The eigenvalue problem

Def: A number $\lambda \in \mathbb{R}$ is an eigenvalue of a matrix A with eigenvector $x \in \mathbb{R}^n$ iff $Ax = \lambda x$.

Applications

1) Polynomial Equations
2) Coupled Oscillators
   (e.g. Quantum Mechanics: Schrödinger equation)

Preliminaries

To treat the problem with generality, we use the complex spaces $\mathbb{C}^n$ and $\mathbb{C}^{n \times n}$.

The vector space $\mathbb{C}^n$

Let $x, y \in \mathbb{C}^n$. The inner product is defined as

$$(x, y) = \sum_{a=1}^{n} x_a \overline{y_a}$$

and $\|x\|_2 = \sqrt{(x,x)}$. Note that

1) $(x,y) = \overline{(y,x)}$, $\forall x,y \in \mathbb{C}^n$

2) $\begin{cases} (\lambda x, y) = \lambda (x,y) \\ (x, \lambda y) = \overline{\lambda} (x,y) \end{cases}$, $\forall x,y \in \mathbb{C}^n$, $\forall \lambda \in \mathbb{C}$.

Depending on which inner product we use, we must distinguish between real orthonality and complex orthogonality.

▶ The space $\mathbb{C}^{n \times n}$

Definitions of
a) Matrix addition $(A+B)$
b) Matrix multiplication (AB)
c) Scalar product (λA)
d) Matrix-vector operation (Ax)

remain the same. However we replace the transpose operation (A^T) with the Hermitian (A^H).

Def: $B = A^H \Leftrightarrow B_{ab} = \overline{A_{ba}}$, $\forall a,b \in [n]$

Now compare the following definitions:

$$\boxed{\begin{array}{lcl} A \text{ orthogonal} & \Leftrightarrow & A^{-1} = A^T \\ A \text{ unitary} & \Leftrightarrow & A^{-1} = A^H \end{array}}$$ (complex orthonormal columns)

and

$$\boxed{\begin{array}{lcl} A \text{ symmetric} & \Leftrightarrow & A = A^T \\ A \text{ hermitian} & \Leftrightarrow & A = A^H \end{array}}$$

▸ Formal solution of eigenvalue problem

$$\begin{aligned}
\lambda \text{ eigenvalue of } A &\Leftrightarrow \exists x \in \mathbb{C}^n \setminus \{0\} : Ax = \lambda x \\
&\Leftrightarrow \exists x \in \mathbb{C}^n \setminus \{0\} : (A - \lambda I)x = 0 \\
&\Leftrightarrow A - \lambda I \text{ singular} \\
&\Leftrightarrow \det(A - \lambda I) = 0 \Leftrightarrow \cdots \Leftrightarrow \\
&\Leftrightarrow a_n \lambda^n + a_{n-1} \lambda^{n-1} + \cdots + a_1 \lambda + a_0 = 0.
\end{aligned}$$

(the characteristic polynomial of A)

The fundamental theorem of algebra guarantees the existence of n complex solutions.

Notation

The set of all eigenvalues of a matrix A is the spectrum of the matrix

$$sp(A) = \{\lambda \in \mathbb{C} \mid \exists x \in \mathbb{C} : Ax = \lambda x\}.$$

The larger in "length" eigenvalue is the spectral radius of the matrix

$$\rho(A) = \max_{\lambda \in sp(A)} |\lambda|.$$

Self-consistency properties

1) The trace of matrix A, defined as the sum of the diagonal elements satisfies:

$$\mathrm{tr} A = \sum_{a=1}^{n} A_{aa} = \sum_{a=1}^{n} \lambda_a$$

2) The determinant equals the product of the eigenvalues.

$$\det A = \prod_{a=1}^{n} \lambda_a$$

Properties of Eigenvalues

1) $\left.\begin{array}{l}\det P \neq 0 \\ B = P^{-1}AP\end{array}\right\} \Rightarrow sp(B) = sp(A)$

<u>Proof</u>

$$\begin{aligned}\det(B-\lambda I) &= \det(P^{-1}AP-\lambda I) \\ &= \det(P^{-1}(A-\lambda I)P) \\ &= \det P^{-1} \det(A-\lambda I) \det P \\ &= \det(A-\lambda I),\ \forall \lambda \in \mathbb{C} \Rightarrow sp(B) = sp(A) \quad \square\end{aligned}$$

2) The diagonal matrix

$$A = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}$$

has eigenvalues

$$sp(A) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$$

This result generalizes as follows

3) If $A \in \mathbb{C}^{n\times n}$ is partitioned as

$$A = \begin{array}{cc} \begin{bmatrix} B & D \\ 0 & C \end{bmatrix} & \begin{array}{c} p \\ q \end{array} \\ \begin{array}{cc} p & q \end{array} & \end{array}$$

with $B \in \mathbb{C}^{p\times p}$ and $C \in \mathbb{C}^{q\times q}$ then
$sp(A) = sp(B) \cup sp(C)$.

