

C S C I 5304

Fall 2021

COMPUTATIONAL ASPECTS OF MATRIX THEORY

Class time: MW 4:00 - 5:15 pm : Keller 3-230 or Online Room Instructor **Daniel Boley**

Lecture notes:

http://www-users.cselabs.umn.edu/classes/Fall-2021/csci5304/

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EIGENVALUE PROBLEMS

- Background on eigenvalues/ eigenvectors / decompositions
- Perturbation analysis, condition numbers..
- Power method
- The QR algorithm
- Practical QR algorithms: use of Hessenberg form and shifts
- The symmetric eigenvalue problem.

Eigenvalue Problems. Introduction

Let A an $n \times n$ real nonsymmetric matrix. The eigenvalue problem:

 $Ax = \lambda x$

 $\lambda \in \mathbb{C}$: eigenvalue $x \in \mathbb{C}^n$: eigenvector

Types of Problems:

- Compute a few λ_i 's with smallest or largest real parts;
- Compute all λ_i 's in a certain region of \mathbb{C} ;
- Compute a few of the dominant eigenvalues;
- Compute all λ_i 's.

Eigenvalue Problems. Their origins

- ullet Structural Engineering $[Ku = \lambda Mu]$
- Stability analysis [e.g., electrical networks, mechanical system,..]
- Bifurcation analysis [e.g., in fluid flow]
- Electronic structure calculations [Schrödinger equation..]
- Application of new era: page ranking on the world-wide web.

GvL 7.1-7.4,7.5.2 - Eigen

GvL 7.1-7.4,7.5.2 - Eigen

Basic definitions and properties

A complex scalar λ is called an eigenvalue of a square matrix A if there exists a nonzero vector u in \mathbb{C}^n such that $Au = \lambda u$. The vector u is called an eigenvector of A associated with λ . The set of all eigenvalues of A is the 'spectrum' of A. Notation: $\Lambda(A)$.

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Basic definitions and properties (cont.)

➤ An eigenvalue is a root of the Characteristic polynomial:

$$p_A(\lambda) = \det(A - \lambda I)$$

- \triangleright So there are n eigenvalues (counted with their multiplicities).
- ightharpoonup The multiplicity of these eigenvalues as roots of p_A are called algebraic multiplicities.
- The geometric multiplicity of an eigenvalue λ_i is the number of linearly independent eigenvectors associated with λ_i .

- $m{\lambda}$ is an eigenvalue iff the columns of $A-\lambda I$ are linearly dependent.
- \triangleright ... equivalent to saying that its rows are linearly dependent. So: there is a nonzero vector w such that

$$w^H(A - \lambda I) = 0$$

- ightharpoonup w is a left eigenvector of A (u= right eigenvector)
- $ightharpoonup \lambda$ is an eigenvalue iff $\overline{\det(A-\lambda I)}=0$

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- ➤ Geometric multiplicity is ≤ algebraic multiplicity.
- An eigenvalue is simple if its (algebraic) multiplicity is one.
- ➤ It is semi-simple if its geometric and algebraic multiplicities are equal.

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GvL 7.1-7.4,7.5.2 – Eiger

∠ Consider

$$A = \begin{pmatrix} 1 & 2 & -4 \\ 0 & 1 & 2 \\ 0 & 0 & 2 \end{pmatrix}$$

Eigenvalues of A? their algebraic multiplicities? their geometric multiplicities? Is one a semi-simple eigenvalue?

Same questions if, in addition, a_{12} is replaced by zero.

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Transformations that preserve eigenvectors

Shift $B = A - \sigma I$: $Av = \lambda v \iff Bv = (\lambda - \sigma)v$ eigenvalues move, eigenvectors remain the same.

Polynomial $B=p(A)=lpha_0I+\cdots+lpha_nA^n$: $Av=\lambda v \Longleftrightarrow Bv=p(\lambda)v$ eigenvalues transformed, eigenvectors remain the same.

Invert $B = A^{-1}$: $Av = \lambda v \iff Bv = \lambda^{-1}v$ eigenvalues inverted, eigenvectors remain the same.

