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:

$$Ax = \lambda x \quad \lambda \in \mathbb{C} : \text{eigenvalue}$$

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

Types of Problems:

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

Eigenvalue Problems. Their origins

- 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.
Basic definitions and properties

A complex scalar $\lambda$ 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 $\lambda$. The set of all eigenvalues of $A$ is the ‘spectrum’ of $A$. Notation: $\Lambda(A)$.

$\lambda$ is an eigenvalue iff the columns of $A - \lambda I$ are linearly dependent.

... equivalent to saying that its rows are linearly dependent. So: there is a nonzero vector $w$ such that

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

$w$ is a left eigenvector of $A$ ($u=$ right eigenvector)

$\lambda$ is an eigenvalue iff $\det(A - \lambda I) = 0$

Geometric multiplicity is $\leq$ algebraic multiplicity.

An eigenvalue is simple if its (algebraic) multiplicity is one.

It is semi-simple if its geometric and algebraic multiplicities are equal.

An eigenvalue is a root of the Characteristic polynomial:

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

So there are $n$ eigenvalues (counted with their multiplicities).

The multiplicity of these eigenvalues as roots of $p_A$ are called algebraic multiplicities.

The geometric multiplicity of an eigenvalue $\lambda_i$ is the number of linearly independent eigenvectors associated with $\lambda_i$.

Basic definitions and properties (cont.)
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 \( a_{33} \) is replaced by one.

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

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

Any Hermitian matrix is unitarily similar to a real diagonal matrix, (i.e. its Schur form is real diagonal).

It is easy to read off the eigenvalues (including all the multiplicities) from the triangular matrix \( R \)

Eigenvectors can be obtained by back-solving.
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 $PAP^H = \begin{pmatrix} \lambda & * \\ 0 & A_2 \end{pmatrix}$.

Apply process recursively to $A_2$.

What happens if $A$ is Hermitian?

Another proof altogether: use Jordan form of $A$ and QR factorization.

Localization: where are the eigenvalues located in $\mathbb{C}$?

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 $\| \cdot \|$ be a matrix norm.

Then:

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

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

More refined result: Gerschgorin

**THEOREM** [Gerschgorin]

$$\forall \lambda \in \Lambda(A), \exists i \text{ such that } |\lambda - a_{ii}| \leq \sum_{\substack{j=1 \atop j \neq i}}^{n} |a_{ij}| .$$

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

Proof: By contradiction. If contrary is true then there is one eigenvalue $\lambda$ 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 \(\square\)
**Gerschgorin’s theorem - example**

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

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

- Refinement: if disks are all disjoint then each of them contains one eigenvalue
- 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 \( \tilde{A} \) is diagonalizable: \( \tilde{A} = XD\tilde{X}^{-1} \), with \( D \) diagonal. Then

\[ \exists \lambda \in \Lambda(A) \quad \text{such that} \quad |\lambda - \tilde{\lambda}| \leq \text{cond}_2(X)\|r\|_2. \]

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

\[ |\lambda - \tilde{\lambda}| \leq \text{cond}_2(X)\|E\|_2. \]

- Very restrictive result - also not too sharp in general.
Assume that \( \lambda \) is a simple eigenvalue with right and left eigenvectors \( u \) and \( w^H \) respectively. Consider the matrices:

\[
A(t) = A + tE
\]

Towards the eigenvalue \( \lambda(t) \), Eigenvector \( u(t) \).

Conditioning of \( \lambda \) of \( A \) relative to \( E \) is

\[
\left| \frac{d\lambda(t)}{dt} \right|_{t=0}
\]

Write

\[
A(t)u(t) = \lambda(t)u(t)
\]

Then multiply both sides to the left by \( w^H \)

\[
w^H(A(t) + tE)u(t) = \lambda(t)w^Hu(t) \rightarrow \lambda(t)w^Hu(t) = w^HAu(t) + tw^Heu(t)
\]

\[
= \lambda w^Hu(t) + tw^Heu(t).
\]

Take the limit at \( t = 0 \),

\[
\lambda'(0) = w^Heu
\]

\[
\frac{\lambda(t) - \lambda}{t} w^Hu(t) = w^Heu(t)
\]

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

\[
|\lambda'(0)| \leq \frac{\|Eu\|_2\|w\|_2}{\|u\|_2\|w\|_2} \leq \frac{\|E\|_2\|u\|_2\|w\|_2}{\|u\|\|w\|}
\]

**Example:** Consider the matrix

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

**Definition.** The condition number of a simple eigenvalue \( \lambda \) of an arbitrary matrix \( A \) is defined by

\[
\text{cond}(\lambda) = \frac{1}{\cos \theta(u,w)}
\]

in which \( u \) and \( w^H \) are the right and left eigenvectors, respectively, associated with \( \lambda \).
\( \Lambda(A) = \{1, 2, 3\} \). Right and left eigenvectors associated with 
\( \lambda_1 = 1 \):
\[
\begin{bmatrix}
0.3162 \\
-0.9487 \\
0.0
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
0.6810 \\
0.2253 \\
0.6967
\end{bmatrix}
\]
So: \( \text{cond}(\lambda_1) \approx 603.64 \)

Perturbing \( a_{11} \) to \(-149.01\) yields the spectrum:
\( \{0.2287, 3.2878, 2.4735\} \).

as expected.