<u>Proof</u>

Let $\lambda \in sp(A)$ be given. Then

$$\exists x_1 \in \mathbb{C}^p : \exists x_2 \in \mathbb{C}^q : \begin{bmatrix} B & D \\ 0 & C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \Rightarrow$$

$$\Rightarrow \begin{cases} Bx_1 + Dx_2 = \cancel{\lambda(x_1+x_2)}\ \lambda x_1 \\ Cx_2 = \lambda x_2 \end{cases}$$

If $\left.\begin{array}{l} x_2 \neq 0 \\ Cx_2 = \lambda x_2 \end{array}\right\} \Rightarrow \lambda \in sp(C)$

If $x_2 = 0 \Rightarrow Bx_1 = \lambda x_1 \Rightarrow \lambda \in sp(B)$

Thus $\lambda \in sp(B) \vee \lambda \in sp(C) \Rightarrow \lambda \in sp(B) \cup sp(C)$

Thus $sp(A) \subseteq sp(B) \cup sp(C)$ (1)

Conversely:

$\lambda \in sp(B) \Rightarrow \exists x \in \mathbb{C}^p - \{0\} : Bx = \lambda x \Rightarrow$

$$\Rightarrow \begin{bmatrix} B & D \\ 0 & C \end{bmatrix} \begin{bmatrix} x \\ 0 \end{bmatrix} = \lambda \begin{bmatrix} x \\ 0 \end{bmatrix}$$

$$\Rightarrow \lambda \in sp(A)$$

and

$\lambda \in sp(C) \Rightarrow \exists x \in \mathbb{C}^q - \{0\} : Cx = \lambda x \Rightarrow$

$$\Rightarrow \begin{bmatrix} B & D \\ 0 & C \end{bmatrix} \begin{bmatrix} 0 \\ x \end{bmatrix} = \lambda \begin{bmatrix} 0 \\ x \end{bmatrix} \Rightarrow \lambda \in sp(A)$$

Thus $sp(A) \supseteq sp(B) \cup sp(C)$ (2)

$(1) \wedge (2) \Rightarrow \quad sp(A) = sp(B) \cup sp(C)$.

↳ An immediate consequence of this result is that the diagonal elements of an upper triangular matrix are its eigenvalues.

Orthogonal / Unitary Decompositions

(I) Schur Decomposition

<u>Thm</u>: If $A \in \mathbb{C}^{n\times n}$, then there is a $Q \in \mathbb{C}^{n\times n}$ such that

a) Q unitary

b) $Q^H A Q = T = D + N$

with $D = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_n\}$

N strictly upper triangular.

From the Schur decomposition, one finds immediately the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of A.

<u>special case</u>: A normal $\Leftrightarrow A^H A = A A^H$

A normal $\Leftrightarrow N = 0$

$\Leftrightarrow$ The Schur decomposition diagonalizes the matrix A.

A hermitian matrix $A = A^H \Rightarrow A A^H = A^H A = A^2$

$\Rightarrow A$ normal

also has diagonalized Schur decomposition.

(2) Real Schur decomposition

Thm: If $A \in \mathbb{R}^{n\times n}$, then there is an orthogonal $Q \in \mathbb{R}^{n\times n}$ such that

$$Q^T A Q = \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{22} & \cdots & R_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{mm} \end{bmatrix}$$

where each R_{aa} is either a 1×1 matrix (gives real eigenvalue) or a 2×2 matrix (gives pair of complex eigenvalues that are conjugate to each other).

For a symmetric real matrix $A = A^T$, all eigenvalues are real (i.e. $sp(A) \subseteq \mathbb{R}$) and the real Schur decomposition gives a diagonal matrix.

Because of Galois theory, it is not possible to calculate the Schur decomposition of a 5×5 or larger matrix numerically with a finite step algorithm that uses elementary operations. One uses iterative algorithms.

What about eigenvectors

Case 1: Assume all n eigenvalues are DISTINCT!

Thm: If $\lambda_1, \lambda_2, \dots, \lambda_k \in sp(A)$ are distinct, and v_m is the eigenvector of λ_m then $v_1, v_2, \dots, v_m$ are linearly independent.

- If A is also Hermitian ($A^H = A$) then $v_1, v_2, \dots, v_m$ are orthogonal.