Shift & $B=(A-\sigma I)^{-1}$: $Av=\lambda v \iff Bv=$ Invert $(\lambda-\sigma)^{-1}v$ eigenvalues transformed, eigenvectors remain the same. spacing between eigenvalues can be radically changed.

ightharpoonup Two matrices A and B are similar if there exists a nonsingular matrix X such that

$$A = XBX^{-1}$$

- $ightharpoonup Av = \lambda v \iff B(X^{-1}v) = \lambda(X^{-1}v)$ eigenvalues remain the same, eigenvectors transformed.
- \triangleright Issue: find X so that B has a simple structure

Definition: A is diagonalizable if it is similar to a diagonal matrix

- ightharpoonup THEOREM: A matrix is diagonalizable iff it has n linearly independent eigenvectors
- > ... iff all its eigenvalues are semi-simple
- \triangleright ... iff its eigenvectors form a basis of \mathbb{R}^n

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THEOREM (Schur form): Any matrix is unitarily similar to a triangular matrix, i.e., for any \boldsymbol{A} there exists a unitary matrix \boldsymbol{Q} and an upper triangular matrix \boldsymbol{R} such that

$$A = QRQ^H$$

- Any Hermitian matrix is unitarily similar to a real diagonal matrix, (i.e. its Schur form is real diagonal).
- \blacktriangleright It is easy to read off the eigenvalues (including all the multiplicities) from the triangular matrix R
- ➤ Eigenvectors can be obtained by back-solving

GvL 7.1-7.4,7.5.2 – Eigen

GvL 7.1-7.4,7.5.2 - Eigen

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Schur Form - Proof

Show that there is at least one eigenvalue and eigenvector of A: $Ax = \lambda x$, with $||x||_2 = 1$

There is a unitary transformation P such that $Px=e_1$. How do you define P?

- Show that $PAP^H = \left(rac{\lambda \mid **}{0 \mid A_2}
 ight)$.

- Another proof altogether: use Jordan form of $m{A}$ and QR factorization

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➤ More refined result: Gerschgorin

THEOREM [Gerschgorin]

$$orall \; \lambda \; \in \Lambda(A), \quad \exists \; i \; \; \mathsf{such \; that} \; \; |\lambda - a_{ii}| \leq \sum_{\substack{j=1 \ j
eq i}}^{j=n} |a_{ij}| \; .$$

In words: eigenvalue λ is located in one of the closed discs of the complex plane centered at a_{ii} and with radius $ho_i = \sum_{j \neq i} |a_{ij}|$.

Localization theorems and perturbation analysis

- \triangleright Localization: where are the eigenvalues located in \mathbb{C} ?
- \triangleright Perturbation analysis: If A is perturbed how does an eigenvalue change? How about an eigenvector?
- ➤ Also: sensitivity of an eigenvalue to perturbations
- ➤ Next result is a "localization" theorem
- ➤ We have seen one such result before. Let ||.|| be a matrix norm.

Then:

$$\forall \ \lambda \in \Lambda(A) : |\lambda| \le ||A||$$

ightharpoonup All eigenvalues are located in a disk of radius $\|A\|$ centered at 0.

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Proof: By contradiction. If contrary is true then there is one eigenvalue λ that does not belong to any of the disks, i.e., such that $|\lambda - a_{ii}| > \rho_i$ for all i. Write matrix $A - \lambda I$ as:

$$A - \lambda I = D - \lambda I - [D - A] \equiv (D - \lambda I) - F$$

where D is the diagonal of A and -F=-(D-A) is the matrix of off-diagonal entries. Now write

$$A - \lambda I = (D - \lambda I)(I - (D - \lambda I)^{-1}F).$$

From assumptions we have $\|(D-\lambda I)^{-1}F\|_{\infty} < 1$. (Show this). The Lemma in P. 5-3 of notes would then show that $A-\lambda I$ is nonsingular – a contradiction \square

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GvL 7.1-7.4,7.5.2 – Eigen

Gerschgorin's theorem - example

Find a region of the complex plane where the eigenvalues of the following matrix are located:

$$A = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 2 & 0 & 1 \\ -1 & -2 & -3 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 & -4 \end{pmatrix}$$

GvL 7.1-7.4,7.5.2 – Eige

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one eigenvalue

GvL 7.1-7.4.7.5.2 - Eigen

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Refinement: if disks are all disjoint then each of them contains

Refinement: can combine row and column version of the theorem

(column version: apply theorem to A^H).

Bauer-Fike theorem

THEOREM [Bauer-Fike] Let $\tilde{\lambda}$, \tilde{u} be an approximate eigenpair with $\|\tilde{u}\|_2=1$, and let $r=A\tilde{u}-\tilde{\lambda}\tilde{u}$ ('residual vector'). Assume A is diagonalizable: $A=XDX^{-1}$, with D diagonal. Then

$$\exists \; \lambda \in \; \Lambda(A) \;\; ext{ such that } \;\; |\lambda - ilde{\lambda}| \leq \mathsf{cond}_2(X) \|r\|_2 \;.$$

Very restrictive result - also not too sharp in general.

