{bmatrix} V_i \\ W_i \end{bmatrix} \begin{matrix} p \\ n-p \end{matrix}$

V_i multiplied by $\left(\frac{\lambda_k}{\lambda_p}\right)^i$, $\left(\frac{\lambda_k}{\lambda_p}\right) \geq 1$

W_i multiplied by $\left(\frac{\lambda_k}{\lambda_p}\right)^i$, $\left(\frac{\lambda_k}{\lambda_p}\right) < 1$

$W_i \to 0$, V_i grows, keeps full rank if V_0 full rank

$A^i Z_0 \to \lambda_p^i S \begin{bmatrix} V_i \\ 0 \end{bmatrix}$ = linear combination of leading p columns of S

i.e. first p eigenvectors, desired invariant subspace

Note that first $k < p$ columns of Z_i are the same as though we started with first k columns of Z_0 because k^{th} column of Q, R in QR decomp of A only depends on first k columns

$\Rightarrow$ Othogonal Iterative gives first p invariant subspaces, assuming $|\lambda_1| > |\lambda_2| > \cdots$

Why not let $p = n$, $Z_0 = I$, compute n invariant subspaces, if $|\lambda_1| > |\lambda_2| > \cdots$

(A real $\Rightarrow$ complex eigenvalues have $|\lambda_i| = |\lambda_{i+1}|$
doesn't work)

Thm Run Orthogonal Iteration on A with $Z_0 = I$, $|\lambda_1| > |\lambda_2| > \cdots$ and all submatrices $S(1{:}k, 1{:}k)$ all have full rank, then $A_i = Z_i^T A Z_i$ (similar to A) converges to Schur form, i.e. upper triangular, evals on diagonal

proof: by previous analysis, for each k, span of first k columns of Z_i converge to invariant subspace spanned by first k evecs of A

$$Z_i = [\overset{k}{Z_{i1}}, \overset{n-k}{Z_{i2}}]$$

$$Z_i^H A Z_i = \begin{bmatrix} Z_{i1}^H \\ Z_{i2}^H \end{bmatrix} A \left[Z_{i1}, Z_{i2}\right]$$

$$= \begin{bmatrix} Z_{i1}^H A Z_{i1} & Z_{i1}^H A Z_{i2} \\ \underbrace{Z_{i2}^H A Z_{i1}}_{\text{converges to } 0} & Z_{i2}^H A Z_{i2} \end{bmatrix}$$

AZ_{i1} converges to $Z_{i1}B$, where B $k \times k$
since $Z_{i1} \to$ invariant subspace

$$Z_{i2}^H A Z_{i1} \to \underbrace{Z_{i2}^H Z_{i1}}_{\to 0 \text{ by orthogonality of } Z_i} B \to 0$$

block upper triangular for all k
$\Rightarrow$ upper triangular, Z_i unitary
$\Rightarrow$ Schur form
(matlab demo: see typed notes for code)

Math 221 Lecture 9 Segment 7

power method $\Rightarrow$ Orthogonal Iteration
$\Rightarrow$ QR Iteration $\Rightarrow$ add inverse iteration
$\to$ lets us converge to any eigenvalue for which we have an approximation (to be supplied by algorithm)

QR: given $A_0 = A$
$i = 0$
repeat
  factor $A_i = Q_i R_i$
  $A_{i+1} = R_i Q_i$
  $i = i + 1$
until convergence

$$A_{i+1} = R_i Q_i = Q_i^T \underbrace{Q_i R_i}\, Q_i = Q_i^T A_i Q_i$$

$\Rightarrow A_{i+1}$ and A_i orthog similar

Thm: A_i from QR iteration identical to $Z_i^T A Z_i$ from orthog. iteration

$\Rightarrow A_i$ converges to Schur form if all eigenvalues have different magnitudes

