# 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:
   a. The eigenvalues of $H$ are real.
   b. The eigenfunctions corresponding to different eigenvalues are orthogonal.
   c. The eigenfunctions of a Hermitian operator form a complete set.

2. Proof of real eigenvalues:
   a. Let $\underset{\sim}{H}$ be Hermitian matrix with eigenvalues $\lambda_i$ and $\lambda_j$ and corresponding eigenvectors $\underset{\sim}{c}_i$ and $\underset{\sim}{c}_j$
   b. Thus
   $$H|c_i\rangle = \lambda_i |c_i\rangle \qquad H|c_j\rangle = \lambda_j |c_j\rangle$$
   c. Multiply by $\langle c_j|$ and $\langle c_i|$
   $$\langle c_j|H|c_i\rangle = \lambda_i \langle c_j|c_i\rangle \qquad \langle c_i|H|c_j\rangle = \lambda_j \langle c_i|c_j\rangle$$
   d. Complex conjugate second equation.
   $$\text{LHS } \langle c_i|H|c_j\rangle^* = \langle Hc_j|c_i\rangle = \langle c_j|H^\dagger c_i\rangle = \langle c_j|H|c_i\rangle$$
   $$\text{RHS } [\lambda_j \langle c_i|c_j\rangle]^* = \lambda_j^* \langle c_j|c_i\rangle$$
   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: $(\lambda_i - \lambda_j^*)\langle c_j|c_i\rangle = \boxed{(\lambda_i - \lambda_j)\langle c_j|c_i\rangle = 0}$ (real)
   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. <u>Degenerate eigenvalues</u>: Note that if $\lambda_i = \lambda_j$ (degenerate eigenvalues), we cannot state anything about orthogonality.
   a. But, for m degenerate eigenvalues, the eigenvectors span and m-dimensional manifold.
   b. We can always use Gram-Schmidt orthogonalization to generate a set of orthogonal eigenvectors spanning the m-dimensional manifold.

5. a. Thus, since an nxn Hermitian matrix has n eigenvectors, and we can make an orthonormal set of eigenvectors, that set spans the space of the matrix ⇒ <u>Complete set.</u>
   b. We can write <u>any vector</u> as a <u>linear combination of basis vectors.</u>

6. These properties are true for <u>Hermitian matrices</u> as well as <u>Hermitian linear operators</u> on a Hilbert space.

B. <u>Hermitian Matrix Diagonalization</u>

1. An alternative approach to solving matrix eigenvalue problems is to <u>diagonalize the matrix</u>, since <u>diagonal elements are the eigenvalues.</u>

2. $\boxed{\text{The eigenvalues of a matrix remain unchanged under unitary transformation.}}$
   a. <u>Proof:</u>
      i. $\underset{\sim}{H}\underset{\sim}{c} = \lambda \underset{\sim}{c} \quad \Rightarrow \underset{\sim}{U}\,\underset{\sim}{H}(\underset{\sim}{U}^{-1}\underset{\sim}{U})\underset{\sim}{c} = \lambda\, \underset{\sim}{U}\underset{\sim}{c} \Rightarrow (\underset{\sim}{U}\underset{\sim}{H}\underset{\sim}{U}^{-1})(\underset{\sim}{U}\underset{\sim}{c}) = \lambda(\underset{\sim}{U}\underset{\sim}{c})$

$$\boxed{\underset{\sim}{H}'\underset{\sim}{c}' = \lambda \underset{\sim}{c}'}$$

3. $\boxed{\text{Any Hermitian matrix can be diagonalized by a unitary transformation, with its eigenvalues as the diagonal elements.}}$

4. NOTE: Once diagonalized

a. $(\underset{\approx}{U}\underset{\approx}{H}\underset{\approx}{U}^{-1})(\underset{\approx}{U}\underset{\sim}{c}_i) \quad \lambda_i(\underset{\approx}{U}\underset{\sim}{c}_i)$

$$\begin{pmatrix} \lambda_1 & & & & 0 \\ & \lambda_2 & & & \\ & & \ddots \lambda_i & & \\ 0 & & & \ddots & \lambda_n \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \lambda_i \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

ith row

b. Thus $\underset{\approx}{U}\underset{\sim}{c}_i = \underset{\sim}{\hat{e}}_i$ for $\lambda_i$ (Unit vector)

c. So $\boxed{\underset{\sim}{c}_i = \underset{\approx}{U}^{-1}\underset{\sim}{\hat{e}}_i}$

d. So, $\boxed{\text{Column vectors of } \underset{\approx}{U}^{-1} \text{ are normalized eigenvectors of } \underset{\approx}{H}}$

where $\underset{\approx}{U}$ is the unitary transformation that makes $\underset{\approx}{H}$ diagonal.