Let $v_1, v_2, \dots, v_n$ are linearly independent eigenvectors of A. Define

$$P = [v_1 \; v_2 \cdots v_n]$$

Linear independence implies that there is P^{-1}.
Now note that

$$\begin{aligned} AP &= A[v_1 \; v_2 \cdots v_n] = [Av_1 \; Av_2 \cdots Av_n] \\ &= [\lambda_1 v_1 \; \lambda_2 v_2 \cdots \lambda_n v_n] \\ &= P \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) \Rightarrow \end{aligned}$$

$$\Rightarrow A = AI = APP^{-1} = P\,\mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)\,P^{-1}$$

$\Rightarrow$ A can be diagonalized!

Case 2 : Some eigenvalues are not distinct.

Repeated eigenvalues arise from repeates solutions of the characteristic polynomial $p(x)$

If $p(x) = (x-\lambda)^k q(x)$ and $q(\lambda) \neq 0$, then $x = \lambda$ is an eigenvalue with algebraic multiplicity k. With the eigenvalue λ we associate an invariant space S_λ defined as

$$S_\lambda = \{ x \in \mathbb{C}^n \mid Ax = \lambda x \}$$

If $\dim S_\lambda = k$ for all eigenvalues $\lambda \in sp(A)$ then A can STILL be diagonalized!

$\dim S_\lambda$ = geometric multiplicity of λ.

If there is an eigenvalue λ such that $\dim S_\lambda < k$ then we say that the matrix A is defective.

A defective matrix is usually "unphysical" and cannot be diagonalized!

The QR algorithm

To find the eigenvalues $\lambda \in sp(A)$ of a matrix A, we define the following sequance:

$$A_0 = A$$
$$A_{m-1} = Q_m R_m \quad [\text{QR decomposition of } A_{m-1}]$$
$$A_m = R_m Q_m$$

It can be shown that A will be driven to triangular form in the limit $m \to +\infty$.
Note that

$$A_m = R_m Q_m = Q_m^{-1} Q_m R_m Q_m = Q_m^{-1} A_{m-1} Q_m \Rightarrow$$
$$\Rightarrow sp(A_m) = sp(A_{m-1}).$$

Thus the diagonal elements of $\lim A_m$ are the eigenvalues of A!
What about eigenvectors? By induction we see that

$$A_m = Q_m^{-1} \cdots Q_2^{-1} Q_1^{-1} A Q_1 Q_2 \cdots Q_m$$

If A can be diagonalized, then the eigenvectors of A are given by the columns of

$$V = \lim_{n \to +\infty} \prod_{k=1}^{n} Q_k$$

One may implement this algorithm as follows:

<u>Algorithm</u> : QR iterations

```
let V = I.
do
  A = QR
  V = VQ
  B = RQ
  test = ||B - A||  (use the minimum of 1-norm
                      and ∞-norm)
  A = B
while (abs(test) > eps)
```

This algorithm works fine, it is adequate, but it slows down as $O(n^3)$ with n the size of A.

The QR algorithm with Hessenberg reduction

We use Hessenberg reduction so that each QR iteration can be done with $O(n^2)$ steps instead of $O(n^3)$.

<u>Def</u> : A matrix A is Hessenberg iff the elements bellow the subdiagonal are zero:

$$A \text{ Hessenberg} \iff \forall a, b \in [n] : a > b+1 \Rightarrow A_{ab} = 0 .$$

It is easy to prove that

<u>Prop</u> : $\left.\begin{array}{l} A \text{ Hessenberg} \\ B \text{ upper triangular} \end{array}\right\} \Rightarrow AB, BA \text{ Hessenberg}.$

<u>Thm</u> : If a matrix A is Hessenberg, then the QR iteration preserves this property.

<u>Proof</u>

Let $A_{m-1} = Q_m R_m$, and $A_m = R_m Q_m$. Then

$$A_m = R_m Q_m = R_m Q_m I = R_m Q_m R_m R_m^{-1} =$$
$$= R_m A_{m-1} R_m^{-1} \text{ , thus}$$

A_{m-1} Hessenberg $\wedge$ R_m, R_m^{-1} upper triangular $\Rightarrow$ A_m Hessenberg

The strategy therefore is to reduce A to Hessenberg form and do QR iterations on the reduced matrix.

Let $U = H_n \cdots H_2 H_1$ be a sequence of Householder transformations that reduce A to Hessenberg as follows:

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix} \xrightarrow{H_1} \begin{bmatrix} x & x & x & x \\ x & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \end{bmatrix} \xrightarrow{H_2}$$

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \end{bmatrix}$$

Then $UA = H_n H_{n-1} \cdots H_1 A$ is Hessenberg and UAU^{-1} can be shown to be Hessenberg too!

Thus: jumstart iteration with $A_0 = U$ and $V = U^{-1}$.

