Lecture #14 Transformations, Invariants, and Matrix Eigenvalue Problems

I. Transformations of Operators

A. Unitary Transformations

1. Unitary transformations describe the transformation of a function from orthonormal basis to another.
2. How do operators undergo the corresponding transformation?
   a. An operator expanded in ϕ basis has the form $A = \sum_{mn} |\phi_m\rangle a_{mn} \langle \phi_n|$
   b. Insert resolutions of identity in ϕ' basis $A = \sum_{mnpq} \underbrace{|\phi'_p\rangle\langle\phi'_p|}_{\text{Identity}}\phi_m\rangle a_{mn} \langle\phi_n\underbrace{|\phi'_q\rangle\langle\phi'_q|}_{\text{Identity}}$
   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 $U^*_{qn} = (U^\dagger)_{nq}$ $\xRightarrow{\text{Corresponds to}}$ $\boxed{\underset{\approx}{A}' = \underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^\dagger = \underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{-1}}$
3. This can also be shown for matrix representation:
   a. $\underset{\approx}{A}\,\underset{\sim}{b} = \underset{\sim}{c} \implies \underset{\approx}{A}(\underset{\approx}{U}^{-1}\underset{\approx}{U})\underset{\sim}{b} = \underset{\sim}{c} \Rightarrow (\underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{\dagger})(\underset{\approx}{U}\,\underset{\sim}{b}) = \underset{\approx}{U}\,\underset{\sim}{c}$
   b. Since $\underset{\sim}{b}' = \underset{\approx}{U}\,\underset{\sim}{b}$ and $\underset{\sim}{c}' = \underset{\approx}{U}\,\underset{\sim}{c}$ $\Rightarrow \boxed{\underset{\approx}{A}'\underset{\sim}{b}' = \underset{\sim}{c}'}$ where $\boxed{\underset{\approx}{A}' = \underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{-1}}$

B. Non-Unitary Transformations

1. The equivalent transformation for a non-unitary transformation $\underset{\approx}{G}$ is called a similarity transformation $(\underset{\approx}{G}\,\underset{\approx}{A}\,\underset{\approx}{G}^{-1})(\underset{\approx}{G}\,\underset{\sim}{b}) = \underset{\approx}{G}\,\underset{\sim}{c}$
2. Does not describe same quantity in a different basis, but a consistently transformed quantity.

II. Invariants

A. Invariant Quantities

1. For physical vectors, coordinate rotations leave invariant the properties of the vectors
2. Similarly, unitary transformation preserve essential features of vector spaces
3. The relationship between quantities <u>must be invariant</u> under unitary transformations.
   a. Take $\underset{\sim}{b} = \underset{\approx}{A}\,\underset{\sim}{c}$
   b. Consider a unitary transformation $\underset{\approx}{U}$ to another orthonormal basis.
   $$\underset{\sim}{b}' = \underset{\approx}{U}\,b \;,\; \underset{\sim}{c}' = \underset{\approx}{U}\,\underset{\sim}{c} \;,\; \underset{\approx}{A}' = (\underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{-1})$$
   c. Thus, check that $\underset{\sim}{b}' = \underset{\approx}{A}'\,\underset{\sim}{c}'$ remains satisfied.
   $$(\underset{\approx}{U}\,\underset{\sim}{b}) = (\underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{-1})(\underset{\approx}{U}\,\underset{\sim}{c}) = \underset{\approx}{U}\,\underset{\approx}{A}\,\cancelto{1}{(\underset{\approx}{U}^{-1}\underset{\approx}{U})}\,\underset{\sim}{c} = \underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\sim}{c}$$
   d. Operate on left with $\underset{\approx}{U}^{-1}$ $\Rightarrow (\underset{\approx}{U}^{-1}\underset{\approx}{U})\underset{\sim}{b} = (\underset{\approx}{U}\,\underset{\approx}{U}^{-1})\underset{\approx}{A}\,\underset{\sim}{c} \Rightarrow \boxed{\underset{\sim}{b} = \underset{\approx}{A}\,\underset{\sim}{c}}$