**Perturbations with Multiple Eigenvalues - Example**

Consider \( A = \begin{pmatrix} 1 & 2 & 0 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{pmatrix} \)

Worst case perturbation is in 3,1 position: set \( A_{31} = \epsilon \).

Eigenvalues of perturbed \( A \) are the roots of
\[ p(\mu) = (\mu - 1)^3 - 4 \cdot \epsilon. \]

Roots:
\[ \mu_k = 1 + (4\epsilon)^{1/3} e^{2k\pi i / 3}, \quad k = 1, 2, 3 \]

Hence eigenvalues of perturbed \( A \) are \( 1 + O(\sqrt{\epsilon}) \).

If index of eigenvalue (dimension of largest Jordan block) is \( k \), then an \( O(\epsilon) \) perturbation to \( A \) leads to \( O(\sqrt{\epsilon}) \) change in eigenvalue. Simple eigenvalue case corresponds to \( k = 1 \).

**Basic algorithm: The power method**

Basic idea is to generate the sequence of vectors \( A^k v_0 \) where
\( v_0 \neq 0 \) – then normalize.

Most commonly used normalization: ensure that the largest component of the approximation is equal to one.
The Power Method

1. Choose a nonzero initial vector $v^{(0)}$.
2. For $k = 1, 2, \ldots$, until convergence, Do:
   3. $\alpha_k = \text{argmax}_{i=1, \ldots, n} |(Av^{(k-1)})_i|$
   4. $v^{(k)} = \frac{1}{\alpha_k} Av^{(k-1)}$
5. EndDo

$\text{argmax}_{i=1, \ldots, n} |x_i| \equiv \text{the component } x_i \text{ with largest modulus}$

Convergence of the power method

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

Proof in the diagonalizable case.

- $v^{(k)}$ is = vector $A^k v^{(0)}$ normalized by a certain scalar $\hat{\alpha}_k$ 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 $\lambda_i$.

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

\[
v^{(k)} = \frac{1}{\text{scaling}} \times \sum_{i=1}^{n} \lambda_i^k \gamma_i u_i = \frac{1}{\text{scaling}} \times \left[ \lambda_1^k \gamma_1 u_1 + \sum_{i=2}^{n} \lambda_i^k \gamma_i u_i \right] = \frac{1}{\text{scaling'}} \times \left[ u_1 + \sum_{i=2}^{n} \left( \frac{\lambda_i}{\lambda_1} \right)^k \frac{\gamma_i}{\gamma_1} u_i \right]
\]
- Second term inside bracket converges to zero. QED
- Proof suggests that the convergence factor is given by
  \[ \rho_D = \frac{|\lambda_2|}{|\lambda_1|} \]
where $\lambda_2$ is the second largest eigenvalue in modulus.
**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 $\lambda = 2$.

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Norm of diff.</th>
<th>Res. norm</th>
<th>Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.639D-01</td>
<td>0.276D-01</td>
<td>1.02591636</td>
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<td>161</td>
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<td>1.00000005</td>
</tr>
</tbody>
</table>

**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 $\sigma$.

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

<table>
<thead>
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<th>Eigenvalue</th>
</tr>
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<td>88</td>
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<td>1.00000002</td>
</tr>
</tbody>
</table>

**Question:** What is the best shift-of-origin $\sigma$ 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 $\sigma$ that yields the best convergence factor is:

$$\sigma_{\text{opt}} = \frac{\lambda_2 + \lambda_n}{2}$$

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

**Inverse Iteration**

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

Idea: use the power method on $A^{-1}$.

Will compute the eigenvalues closest to zero.

Shift-and-invert Use power method on $[A - \sigma I]^{-1}$.

will compute eigenvalues closest to $\sigma$.

Rayleigh-Quotient Iteration: use $\sigma = \frac{v^T Av}{v^T v}$ (best approximation to $\lambda$ given $v$).

Advantages: fast convergence in general.

Drawbacks: need to factor $A$ (or $A - \sigma I$) into LU.