

Lecture #14 Transformations, Invariants, and Matrix Eigenvalue Problems

I. Transformations of Operators

A. Unitary Transformations

1. Unitary transformations describe the transformation of a linear operator from orthonormal basis to another.

2. How do operators undergo the corresponding transformation?

a. An operator expanded in  $\phi$  basis has the form  $A = \sum_{mn} |\phi_m\rangle a_{mn} \langle \phi_n|$

b. Insert resolutions of identity in  $\phi'$  basis  $A = \sum_{mnpq} |\phi'_p\rangle \underbrace{\langle \phi'_p | \phi_m \rangle}_{\text{Identity}} a_{mn} \underbrace{\langle \phi_n | \phi'_q \rangle}_{\text{Identity}} \langle \phi'_q|$

c. Remembering  $U_{pm} = \langle \phi'_p | \phi_m \rangle$  and  $U_{qn}^* = \langle \phi_n | \phi'_q \rangle$ , we obtain

$$A = \sum_{mnpq} |\phi'_p\rangle U_{pm} a_{mn} U_{qn}^* \langle \phi'_q| = \sum_{pq} |\phi'_p\rangle a'_{pq} \langle \phi'_q|$$

d. So  $a'_{pq} = \sum_{mn} U_{pm} a_{mn} U_{qn}^*$  Unitary Operator Transformation

where  $U_{qn}^* = (U^\dagger)_{nq}$  Corresponds to 
 $A' = U A U^\dagger = U A U^{-1}$

3. This can also be shown for matrix representation:

a.  $A b = c \Rightarrow \underbrace{A}_{\approx} \underbrace{(U^\dagger U)}_{\approx} \underbrace{b}_{\approx} = \underbrace{c}_{\approx} \Rightarrow \underbrace{(U A U^\dagger)}_{\approx} \underbrace{(U b)}_{\approx} = \underbrace{U c}_{\approx}$

b. Since  $b' = U b$  and  $c' = U c \Rightarrow \boxed{A' b' = c'}$  where  $\boxed{A' = U A U^\dagger}$

B. Non-Unitary Transformations

1. The equivalent transformation for a non-unitary transformation  $G$  is called a similarity transformation.  $(G A G^{-1})(G b) = G c$

2. Does not describe same quantity in a different basis, but a consistently transformed quantity.

## III. Invariants

### A. Invariant Quantities

1. For physical vectors, coordinate rotations leave invariant the properties of the vectors
2. Similarly, unitary transformations preserve essential features of vector spaces
3. The relationship between quantities must be invariant under unitary transformations.

a. Take  $\underline{b} = \underline{A} \underline{c}$

b. Consider a unitary transformation  $\underline{U}$  to another orthonormal basis.

$$\underline{b}' = \underline{U} \underline{b}, \quad \underline{c}' = \underline{U} \underline{c}, \quad \underline{A}' = (\underline{U} \underline{A} \underline{U}^{-1})$$

c. Thus, check that  $\underline{b}' = \underline{A}' \underline{c}'$  remains satisfied.

$$(\underline{U} \underline{b}) = (\underline{U} \underline{A} \underline{U}^{-1}) (\underline{U} \underline{c}) = \underline{U} \underline{A} (\underline{U}^{-1} \underline{U}) \underline{c} = \underline{U} \underline{A} \underline{c}$$

d. Operate on left

with  $\underline{U}^{-1} \Rightarrow (\underline{U}^{-1} \underline{U}) \underline{b} = (\underline{U}^{-1} \underline{U} \underline{A} \underline{c}) \Rightarrow \underline{b} = \underline{A} \underline{c}$

### B. Examples of Invariants

1. Ex: Scalar Product:  $\langle f | g \rangle$

a. In some orthonormal basis  $f \rightarrow \underline{a}$      $g \rightarrow \underline{b}$

$$\text{Thus } \langle f | g \rangle = \underline{a}^{\dagger} \underline{b}$$

b.  $\underline{a}' = \underline{U} \underline{a}$  and  $\underline{b}' = \underline{U} \underline{b}$  (Unitary transform from  $\phi_i$  to  $\phi_i'$ )

c. Check  $\langle f | g \rangle$  in  $\phi_i'$  basis.