B. Examples of Invariants

1. <u>Ex:</u> Scalar Product: $\langle f|g\rangle$
   a. In some orthonormal basis $f \to \underset{\sim}{a}$ $\quad g \to \underset{\sim}{b}$
   Thus $\langle f|g\rangle = \underset{\sim}{a}^{\dagger}\,\underset{\sim}{b}$
   b. $\underset{\sim}{a}' = \underset{\approx}{U}\,\underset{\sim}{a}$ and $\underset{\sim}{b}' = \underset{\approx}{U}\,\underset{\sim}{b}$ (Unitary transform from ϕ_i to ϕ_i')
   c. Check $\langle f|g\rangle$ in ϕ_i' basis.
   $$\langle f|g\rangle = (\underset{\sim}{a}')^{\dagger}\,\underset{\sim}{b}' = (\underset{\approx}{U}\,\underset{\sim}{a})^{\dagger}(\underset{\approx}{U}\,\underset{\sim}{b}) = \underset{\sim}{a}^{\dagger}\underbrace{(\underset{\approx}{U}^{\dagger}\underset{\approx}{U})}_{=\underset{\approx}{U}^{-1}\underset{\approx}{U}=1}\underset{\sim}{b} = \underset{\sim}{a}^{\dagger}\,\underset{\sim}{b} \Rightarrow \text{Invariant!}$$

2. <u>Ex:</u> Expectation Value $\langle A\rangle$
   a. Take $\psi = \sum_i c_i \phi_i$ so that $\langle\psi|A|\psi\rangle \Rightarrow \underset{\sim}{c}^{\dagger}\,\underset{\approx}{A}\,\underset{\sim}{c}$
   b. $(\underset{\sim}{c}')^{\dagger}\,\underset{\approx}{A}'\,\underset{\sim}{c}' = (\underset{\approx}{U}\,\underset{\sim}{c})^{\dagger}(\underset{\approx}{U}\,\underset{\approx}{A}\,\underset{\approx}{U}^{-1})(\underset{\approx}{U}\,\underset{\sim}{c}) = \underset{\sim}{c}^{\dagger}(\underset{\approx}{U}^{\dagger}\underset{\approx}{U})\underset{\approx}{A}(\underset{\approx}{U}^{-1}\underset{\approx}{U})\underset{\sim}{c} = \boxed{\underset{\sim}{c}^{\dagger}\,\underset{\approx}{A}\,\underset{\sim}{c}}$ ✓

II. B. (Continued)

3. Both the trace of a matrix and the determinant are also invariant under unitary transformations.

III. Eigenvalue Problems

A. Eigenvalue Equations

1. In physics, many problems can be cast in the form

$$\underbrace{A}_{\text{linear operator}} \psi = \underbrace{\lambda}_{\text{constant}} \psi \leftarrow \text{function}$$

Known → a. Operator A leaves ψ unchanged except for scale factor λ.

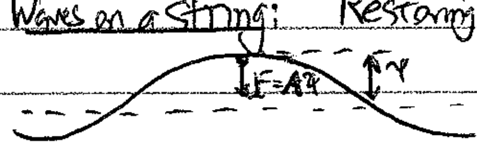
⇒ Eigenvalue equation Eigen → "It's own"

Unknown → b. Eigenfunction, ψ

Unknown → c. Eigenvalue, λ

2. Examples:

a. Waves on a string: Restoring Force $A\psi$, displacement ψ



b. Angular Momentum of Rigid Body: $\underset{\sim}{L} = \underset{\approx}{I}\,\underset{\sim}{\omega}$ ← Moment of Inertia

i. Axes for $\underset{\sim}{L}$ & $\underset{\sim}{\omega}$ are coincident, so $\underset{\sim}{L} = \lambda \underset{\sim}{\omega} \Rightarrow \boxed{\underset{\approx}{I}\,\underset{\sim}{\omega} = \lambda \underset{\sim}{\omega}}$

c. Time Independent Schrödinger Eq: $\underbrace{H}_{\text{Hamiltonian}}|\psi\rangle = \underbrace{E}_{\text{Energy}}|\psi\rangle$ ← Wave function

