

Lecture #15: Hermitian and Normal Matrix Eigenvalue Problems

I. Hermitian Eigenvalue Problems

A. Important Properties of Hermitian Matrices and Hermitian Operators.

1. If H is a linear Hermitian operator on a Hilbert space:

- The eigenvalues of H are real.
- The eigenfunctions corresponding to different eigenvalues are orthogonal.
- The eigenfunctions of a Hermitian operator form a complete set.

2. Proof of real eigenvalues:

a. Let H be Hermitian matrix with eigenvalues λ_i and λ_j and corresponding eigenvectors $|c_i\rangle$ and $|c_j\rangle$

b. Thus $H|c_i\rangle = \lambda_i|c_i\rangle$ $H|c_j\rangle = \lambda_j|c_j\rangle$

c. Multiply by $\langle c_j|$ and $\langle c_i|$

$$\langle c_j|H|c_i\rangle = \lambda_i \langle c_j|c_i\rangle \quad \langle c_i|H|c_j\rangle = \lambda_j \langle c_i|c_j\rangle$$

d. Complex conjugate second equation.

$$\text{LHS } \langle c_i|H|c_j\rangle^* = \langle H|c_j|c_i\rangle = \langle c_j|H^\dagger|c_i\rangle = \langle c_j|H|c_i\rangle$$

$$\text{RHS } [\lambda_j \langle c_i|c_j\rangle]^* = \lambda_j^* \langle c_j|c_i\rangle$$

e. Thus $\langle c_j|H|c_i\rangle = \lambda_i \langle c_j|c_i\rangle$ and $\langle c_j|H|c_i\rangle = \lambda_j^* \langle c_j|c_i\rangle$

f. If $i=j$, then $\langle c_i|c_i\rangle > 0$, so $\lambda_i = \lambda_i^* \Rightarrow \boxed{\lambda_i \text{ is real}}$

3. Proof of orthogonal eigenvectors:

a. Subtract eqs in 2e. above: $(\lambda_i - \lambda_j^*) \langle c_j|c_i\rangle = (\lambda_i - \lambda_j) \langle c_j|c_i\rangle = 0$

b. Thus, if $\lambda_i \neq \lambda_j$, then $\langle c_j|c_i\rangle = 0 \Rightarrow \boxed{\text{Eigenvectors are orthogonal}}$

I. A. (Continued)

4. Degenerate eigenvalues: Note that if $\lambda_i = \lambda_j$ (degenerate eigenvalues), we cannot state anything about orthogonality.
 - a. But, for m degenerate eigenvalues, the eigenvectors span an m -dimensional manifold.
 - b. We can always use Gram-Schmidt orthogonalization to generate a set of orthogonal eigenvectors spanning the m -dimensional manifold.
5. Thus, since an $n \times n$ Hermitian matrix has n eigenvectors, and we can make an orthonormal set of eigenvectors, that set spans the space of the matrix \Rightarrow Complete set.
 - a. We can write any vector as a linear combination of basis vectors.
6. These properties are true for Hermitian matrices as well as Hermitian linear operators on a Hilbert space.

B. Hermitian Matrix Diagonalization

1. An alternative approach to solving matrix eigenvalue problems is to diagonalize the matrix, since diagonal elements are the eigenvalues.
2. The eigenvalues of a matrix remain unchanged under unitary transformation.
 - a. Proof:
 - i. $\tilde{H} \tilde{c} = \lambda \tilde{c} \Rightarrow \tilde{U} H (\tilde{U}^{-1} \tilde{U}) \tilde{c} = \lambda \tilde{U} \tilde{c} \Rightarrow \underbrace{(\tilde{U} H \tilde{U}^{-1})}_{\tilde{H}'} (\underbrace{\tilde{U} \tilde{c}}_{\tilde{c}'}) = \lambda (\tilde{U} \tilde{c})$
 $\tilde{H}' \tilde{c}' = \lambda \tilde{c}'$
3. Any Hermitian matrix can be diagonalized by a unitary transformation, with its eigenvalues as the diagonal elements.