proof: Induction: assume $A_i = Z_i^T A Z_i$

One step of Orthog It $\rightarrow$

$$A Z_i = Z_{i+1} R_{i+1} \quad \ldots \text{ QR decomp}$$

$$A_i = Z_i^T A Z_i = \underbrace{Z_i^T Z_{i+1}}\, \underline{R_{i+1}}$$

$$= \text{orthog} \cdot \text{triangular}$$

$= \underline{QR}$ decomp of A_i by uniqueness

$$Z_{i+1}^T A Z_{i+1} = Z_{i+1}^T A\, Z_i Z_i^T Z_{i+1}$$

$$= (Z_{i+1}^T A Z_i)(Z_i^T Z_{i+1})$$

$$= R_{i+1} \cdot (Z_i^T Z_{i+1})$$

$$= \underline{RQ} \quad \text{where } QR = Z_i^T A Z_i$$

$$= A_{i+1}$$

i.e. we have taken one step of QR iteration

Add inverse iteration

QR iteration with a shift: given $A_0 = A$

$i = 0$

repeat

choose shift σ_i near an eigenvalue

factor $A_i - \sigma_i I = Q_i R_i$

$A_{i+1} = R_i Q_i + \sigma_i I$

$i = i+1$

until convergence

Lemma: A_i and A_{i+1} orthog. similar

pf: $A_{i+1} = R_i Q_i + \sigma_i I$

$$= Q_i^T \underbrace{Q_i R_i} Q_i + \sigma_i I$$

$$= Q_i^T (A_i - \underbrace{\sigma_i I}) Q_i + \underbrace{\sigma_i I}_{\text{cancel}}$$

$$= Q_i^T A_i Q_i$$

If R_i nonsingular we can write

$$A_{i+1} = R_i Q_i + \sigma_i I$$

$$= R_i \underbrace{Q_i R_i} R_i^{-1} + \sigma_i I$$

$$= R_i (A_i - \underline{\sigma_i I}) R_i^{-1} + \underline{\sigma_i I} \quad \text{cancel}$$

$= R_i A_i R_i^{-1}$

If σ_i exact eval of A, QR iteration with shift converges in 1 step:

$A_i - \sigma_i I$ singular $\Rightarrow R_i$ singular

$\Rightarrow$ some diagonal entry of R_i is 0

Suppose that $R_i(n,n) = 0$

$\Rightarrow$ whole last row of R_i is 0

$\Rightarrow$ last row of $R_i Q_i$ is 0

$\Rightarrow$ last row of $A_{i+1} = R_i Q_i + \sigma_i I$

is zero except $A_{i+1}(n,n) = \sigma_i$

$$n-1\left\{\begin{bmatrix} \overbrace{\ast}^{n-1} & \ast \\ 0 & \sigma_i \end{bmatrix}\right. \leftarrow \text{eigenvalue}$$

$\Rightarrow$ continue working on leading $n-1 \times n-1$ submatrix

If σ_i not exact eval, declare convergence if $A_{i+1}(n, 1{:}n-1)$ small enough ($\le O(\epsilon)\cdot\|A\|$ $\Rightarrow$ backward stable)

Previous analysis $\Rightarrow$ expect $A_{i+1}(n, 1:n-1)$ to shrink by factor

$$|\lambda_k - \sigma_i| / \min_{j \neq k} |\lambda_j - \sigma_i|$$

This is implicitly inverse iteration

Suppose eval is real

$$A_i - \sigma_i I = Q_i R_i$$

$\Rightarrow Q_i^T (A_i - \sigma_i I) = R_i$

$\Rightarrow$ if σ_i were exact eval, $\Rightarrow$

$R_i(n,n) = 0 \Rightarrow$

last row of $Q_i^T (A_i - \sigma_i I)$ is 0

$\Rightarrow$ last col of Q_i is left evec of A_i for eval σ_i

Now suppose σ_i just close to an eval

$$A_i - \sigma_i I = Q_i R_i$$

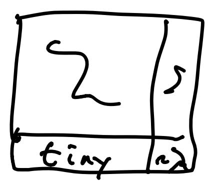
$$(A_i - \sigma_i I)^{-1} = R_i^{-1} Q_i^T$$

$$(A_i - \sigma_i I)^{-T} = Q_i R_i^{-T}$$

$$(A_i - \sigma_i I)^{-T} \underbrace{R_i^T}_{\triangle} = Q_i$$

take last column of both sides

$(A_i - \sigma_i I)^{-T} e_n$ and last col of Q_i
are parallel $\Rightarrow$ last col of Q_i
gotten by one step of inverse iteration
starting with e_n
$\Rightarrow$ last col of Q_i closer to evec of A_i^T
$\Rightarrow$ last col of $A_i^T Q_i$ closer to $\lambda \cdot$ last col of Q_i
$\Rightarrow$ last col of $Q_i^T A_i^T Q_i$ closer to λe_n
$\Rightarrow$ last row of $Q_i^T A_i Q_i$ closer to λe_n^T
i.e. tiny in first $n-1$ entries
close to λ on diagonal



Where do we get approx eval?