3. Eigenvalue equations can be expressed in orthonormal basis ϕ_i

a. Vector ψ: $\psi = \sum_i c_i \phi_i$ where $c_i = \langle \phi_i | \psi \rangle \rightarrow \underset{\sim}{c}$

b. Operator: $a_{ij} = \langle \phi_i | A | \phi_j \rangle$ defined elements of $\underset{\approx}{A}$

c. Matrix Eigenvalue Equation $\underset{\approx}{A}\,\underset{\sim}{c} = \underbrace{\lambda}_{\text{eigenvalue}} \underset{\sim}{c}$ ← eigenvector

↓

Defines eigenfunction

$\psi_i = \sum_i c_i \phi_i$

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

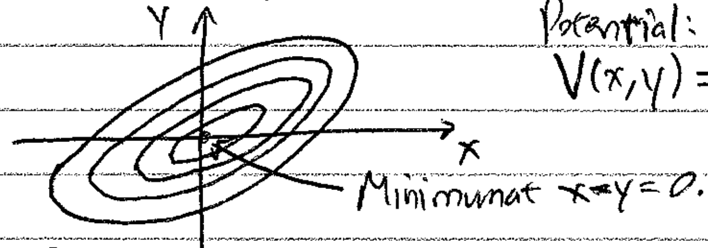
$\Rightarrow$ This leads to a <u>Matrix Eigenvalue Equation</u>

$\Rightarrow$ equivalent to original problem.

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

B. <u>Matrix Eigenvalue Problems: Example: Particle in Ellipsoidal Basin</u>

1.



Potential:

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

2. Find positions in which trajectory is toward minimum
 a. $F_x = \frac{-\partial V}{\partial x} = -2ax - by \qquad F_y = -\frac{\partial V}{\partial y} = -bx - 2cy$
 b. Force will be in direction of origin when $\frac{F_x}{F_y} = \frac{x}{y}$.

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

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

$$\underset{\sim}{f} = \boxed{\underset{\approx}{H}\,\underset{\sim}{r} = \lambda\,\underset{\sim}{r}}$$

 a. $\underset{\approx}{H}$ is known matrix
 b. λ and $\underset{\sim}{r}$ are unknown.

5. Convert to homogeneous system of linear equations:

$$(\underset{\approx}{H} - \lambda\underset{\approx}{1})\underset{\sim}{r} = 0$$

 a. From Chap 2, unique solution $\underset{\sim}{r} = 0$ <u>unless</u> $\det(\underset{\approx}{H} - \lambda\underset{\approx}{1}) = 0$.
 b. Solve for values of λ that cause $\det(\underset{\approx}{H} - \lambda\underset{\approx}{1}) = 0$.

$$\det(\underset{\approx}{H} - \lambda\underset{\approx}{1}) = \begin{vmatrix} h_{11}-\lambda & h_{12} \\ h_{21} & h_{22}-\lambda \end{vmatrix} = \underbrace{\boxed{(h_{11}-\lambda)(h_{22}-\lambda) - h_{12}h_{21} = 0.}}_{\text{Secular/Characteristic Equation}}$$

III. B5 (Continued)

c. Once a solution λ is obtained, solve for $\underset{\sim}{r}$ — eigenvalue, its associated eigenvector Hmes ⑤

6. <u>Numerical Example</u>: Take $a=1,\ b=-\sqrt{5},\ c=3$

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

b. $$\det(\underset{\sim}{H}-\lambda\underset{\sim}{1})=\begin{vmatrix}-2-\lambda & +\sqrt{5}\\ \sqrt{5} & -6-\lambda\end{vmatrix}=\underbrace{\lambda^2+8\lambda+7=0}_{(\lambda+1)(\lambda+7)=0}\Rightarrow \boxed{\lambda=\begin{cases}-1\\-7\end{cases}}$$