5. Additional consequences for Hermitian Matrices:

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

b. $\boxed{\text{Trace of a Hermitian matrix is the sum of its eigenvalues}}$

c. Note that both these quantities are <u>invariant</u> under <u>unitary</u> transformation.

6. <u>Ex:</u> <u>Find Diagonalizing Unitary Matrix, $\underset{\approx}{U}$.</u>

a. $\underset{\approx}{H} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

b. Same example from Lec#14, with eigenvectors $\underset{\sim}{c}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \underset{\sim}{c}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \underset{\sim}{c}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

c. Therefore $\underset{\approx}{U}^{-1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix} \Rightarrow \underset{\approx}{U} = (\underset{\approx}{U}^{+})^{+} = (\underset{\approx}{U}^{-1})^{+} = \boxed{\begin{pmatrix} 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} = \underset{\approx}{U}}$

d. You may verify that

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

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

$\det(\underset{\approx}{H}) = -2$

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

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

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

a. <u>NOTE</u>: $\underset{\approx}{A}$ & $\underset{\approx}{B}$ need <u>not</u> have the same eigenvalues.

9. <u>Spectral Decomposition of a Hermitian Matrix</u>

a. Set of eigenvalues of a matrix $\underset{\approx}{H}$ is called its <u>Spectrum</u>.

b. Spectral Decomposition.

$$\boxed{\underset{\approx}{H} = \sum_n |c_n\rangle \lambda_n \langle c_n|}$$ where $\underset{\sim}{c}_n$ satisfies $\underset{\approx}{H}\underset{\sim}{c}_n = \lambda_n \underset{\sim}{c}_n$ and $\langle c_m|c_n\rangle = 1$.

c. <u>NOTE</u>: If $\underset{\approx}{H}\underset{\sim}{c}_n = \lambda_n \underset{\sim}{c}_n$, then $\underset{\approx}{H}^m \underset{\sim}{c}_n = (\lambda_n)^m \underset{\sim}{c}_n$.

i. Thus, all positive powers of $\underset{\approx}{H}$ have <u>same eigenvectors</u>!

ii. Therefore, for any function that has a <u>power series expansion</u>,

$$f(\underset{\approx}{H}) = \sum_n |\underset{\sim}{c}_n\rangle f(\lambda_n) \langle \underset{\sim}{c}_n|$$ Express function in terms of eigenvalues!

iii. Also $$\underset{\approx}{H}^{-1} \underset{\sim}{c}_n = \frac{1}{\lambda_n} \underset{\sim}{c}_n$$ $\Rightarrow$ Negative powers of $\underset{\approx}{H}$ have <u>same eigenvectors</u> also!

## C. <u>Bounds on Expectation Values</u>

1. Let us evaluate $\langle H\rangle = \langle\psi|H|\psi\rangle$ for <u>normalized function</u> $\psi = \sum_m a_m \phi_m$ and $H = \sum_n |\phi_n\rangle \lambda_n \langle\phi_n|$ expressed in orthonormal basis $\phi_i$

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

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)

4. NOTE: Since $\psi$ 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 $\boxed{\lambda_{min} \leq \langle H \rangle \leq \lambda_{max}}$

Finite bounds of expectation value of H depend on eigenvalues of $\underset{\approx}{H}$.

6. If all eigenvalues $\lambda_i > 0$, $\underset{\approx}{H}$ 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,

$$[\underset{\approx}{A}, \underset{\approx}{A}^{\dagger}] = 0.$$

2. $\boxed{\text{All normal matrices can be diagonalized by unitary transformation.}}$

$\Rightarrow$ need not be Hermitian!