Alternative formulation. If E is a perturbation to A then for any eigenvalue $\tilde{\lambda}$ of A+E there is an eigenvalue λ of A such that:

$$|\lambda - ilde{\lambda}| \leq \mathsf{cond}_2(X) \|E\|_2$$
 .

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GvL 7.1-7.4,7.5.2 – Eigen

Conditioning of Eigenvalues

 \triangleright Assume that λ is a simple eigenvalue with right and left eigenvectors u and w^H respectively. Consider the matrices:

$$A(t) = A + tE$$

Eigenvalue $\lambda(t)$. Eigenvector u(t).

Conditioning of λ of A relative to E is $\left|\frac{d\lambda(t)}{dt}\right|_{t=0}$.

- $ightarrow rac{\lambda(t) \lambda}{t} w^H u(t) = w^H E u(t)$
- Take the limit at t=0, $\lambda'(0)=rac{w^HEu}{mHe}$
- Note: the left and right eigenvectors associated with a simple eigenvalue cannot be orthogonal to each other.
- Actual conditioning of an eigenvalue, given a perturbation "in the direction of E" is $|\lambda'(0)|$.
- In practice only estimate of ||E|| is available, so

$$|\lambda'(0)| \leq rac{\|Eu\|_2 \|w\|_2}{|(u,w)|} \leq \|E\|_2 rac{\|u\|_2 \|w\|_2}{|(u,w)|}$$

Write

 $A(t)u(t) = \lambda(t)u(t)$

Then multiply both sides to the left by w^H

$$egin{aligned} w^H(A+tE)u(t) &= \lambda(t)w^Hu(t) &
ightarrow \ \lambda(t)w^Hu(t) &= w^HAu(t) + tw^HEu(t) \ &= \lambda w^Hu(t) + tw^HEu(t). \end{aligned}$$

Definition. The condition number of a simple eigenvalue λ of an arbitrary matrix A is defined by

$$\mathsf{cond}(\pmb{\lambda}) = rac{1}{\cos heta(u,w)}$$

in which u and w^H are the right and left eigenvectors, respectively. associated with λ .

Example: Consider the matrix

$$A = \begin{pmatrix} -149 & -50 & -154 \\ 537 & 180 & 546 \\ -27 & -9 & -25 \end{pmatrix}$$

 $ightharpoonup \Lambda(A) = \{1,2,3\}$. Right and left eigenvectors associated with $\lambda_1 = 1$:

$$u = egin{pmatrix} 0.3162 \\ -0.9487 \\ 0.0 \end{pmatrix} \quad ext{and} \quad w = egin{pmatrix} 0.6810 \\ 0.2253 \\ 0.6967 \end{pmatrix}$$

So:

 $cond(\lambda_1) \approx 603.64$

 \blacktriangleright Perturbing a_{11} to -149.01 yields the spectrum:

 $\{0.2287, 3.2878, 2.4735\}.$

> as expected..

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GVL 7.1-7.4,7.5.2 – Eiger

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For Hermitian (also normal matrices) every simple eigenvalue is

well-conditioned, since cond(λ) = 1.

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$Perturbations\ with\ Multiple\ Eigenvalues\ -\ Example$

- Worst case perturbation is in 3,1 position: set $A_{31} = \epsilon$.
- $m ilde{p}$ Eigenvalues of perturbed A are the roots of $p(\mu) = (\mu-1)^3 4 \cdot \epsilon.$
- $\mu_k = 1 + (4\epsilon)^{1/3} \ e^{rac{2ki\pi}{3}}, \quad k = 1, 2, 3$
- \blacktriangleright Hence eigenvalues of perturbed A are $1+O(\sqrt[3]{\epsilon})$.
- If index of eigenvalue (dimension of largest Jordan block) is k, then an $O(\epsilon)$ perturbation to A leads to $O(\sqrt[k]{\epsilon})$ change in eigenvalue. Simple eigenvalue case corresponds to k=1.

Basic algorithm: The power method

- ightharpoonup Basic idea is to generate the sequence of vectors $A^k v_0$ where $v_0
 eq 0$ then normalize.
- Most commonly used normalization: ensure that the largest component of the approximation is equal to one.

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GvL 7.1-7.4,7.5.2 - Eigen

The Power Method

- 1. Choose a nonzero initial vector $v^{(0)}$.
- 2. For $k = 1, 2, \ldots$, until convergence, Do:
- 3. $lpha_k = \operatorname*{argmax}_{i=1,...,n} |(Av^{(k-1)})_i|$ 4. $v^{(k)} = \frac{1}{lpha_k} Av^{(k-1)}$
- 5. EndDo
- $\operatorname{argmax}_{i=1,...n}|\mathbf{x}_i| \equiv \text{the component } x_i \text{ with largest modulus}$

Proof in the diagonalizable case.