$$\langle f | g \rangle = (\underline{a}')^{\dagger} \underline{b}' = (\underline{U} \underline{a})^{\dagger} (\underline{U} \underline{b}) = \underline{a}^{\dagger} (\underline{U}^{\dagger} \underline{U}) \underline{b} = \underline{a}^{\dagger} \underline{b} \Rightarrow \text{Invariant!}$$

2. Ex: Expectation Value  $\langle A \rangle$

a. Take  $\psi = \sum c_i \phi_i$  so that  $\langle \psi | A | \psi \rangle \Rightarrow \underline{c}^{\dagger} \underline{A} \underline{c}$

b.  $(\underline{c}')^{\dagger} \underline{A}' \underline{c}' = (\underline{U} \underline{c})^{\dagger} (\underline{U} \underline{A} \underline{U}^{-1}) (\underline{U} \underline{c}) = \underline{c}^{\dagger} (\underline{U}^{\dagger} \underline{U}) \underline{A} (\underline{U}^{-1} \underline{U}) \underline{c} = \underline{c}^{\dagger} \underline{A} \underline{c} \checkmark$



### III.A (Continued)

Haves (4)

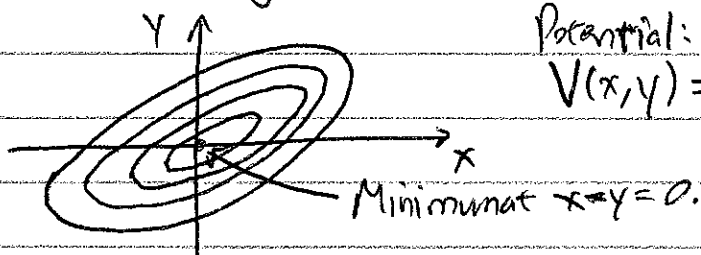
4. a. Operator is linear, operating on elements of a Hilbert space  
 b. Thus, operator and function can be expanded in a basis

⇒ This leads to a Matrix Eigenvalue Equation  
 ⇒ equivalent to original problem.

c. Properties of Matrix influence nature of solutions (e.g. Hermitian)

### B. Matrix Eigenvalue Problems: Example: Particle in Ellipsoidal Basin

1.



Potential:

$$V(x,y) = ax^2 + bxy + cy^2$$

2. Find positions in which trajectory is toward minimum

a.  $F_x = -\frac{\partial V}{\partial x} = -2ax - by$        $F_y = -\frac{\partial V}{\partial y} = -bx - 2cy$

b. Force will be in direction of origin when  $\frac{F_x}{F_y} = \frac{x}{y}$ .

3. Matrix Eq for Force,  $\underline{f}$ :  $\underline{f} = \begin{pmatrix} F_x \\ F_y \end{pmatrix} = \begin{pmatrix} -2a & -b \\ -b & -2c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \underline{H} \underline{r}$

4. Condition  $\frac{F_x}{F_y} = \frac{x}{y}$  is equivalent to  $\underline{f} \propto \underline{r}$ . Thus

$$\underline{f} = \underline{H} \underline{r} = \lambda \underline{r}$$

a.  $\underline{H}$  is known matrix  
 b.  $\lambda$  and  $\underline{r}$  are unknown.