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

3. $\boxed{\text{Eigenvectors of } \underset{\approx}{A} \text{ and } \underset{\approx}{A}^{\dagger} \text{ are same for normal matrices, and eigenvalues are complex conjugates.}}$

Proof: a. $\underset{\approx}{A} | \underset{\sim}{x} \rangle = \lambda | \underset{\sim}{x} \rangle \Rightarrow (\underset{\approx}{A} - \lambda \underset{\approx}{1}) | \underset{\sim}{x} \rangle = 0$

b. Multiply by $\langle \underset{\sim}{x} | (\underset{\approx}{A}^{\dagger} - \lambda^* \underset{\approx}{1})$ on left: $\langle \underset{\sim}{x} | (\underset{\approx}{A}^{\dagger} - \lambda^* \underset{\approx}{1})(\underset{\approx}{A} - \lambda \underset{\approx}{1}) | \underset{\sim}{x} \rangle = 0$

c. Since $[A, A^\dagger]$ 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 $\boxed{A^\dagger |x\rangle = \lambda^* |x\rangle}$ Same eigenvectors
Complex conjugate eigenvalues.

4. $\boxed{\text{Eigenvectors for different eigenvalues of normal matrices are orthogonal}}$

a. Proof is essentially the same as for Hermitian matrices.

5. Complex conjugate nature of eigenvalues implies:

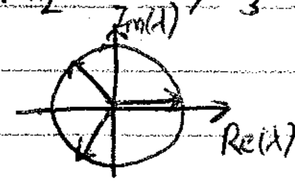
a. Eigenvalues of anti-Hermitian matrix are purely imaginary.
(Since $A^\dagger = -A$, then $\lambda^* = -\lambda$)

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 $\omega \equiv e^{2\pi i/3}$

$\lambda_1 = 1 \quad c_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \lambda_2 = \omega \quad c_2 = \begin{pmatrix} 1 \\ \omega^* \\ \omega \end{pmatrix}, \quad \lambda_3 = \omega^* \quad c_3 = \begin{pmatrix} 1 \\ \omega \\ \omega^* \end{pmatrix}$

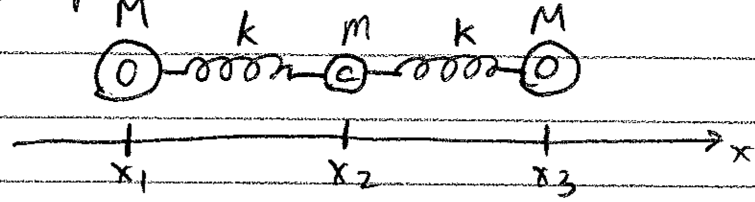
B. Nonnormal Matrices

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

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

II. (Continued) 

C. <u>Example</u>: <u>Normal Modes</u>: Three masses on springs, $CO_2$

1. 


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 <u>normal modes of vibration</u>, 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

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

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

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

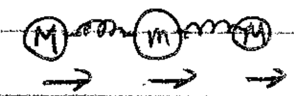
4. This can be written as a matrix eigenvalue equation,

$$\underset{\approx}{A}\,\underset{\sim}{x} = \begin{pmatrix} \frac{k}{M} & -\frac{k}{M} & 0 \\ -\frac{k}{m} & +\frac{2k}{m} & -\frac{k}{m} \\ 0 & -\frac{k}{M} & \frac{k}{M} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

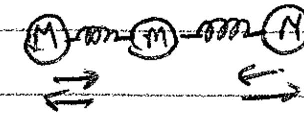
5. a. $\det(\underset{\approx}{A} - \omega^2 \underset{\approx}{1}) = \omega^2\left(\frac{k}{M} - \omega^2\right)\left(\omega^2 - \frac{2k}{m} - \frac{k}{M}\right) = 0$

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

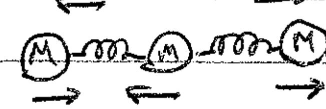
6. Eigenfunctions:

   a. $\boxed{\omega_1^2 = 0} \Rightarrow \boxed{x_1 = x_2 = x_3}$ 

Pure translation

   b. $\boxed{\omega_2^2 = \frac{k}{M}}$ $\boxed{\begin{matrix} x_1 = -x_3 \\ x_2 = 0 \end{matrix}}$ 

Symmetric Stretching

   c. $\boxed{\omega_3^2 = \frac{k}{M} + \frac{2k}{m}}$ $\boxed{\begin{matrix} x_1 = x_3 \\ x_2 = -\frac{2M}{m} x_1 \end{matrix}}$ 

Asymmetric Stretching