I. B. (Continued)

Homes ③

4. NOTE: are diagonalized

a. $(\underline{U} \underline{H} \underline{U}^{-1}) (\underline{U} \underline{c}_i) = \lambda_i (\underline{U} \underline{c}_i)$ b. Thus $\underline{U} \underline{c}_i = \hat{\underline{e}}_i$ for λ_i
 (Unit vector)

$$\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 1 \text{ (ith row)} \\ \vdots \\ 0 \end{pmatrix} = \lambda_i \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

c. So $\underline{c}_i = \underline{U}^{-1} \hat{\underline{e}}_i$

d. So, Column vectors of \underline{U}^{-1} are normalized eigenvectors of \underline{H}

where \underline{U} is the unitary transformation that makes \underline{H} diagonal.

5. Additional consequences for Hermitian Matrices:

a. Determinant of a Hermitian matrix is the product of its eigenvalues

b. Trace of a Hermitian matrix is the sum of its eigenvalues

c. Note that both these quantities are invariant under unitary transformation.

6. Ex: Find Diagonalizing Unitary Matrix, \underline{U}

a. $\underline{H} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}$ b. Same example from Lect #14, with eigenvectors $\underline{c}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, $\underline{c}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$, $\underline{c}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

c. Therefore $\underline{U}^{-1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix} \Rightarrow \underline{U} = (\underline{U}^{-1})^\dagger = (\underline{U}^{-1})^\dagger = \begin{pmatrix} 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} = \underline{U}$

d. You may verify that

$$\underline{U} \underline{H} \underline{U}^{-1} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

e. $\text{trace}(\underline{H}) = 2$

$\text{det}(\underline{H}) = -2$

7a. In practice, we want to diagonalize a matrix when we do not know eigenvalues.

b. Sophisticated numerical methods for solving very large matrices ($n \geq 10^6$) by successive approximations (Jacobi method, etc.).

8. Hermitian matrices \underline{A} & \underline{B} have a complete set of eigenvectors in common if and only if they commute,
 $[\underline{A}, \underline{B}] = 0$.

a. NOTE: \underline{A} & \underline{B} need not have the same eigenvalues.

9. Spectral Decomposition of a Hermitian Matrix

a. Set of eigenvalues of a matrix \underline{H} is called its spectrum.

b. Spectral Decomposition.

$$\underline{H} = \sum_n |\underline{c}_n\rangle \lambda_n \langle \underline{c}_n| \quad \text{where } \underline{c}_n \text{ satisfies } \underline{H}\underline{c}_n = \lambda_n \underline{c}_n \text{ and } \langle \underline{c}_n | \underline{c}_n \rangle = 1.$$

c. NOTE: If $\underline{H}\underline{c}_n = \lambda_n \underline{c}_n$, then $\underline{H}^m \underline{c}_n = (\lambda_n)^m \underline{c}_n$.

i. Thus, all positive powers of \underline{H} have same eigenvectors!

ii. Therefore, for any function that has a power series expansion.

$$F(\underline{H}) = \sum_n |\underline{c}_n\rangle F(\lambda_n) \langle \underline{c}_n| \quad \text{Express function in terms of eigenvalues!}$$

iii. Also $\underline{H}^{-1} \underline{c}_n = \frac{1}{\lambda_n} \underline{c}_n \Rightarrow$ Negative powers of \underline{H} have same eigenvectors also!