5. Convert to homogeneous system of linear equations:

$$(\underline{H} - \lambda \underline{1}) \underline{r} = 0$$

a. From Chap 2, unique solution  $\underline{r} = 0$  unless  $\det(\underline{H} - \lambda \underline{1}) = 0$ .

b. Solve for values of  $\lambda$  that cause  $\det(\underline{H} - \lambda \underline{1}) = 0$ .

$$\det(\underline{H} - \lambda \underline{1}) = \begin{vmatrix} h_{11} - \lambda & h_{12} \\ h_{21} & h_{22} - \lambda \end{vmatrix} = \boxed{(h_{11} - \lambda)(h_{22} - \lambda) - h_{12}h_{21} = 0.}$$

Scalar/Characteristic Equation

III. B5 (Continued)  $\leftarrow$  eigenvalue, its associated eigenvector  $H$  has (5)  
 c. Once a solution  $\lambda$  is obtained, solve for  $\vec{v}$

6. Numerical Example: Take  $a=1$ ,  $b=\sqrt{5}$ ,  $c=3$

a. 
$$H = \begin{pmatrix} -2 & +\sqrt{5} \\ +\sqrt{5} & -6 \end{pmatrix}$$

b. 
$$\det(H - \lambda I) = \begin{vmatrix} -2-\lambda & \sqrt{5} \\ \sqrt{5} & -6-\lambda \end{vmatrix} = \lambda^2 + 8\lambda + 7 = 0$$
  

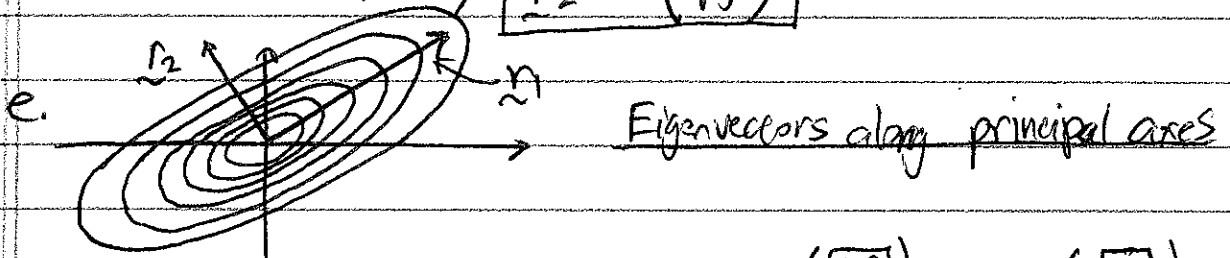
$$(\lambda+1)(\lambda+7) = 0 \Rightarrow \lambda = \begin{cases} -1 \\ -7 \end{cases}$$
 Eigenvalues

c. Eigenvector  $\vec{v}_1$  for  $\lambda = -1$ :  $\begin{pmatrix} -1 & \sqrt{5} \\ \sqrt{5} & -5 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$

ii.  $-x + \sqrt{5}y = 0$  Same Solution  
 $\sqrt{5}x - 5y = 0 \Rightarrow x = \sqrt{5}y$

iii. 
$$\vec{v}_1 = C \begin{pmatrix} \sqrt{5} \\ 1 \end{pmatrix}$$
  $C$  is arbitrary,  $\vec{v}_1$  defines direction!

d. Similarly, for  $\lambda = -7$ , 
$$\vec{v}_2 = C' \begin{pmatrix} -1 \\ \sqrt{5} \end{pmatrix}$$

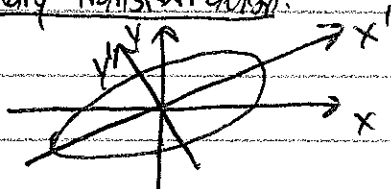


f. Normalize Eigenvectors to unity.  $\vec{v}_1 = \begin{pmatrix} \sqrt{5/6} \\ \sqrt{1/6} \end{pmatrix}$ ,  $\vec{v}_2 = \begin{pmatrix} -\sqrt{1/6} \\ \sqrt{5/6} \end{pmatrix}$

7. General Properties of Solution:

- a. Number of eigenvalues equal to dimension of matrix  $H$ .  
 From Fundamental Thm of Algebra:  $n$  degree equation has  $n$  roots.
- b. Eigenvalues are real
- c. Eigenvectors are orthogonal (proportional to eigenvalues!)