Ma221 Lecture 9 Segment 8

where do we get shift σ_i:
an approximate eigenvalue?

Since we expect $A_i(n,n) \to$ eval

use $\sigma_i = A_i(n,n)$

Get asymptotic quadratic convergence

$$\|A_i(n,1:n-1)\| = \varepsilon << 1$$

$$|A_i(n,n) - \lambda_k| = O(\varepsilon)$$

By previous analysis

$\|A_i(n,1:n-1)\|$ will get multiplied by

$$|\lambda_k - \sigma_i| / \min_{j \neq k} |\lambda_j - \sigma_i| = O(\varepsilon)$$

So on next iteration

$$\|A_i(n,1:n-1)\| = O(\varepsilon^2)$$

(matlab demo - see typed notes for code)

Ma221 Lecture 9 Segment 9

Making QR iteration Practical

1) Each iteration costs one QR fact. + 1 matmul $= O(n^3)$. Constant # of iterations per eval $\Rightarrow$ cost $O(n^4)$
Want total cost of $O(n^3)$

2) How to shift to converge to complex eval of real matrix, i.e. real Schur form?

3) How to decide convergence?

4) How to minimize data movement?

Answers:

(1) preprocess $A = QHQ^T$ where Q orthog and H upper Hessenberg

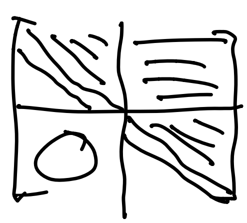

zero below first subdiagonal

QR iteration on H keeps it upper Hessenberg $\Rightarrow$ cost $= O(n^2)$
$\Rightarrow$ cost $O(n)$ iterations $= O(n^3)$

If $A = A^T$, then $H = H^T \Rightarrow H$ tridiagonal
$\Rightarrow$ cost one QR iteration $O(n)$ (Chap 5)

(2) Real Schur form: since evals of real matrices either real or complex conjugate pairs, take 2 consecutive QR iterations with shifts σ and $\bar{\sigma}$; merging these 2 iterations, all imaginary parts cancel, final result real; avoid computing any imaginary parts

(3) Converged? look at any subdiagonal $H(i+1,i)$, set to zero when $= O(\varepsilon)\|H\|$; splits matrix into block upper Hessenberg form



apply QR iteration to diagonal blocks

If block 1×1 or 2×2, done, part of final real Schur form

(4) How to reduce data movement? No known way to attain $O\left(\frac{n^3}{\sqrt{\text{fast mem size}}}\right)$ for QR iteration

Many improvements (SIAM Linear Algebra Prize 2003, Byers/Mathias/Braman) used in LAPACK. reduces communication by constant factor, doesn't hit lower bound

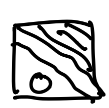
There are non-QR based algorithms that do hit lower bound in theory, do $O(n^3)$ flops (randomized algorithms) but constant in $O(n^3)$ much larger than QR iteration, so not yet practical ("Minimizing communication for Eigenproblems and SVD" at bebop.cs.berkeley.edu)

Ma221 Lecture 9 Segment 10

More detail on Hessenberg QR

How to reduce $A = QHQ^T$

$$H = Q^T A Q$$



Analogous to QR

$$\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & H^{2\times2} \end{bmatrix}
\begin{bmatrix} 1 & & 0 \\ & 1 & \\ 0 & & H^{3\times3} \end{bmatrix}
\begin{bmatrix} 1 & 0 \\ 0 & H^{4\times4} \end{bmatrix}
\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}
\begin{bmatrix} 1 & 0 \\ 0 & H^{4\times4} \end{bmatrix}
\begin{bmatrix} 1 & & 0 \\ & 1 & \\ 0 & & H^{3\times3} \end{bmatrix}
\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & H^{2\times2} \end{bmatrix}$$

$$H$$

Code:

for $i = 1$ to $n-2$ ... zero out $A(i+2:n, i)$

$v = \text{House}(A(i+1:n, i))$

$A(i+1:n, i:n) = A(i+1:n, i:n) - 2v(v^T A(i+1:n, i:n))$

$A(1:n, i+1:n) = A(1:n, i+1:n) - 2(A(1:n, i+1:n) \cdot v) \cdot v^T$

Cost: $\frac{10}{3} n^3 + O(n^2)$ just for H

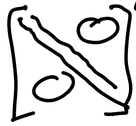
or $\frac{14}{3} n^3 + O(n^2)$ to get Q

Lot more than LU or QR, cheapest part of algorithm

When $A = A^T$ then Hessenberg $H = QAQ^T$ also symmetric $\Rightarrow$ tridiagonal T

process called tridiagonal reduction (used in Chap 5)

SVD: similar, but different orthog matrices on left and right:

$Q_L A Q_R^T = B =$  bidiagonal

$$Q_{Lk} Q_{L3} Q_{L2} Q_{L1} \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix} Q_{R1}^T Q_{R2}^T Q_{R3}^T$$

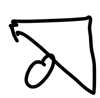
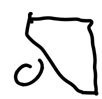
QR iteration on upper Hessenberg matrix

Lemma: Hessenberg form is maintained by QR iteration

proof A upper Hessenberg $\Rightarrow A - \sigma I$ is too

$A - \sigma I = QR$, Q upper Hessenberg

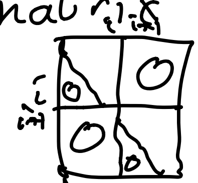
(i^{th} column of Q linear combination of columns $1 \cdots i$ of $A - \sigma I$)

then $R \cdot Q =$   also upper Hessenberg

How to do one step of QR iteration with shift on $H = A - \sigma I$ in $O(n^2)$, not $O(n^3)$

Def: an upper Hessenberg matrix unreduced if all $H(i+1,i)$ nonzero.

Other wise, if $H(i+1,i)=0$, matrix is block upper triangular



run QR on 2 diagonal blocks separately

Implicit Q Thm: suppose $Q^T A Q$ upper Hessenberg and unreduced. Then columns 2 through n of Q are uniquely determined (up to factor ± 1) by column 1 of Q

1 step of QR iteration in $O(n^2)$ flops:

$A - \sigma I = QR$, so first column of Q proportional to 1st column of A:

$$\begin{bmatrix} A(1,1)-\sigma \\ A(2,1) \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Let Q_1 be Givens rotation s.t.

$$\text{first col of } Q \longrightarrow Q_1^T \begin{bmatrix} A(1,1)-\sigma \\ A(2,1) \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} x \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$Q_1^T A Q_1 = Q_1^T \begin{bmatrix} x & x & x & x & x \\ \oplus & x & x & x & x \\ + & x & x & x & x \\ & & x & x & x \\ & & & x & x \end{bmatrix} Q_1$$

"bulge"

$$\begin{bmatrix} x & x & x & x & x \\ \oplus & x & x & x & x \\ \oplus & x & x & x & x \\ & \oplus & x & x & x \\ & & \oplus & x & x \end{bmatrix}$$

"chasing the bulge"

all zero $\Rightarrow$ upper Hessenberg

cost $= O(n^2)$

Proof of Implicit Q Theorem

Let q_i be column i of Q

$$Q^T A Q = H \Rightarrow AQ = QH$$

Column 1: $Aq_1 = H(1,1)\cdot q_1 + H(2,1)\cdot q_2$

$\Rightarrow$ determines $H(1,1)$, $H(2,1)$, q_2 via QR on

$$[q_1, Aq_1] = [q_1, q_2]\begin{bmatrix} 1 & H(1,1) \\ 0 & H(2,1) \end{bmatrix}$$

More generally suppose we have $q_2, q_3 \cdots q_i$ and columns $1:i-1$ of H. Get next column

$$Aq_i = \sum_{j=1}^{i+1} q_j H(j,i) \quad \text{from } AQ = QH$$

$$q_j^T A q_i = H(j,i) \text{ for } j = 1 \text{ to } i$$

$$Aq_i - \sum_{j=1}^{i} q_j H(j,i) = q_{i+1} H(i+1,i)$$

gives us q_{i+1} and $H(i+1,i)$.

This is in LAPACK xGEES (Schur form) or xGEEV (for evecs), used in eig() in Matlab