Let $U = H_1 H_2 \cdots H_n$ be a sequence of Householder transformations that can reduce A to Hessenberg form: $A' = U^{-1} A$:

$$\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix} \xrightarrow{H_1} \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ 0 & x & x & x & x \\ 0 & x & x & x & x \\ 0 & x & x & x & x \end{bmatrix} \xrightarrow{H_2}$$

$$\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ 0 & x & x & x & x \\ 0 & 0 & x & x & x \\ 0 & 0 & x & x & x \end{bmatrix} \xrightarrow{H_3} \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ 0 & x & x & x & x \\ 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x \end{bmatrix}$$

If $U^{-1}A$ is Hessenberg it can be shown that $U^{-1}AU$ is also Hessenberg because applying the the transformations from the other side has an effect only on the matrix elements above the diagonal. Thus, the zeroes are not affected.

The QR algorithm with Hessenberg reduction is:

Algorithm : QR iterations with Hessenberg reduction

~~let~~
$A_0 = U^{-1} A U$ (Hessenberg reduction)
let $V = U$
do
    $A = QR$
    $V = VQ$
    $B = RQ$
    $test = \|B - A\|$
    $A = B$
while $(test > eps)$

Deflation

The algorithm converges when the subdiagonal elements converge to 0. In practice there is some $\pm eps$ "noise" in the subdiagonal elements due to roundoff error.
Deflation means that we set subdiagonal elements $A_{a+1,a}$ exactly equal to zero when they satisfy:

$$|A_{a+1,a}| \leqslant c(eps)\left(|A_{aa}| + |A_{a+1,a+1}|\right)$$

for some small constant ~~eps~~ c.

Other Improvements

1) Shifted QR iteration
   a) Single shift strategy
   b) Double shift strategy
   c) Double implicit shift strategy
   - Goal is to improve rate of convergence.

2) **Balance**: Let $r_a \in \mathbb{R}^n$ be the ROWS of matrix $A \in \mathbb{R}^{n \times n}$ and $c_a \in \mathbb{R}^n$ be the COLUMNS of the same matrix. We say that A is balanced iff $\|r_a\|_\infty = \|c_a\|_\infty$, $\forall a \in [n]$.
To minimize roundoff error in the calculation of eigenvalues, one BALANCES the matrix A by setting

$$A_0 = D^{-1} A D$$

with

$$D = \operatorname{diag}\{b^{a_1}, b^{a_2}, \dots, b^{a_n}\}$$

where b is the floating point base.
A balance subroutine is available in most software packages.

Polynomial Equations

The problem is to find all $z \in \mathbb{C}$ such that

$$p(z) \equiv a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0 = 0 .$$

1) $\deg p = n =$ degree of $p(z)$
2) $\mathbb{R}[x] =$ the set of all polynomials with real coefficients $(a_k \in \mathbb{R})$
3) $\mathbb{C}[x] =$ the set of all polynomials with complex coefficients. $(a_k \in \mathbb{C})$.

Theoretical results.

1) Closed form solutions are available for $n \leq 4$
2) Galois Theory: closed form solutions are not available for $n \geq 5$.
3) Fundamental Theorem of algebra
$\forall p \in \mathbb{C}[x] : \exists z_0 \in \mathbb{C} : p(z_0) = 0$
4) Factorization theorem
$$p(z_0) = 0 \Rightarrow \exists q \in \mathbb{C}[x] : \begin{cases} p(z) = (z - z_0) q(z) \\ \deg q = \deg p - 1 \end{cases}$$

The statements 3 and 4 imply that each polynomial has n roots!
If $z_1, z_2, \dots, z_n$ all satisfy

$$p(z_k) = 0 \ , \forall k \in [n]$$

then $p(z)$ can be factored as:

$$p(z) = a_n (z - z_1)(z - z_2) \cdots (z - z_n)$$

Numerical Method

We define the matrix C as

$$C = \begin{bmatrix} 0 & 0 & \cdots & 0 & -a_0 \\ 1 & 0 & \cdots & 0 & -a_1 \\ 0 & 1 & \cdots & 0 & -a_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -a_{n-1} \end{bmatrix}$$

Then, one can show by induction that

$$\det(zI - C) = z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0 = p(z)$$

Thus,

1) The eigenvalues of the matrix C are the solutions to the equation $p(z)=0$

2) The matrix C is already Hessenberg by definition so QR iterations are efficient!

3) For a general equation

$$a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0 = 0$$

we must rewrite it as

$$z^n + \frac{a_{n-1}}{a_n} z^{n-1} + \cdots + \frac{a_1}{a_n} z + \frac{a_0}{a_n} = 0$$

Before constructing the matrix C.