- $m{v}^{(k)}$ is = vector $m{A}^k m{v}^{(0)}$ normalized by a certain scalar $\hat{m{lpha}}_k$ in such a way that its largest component is 1.
- Decompose initial vector $v^{(0)}$ in the eigenbasis as:

$$v^{(0)} = \sum_{i=1}^n \gamma_i u_i$$

Each u_i is an eigenvector associated with λ_i .

Convergence of the power method

THEOREM Assume there is one eigenvalue λ_1 of A, s.t. $|\lambda_1| >$ $|\lambda_i|$, for $j \neq i$, and that λ_1 is semi-simple. Then either the initial vector $v^{(0)}$ has no component in $\operatorname{Null}(A-\lambda_1 I)$ or $v^{(k)}$ converges to an eigenvector associated with λ_1 and $\alpha_k \to \lambda_1$.

ightharpoonup Note that $A^k u_i = \lambda_i^k u_i$

$$egin{aligned} v^{(k)} &= rac{1}{scaling} \, imes \, \sum_{i=1}^n \lambda_i^k \gamma_i u_i \ &= rac{1}{scaling} \, imes \, \left[\lambda_1^k \gamma_1 u_1 + \sum_{i=2}^n \lambda_i^k \gamma_i^k u_i
ight] \ &= rac{1}{scaling'} \, imes \, \left[u_1 + \sum_{i=2}^n \left(rac{\lambda_i}{\lambda_1}
ight)^k rac{\gamma_i}{\gamma_1} u_i
ight] \end{aligned}$$

- Second term inside bracket converges to zero. QED
- Proof suggests that the convergence factor is given by

$$ho_D = rac{|\lambda_2|}{|\lambda_1|}$$

where λ_2 is the second largest eigenvalue in modulus.

GvL 7.1-7.4,7.5.2 - Eigen

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Example: Consider a 'Markov Chain' matrix of size n=55. Dominant eigenvalues are $\lambda=1$ and $\lambda=-1$ the power method applied directly to A fails. (Why?)

We can consider instead the matrix I+A The eigenvalue $\lambda=1$ is then transformed into the (only) dominant eigenvalue $\lambda=2$

The second	NI C I.CC	Б	F: 1
Iteration	Norm of diff.	Res. norm	Eigenvalue
20	0.639D-01	0.276D-01	1.02591636
40	0.129D-01	0.513D-02	1.00680780
60	0.192D-02	0.808D-03	1.00102145
80			1.00014720
100	0.400D-04	0.174D-04	1.00002078
120	0.562D-05	0.247D-05	1.00000289
140	0.781D-06	0.344D-06	1.00000040
161	0.973D-07	0.430D-07	1.00000005

GvL 7.1-7.4,7.5.2 – Eige

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- Question: What is the best shift-of-origin σ to use?
- Easy to answer the question when all eigenvalues are real.

Assume all eigenvalues are real and labeled decreasingly:

$$\lambda_1 > \lambda_2 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

Then: If we shift A to $A - \sigma I$:

The shift σ that yields the best convergence factor is:

$$\sigma_{opt} = rac{\lambda_2 + \lambda_n}{2}$$

Plot a typical convergence factor $\phi(\sigma)$ as a function of σ . Determine the minimum value and prove the above result.

The Shifted Power Method

In previous example shifted A into B=A+I before applying power method. We could also iterate with $B(\sigma)=A+\sigma I$ for any positive σ

Example: With $\sigma = 0.1$ we get the following improvement.

Iteration	Norm of diff.	Res. Norm	Eigenvalue
20			1.00524001
40			1.00016755
60	0.183D-04	0.509D-05	1.00000446
80	0.437D-06	0.118D-06	1.00000011
88	0.971D-07	0.261D-07	1.00000002

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Inverse Iteration

Observation: The eigenvectors of A and A^{-1} are identical.

- \blacktriangleright Idea: use the power method on A^{-1} .
- Will compute the eigenvalues closest to zero.
- lacksquare Shift-and-invert Use power method on $\overline{(A-\sigma I)^{-1}}$.
- \triangleright will compute eigenvalues closest to σ .
- Rayleigh-Quotient Iteration: use $\sigma = \frac{v^T A v}{v^T v}$ (best approximation to λ given v).
- Advantages: fast convergence in general.
- \blacktriangleright Drawbacks: need to factor A (or $A-\sigma I$) into LU.

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GvL 7.1-7.4,7.5.2 – Eigen