C. Bands on Expectation Values

1. Let us evaluate $\langle H \rangle = \langle \Psi | H | \Psi \rangle$ for normalized function

$\Psi = \sum_m a_m \phi_m$ and $H = \sum_n |\phi_n\rangle \lambda_n \langle \phi_n|$ expressed in orthonormal basis ϕ_i

$$2. H|\Psi\rangle = \left(\sum_n |\phi_n\rangle \lambda_n \langle \phi_n| \right) \left(\sum_m a_m |\phi_m\rangle \right) = \sum_{nm} \underbrace{\langle \phi_n | \phi_m \rangle}_{=\delta_{nm}} a_m \lambda_n |\phi_n\rangle = \sum_n a_n \lambda_n |\phi_n\rangle$$

3. $\langle \Psi | = \sum_m a_m^* \langle \phi_m |$, so

$$\langle \Psi | H | \Psi \rangle = \sum_{nm} a_m^* a_n \lambda_n \underbrace{\langle \phi_m | \phi_n \rangle}_{=\delta_{mn}} = \sum_n a_n^* a_n \lambda_n = \sum_n |a_n|^2 \lambda_n$$

I.C. (Continued)

Haves ⑤

4. NOTE: Since ψ is a normalized function,

$$\langle \psi | \psi \rangle = \sum_n |a_n|^2 = 1$$

5. Thus $\langle H \rangle$ is a weighted sum of eigenvalues, $\langle H \rangle = \sum_n |a_n|^2 \lambda_n$.

a. So $\lambda_{\min} \leq \langle H \rangle \leq \lambda_{\max}$

Finite bounds of expectation value of H depend on eigenvalues of H .

6. If all eigenvalues $\lambda_i > 0$, H is termed positive definite.

7. Singular matrix

a. If any eigenvalues of a matrix are zero, then ^{some} rows (or columns) of a matrix are linearly dependent, and matrix is singular. ($\det = 0$)

b. If $n \times n$ matrix has m zero eigenvalues, rank is $n - m$.

II. Normal Matrices

A. Basic Properties

1. Def: Normal Matrix: A matrix that commutes with its adjoint,

$$[A, A^\dagger] = 0.$$

2. All normal matrices can be diagonalized by unitary transformation.

\Rightarrow need not be Hermitian!

a. Includes Hermitian, anti-Hermitian, and unitary matrices.

3. Eigenvectors of A and A^\dagger are same for normal matrices, and eigenvalues are complex conjugates.

Proof: a. $A|x\rangle = \lambda|x\rangle \Rightarrow (A - \lambda I)|x\rangle = 0$

b. Multiply by $\langle x|(A^\dagger - \lambda^* I)$ on left: $\langle x|(A^\dagger - \lambda^* I)(A - \lambda I)|x\rangle = 0$

II. A3 (Continued)

Hases ⑥

c. Since $[A, A^\dagger] = 0$ and $[1, M] = 0$, we can exchange order of operators $\langle x | (A - \lambda 1) (A^\dagger - \lambda^* 1) | x \rangle = 0$

d. $\langle (A^\dagger - \lambda^* 1)x | (A^\dagger - \lambda^* 1)x \rangle = 0$ only if $(A^\dagger - \lambda^* 1)|x\rangle = 0$.

e. Thus $A^\dagger |x\rangle = \lambda^* |x\rangle$ Same eigenvalues
Complex conjugate eigenvalues.

4. Eigenvectors for different eigenvalues of normal matrices are orthogonal
a. Proof is essentially the same as for Hermitian matrices.

5. Complex conjugate nature of eigenvalues implies:

a. Eigenvalues of anti-Hermitian matrix are purely imaginary.

(Since $A^\dagger = -A$, then $\lambda^* = -\lambda$)

b. Eigenvalues of unitary matrix are of unit magnitude,

($U^\dagger = U^{-1} \Rightarrow \lambda^* = \frac{1}{\lambda}$, or $\lambda^* \lambda = 1$)

6. Ex: Unitary Matrix

$$a. U = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \Rightarrow \begin{vmatrix} -\lambda & 0 & 1 \\ 1 & -\lambda & 0 \\ 0 & 1 & -\lambda \end{vmatrix} = -\lambda^3 + 1 = 0 \Rightarrow \lambda^3 = 1$$