8. Unitary Transformation:



$$V = \frac{1}{2}(x')^2 + \frac{1}{2}(y')^2$$
  
 where 
$$\vec{v}' = U \vec{v} = \begin{pmatrix} \sqrt{5/6} & \sqrt{1/6} \\ \sqrt{1/6} & -\sqrt{5/6} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

### III. C. Block Diagonal Matrix: Example

Expand by minors!

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$$1. H = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix} \Rightarrow \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & 2-\lambda \end{vmatrix} = (2-\lambda) \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = (2-\lambda)(\lambda^2-1) = 0$$

Eigenvalues  $\lambda=2, \lambda=1, \lambda=-1$

2. Eigenvector for  $\lambda=2$ :

$$a. \begin{cases} -2c_1 + c_2 = 0 \\ c_1 - 2c_2 = 0 \\ 0 = 0 \end{cases} \Rightarrow \begin{cases} c_1 = \frac{1}{2}c_2 \\ c_1 = 2c_2 \end{cases} \Rightarrow \begin{cases} c_1 = c_2 = 0 \\ c_3 \text{ is arbitrary} \end{cases}$$

b. Thus  $\underline{c}_1 = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}$  for  $\lambda_1 = 2$

3. Eigenvector for  $\lambda=1$ :

$$a. \begin{cases} -c_1 + c_2 = 0 \\ c_1 - c_2 = 0 \\ c_3 = 0 \end{cases} \Rightarrow \begin{cases} c_1 = c_2 \\ c_1 = c_2 \\ c_3 = 0 \end{cases} \Rightarrow \begin{cases} c_1 = c_2 \\ c_3 = 0 \end{cases}$$

b. Thus  $\underline{c}_2 = \begin{pmatrix} c \\ c \\ 0 \end{pmatrix}$  for  $\lambda_2 = +1$

4. Similarly, we obtain  $\underline{c}_3 = \begin{pmatrix} c \\ -c \\ 0 \end{pmatrix}$  for  $\lambda_3 = -1$

5. NOTE: Block diagonal matrix separated into two problems:

- $\lambda_1$  and  $\underline{c}_1$
  - $\lambda_2, \underline{c}_2$  and  $\lambda_3, \underline{c}_3$
- } uncoupled.

### D. Degenerate Eigenvalues: Example

1. When secular equation has a multiple root, eigensystem is degenerate.

$$2. H = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \Rightarrow \begin{vmatrix} -\lambda & 0 & 1 \\ 0 & 1-\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = \lambda^2(1-\lambda) - (1-\lambda) = (\lambda^2-1)(1-\lambda) = 0$$

$$\Rightarrow \lambda_1 = -1, \lambda_2 = +1, \lambda_3 = +1$$

degenerate

3. Non-degenerate eigenvalue,  $\lambda = -1$ .

a.  $c_1 = -c_3, c_2 = 0 \Rightarrow \underline{c}_1 = c \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$

### III. D. (Continued)

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4. Degenerate eigenvalue,  $\lambda_2 = \lambda_3 = +1$

$$\begin{aligned} \text{a. } -c_1 + c_3 &= 0 \\ 0 &= 0 \\ c_1 - c_3 &= 0 \end{aligned}$$

$$\boxed{\begin{aligned} c_1 &= c_3 \\ c_3 &\text{ has any value} \end{aligned}}$$

→ Corresponds to eigenvectors on a 2D manifold.

$$\text{b. } \lambda = +1 \quad \underline{\xi} = \begin{pmatrix} c \\ c' \\ c \end{pmatrix} \quad \text{where } c \text{ \& } c' \text{ are independent.}$$

$$\text{c. Choose } \boxed{\lambda_2 = +1 \quad \underline{\xi}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad \lambda_3 = +1 \quad \underline{\xi}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}$$

d. Can use the Gram-Schmidt process to ensure that  $\underline{\xi}_2$  and  $\underline{\xi}_3$  are orthogonal.