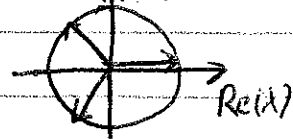
$$\Rightarrow \lambda_1 = 1, \lambda_2 = e^{2\pi i/3}, \lambda_3 = e^{-2\pi i/3}$$

b. Trace = 0

Det = +1

c. Letting $\omega = e^{2\pi i/3}$

$$\lambda_1 = 1 \quad \underline{\zeta}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \lambda_2 = \omega \quad \underline{\zeta}_2 = \begin{pmatrix} 1 \\ \omega^* \\ \omega \end{pmatrix}, \quad \lambda_3 = \omega^* \quad \underline{\zeta}_3 = \begin{pmatrix} 1 \\ \omega \\ \omega^* \end{pmatrix}$$



B. Nonnormal Matrices

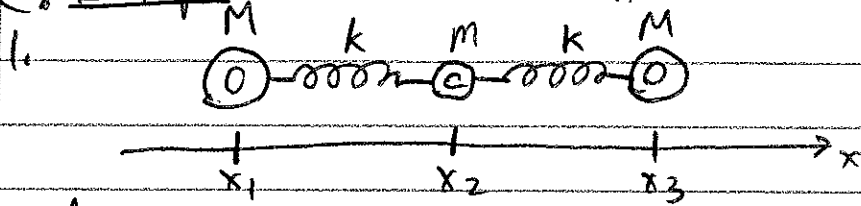
1. A^\dagger still has eigenvalues λ^* , if A has eigenvalues λ .

2. But, A and A^\dagger have neither common eigenvectors nor orthogonal eigenvectors

II. (Continued)

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C. Example: Normal Modes: Three masses on springs, CO₂



2. Assume 1D motion and Hooke's Law $F = -kx$

a. $F_1 = M \ddot{x}_1 = -k(x_1 - x_2)$

$F_2 = m \ddot{x}_2 = -k(x_2 - x_1) - k(x_2 - x_3)$

$F_3 = m \ddot{x}_3 = -k(x_3 - x_2)$

3. We want to determine normal modes of vibration, finding solutions in which all masses move with same frequency.

a. Assume $x_n = \hat{x}_n e^{-i\omega t} \Rightarrow \ddot{x}_n = \frac{d^2 x_n}{dt^2} = -\omega^2 \hat{x}_n e^{-i\omega t} = -\omega^2 x_n$

b. Thus

$$-\omega^2 x_1 = -\frac{k}{M} x_1 + \frac{k}{m} x_2$$

$$-\omega^2 x_2 = +\frac{k}{m} x_1 - \frac{2k}{m} x_2 + \frac{k}{m} x_3$$

$$-\omega^2 x_3 = \frac{k}{M} x_2 - \frac{k}{M} x_3$$

4. This can be written as a matrix eigenvalue equation,

$$\hat{A} \vec{x} = \omega^2 \vec{x}$$

$$\begin{pmatrix} \frac{k}{M} & -\frac{k}{m} & 0 \\ -\frac{k}{m} & \frac{2k}{m} & -\frac{k}{m} \\ 0 & -\frac{k}{M} & \frac{k}{M} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

5. a. $\det(\hat{A} - \omega^2 \mathbf{1}) = \omega^2 \left(\frac{k}{M} - \omega^2 \right) \left(\omega^2 - \frac{2k}{m} - \frac{k}{M} \right) = 0$

b. Eigenvalue solutions $\omega_1^2 = 0, \omega_2^2 = \frac{k}{M}, \omega_3^2 = \frac{k}{M} + \frac{2k}{m}$

6. Eigenfunctions:

a. $\omega_1^2 = 0 \Rightarrow x_1 = x_2 = x_3$ Pure translation

b. $\omega_2^2 = \frac{k}{M}$ $x_1 = -x_3, x_2 = 0$ Symmetric Stretching

c. $\omega_3^2 = \frac{k}{M} + \frac{2k}{m}$ $x_1 = x_3, x_2 = -\frac{2m}{M} x_1$ Asymmetric stretching