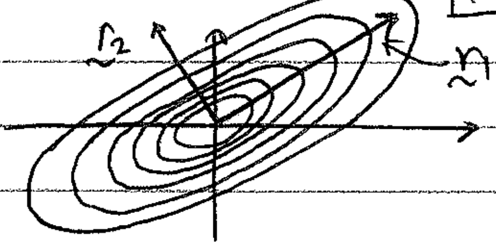
Eigenvalues

c. <u>Eigenvector r_1 for $\lambda=-1$</u>: i. $$\begin{pmatrix}-1 & \sqrt{5}\\ \sqrt{5} & -5\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}=0$$

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

iii. $\boxed{\underset{\sim}{r}_1=C\begin{pmatrix}\sqrt{5}\\ 1\end{pmatrix}}$ C is arbitrary, $\underset{\sim}{r}_1$ defines direction!

d. Similarly, for $\lambda=-7$, $\boxed{\underset{\sim}{r}_2=C'\begin{pmatrix}-1\\ \sqrt{5}\end{pmatrix}}$

e. 

<u>Eigenvectors along principal axes</u>

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

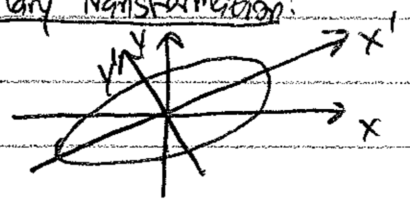
7. <u>General Properties of Solution</u>:

a. <u>Number of eigenvalues</u> equal to dimension of matrix $\underset{\sim}{H}$.
From <u>Fundamental Thm of Algebra</u>: n degree equation has n roots.

b. Eigenvalues are <u>real</u>

c. Eigenvectors are <u>orthogonal</u>

8. <u>Unitary Transformation</u>:



proportional to eigenvalues!

$$V=\frac{1}{2}(x')^2+\frac{7}{2}(y')^2$$

where $$\underset{\sim}{r}'=\underset{\sim}{U}\underset{\sim}{r}=\begin{pmatrix}\sqrt{5/6} & \sqrt{1/6}\\ \sqrt{1/6} & -\sqrt{5/6}\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}$$

III. C. Block Diagonal Matrix: Example

Expand by minors!

1. $\underset{\sim}{H} = \left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 2 \end{array}\right) \Rightarrow \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & 2-\lambda \end{vmatrix} = (2-\lambda)\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = (2-\lambda)(\lambda^2-1) = 0$

Eigenvalues $\boxed{\lambda=2,\ \lambda=1,\ \lambda=-1}$

2. Eigenvector for $\lambda = 2$:

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

b. Thus $\boxed{\underset{\sim}{c}_1 = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} \text{ for } \lambda_1 = 2}$

3. Eigenvector for $\lambda = 1$:

a. $-c_1 + c_2 = 0 \quad c_1 = c_2$
$c_1 - c_2 = 0 \quad c_1 = c_2$
$c_3 = 0 \quad c_3 = 0$
$\Rightarrow \boxed{c_1 = c_2,\ c_3 = 0}$

b. Thus $\boxed{\underset{\sim}{c}_2 = \begin{pmatrix} c \\ c \\ 0 \end{pmatrix} \text{ for } \lambda_2 = +1}$

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

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

a. λ_1 and $\underset{\sim}{c}_1$
b. $\lambda_2, \underset{\sim}{c}_2$ and $\lambda_3, \underset{\sim}{c}_3$
} Uncoupled.

D. Degenerate Eigenvalues: Example

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

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

$\Rightarrow \lambda_1 = -1, \underbrace{\lambda_2 = +1,\ \lambda_3 = +1}_{\text{degenerate}}$

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

a. $C_1 = -C_3,\ C_2 = 0 \Rightarrow \underset{\sim}{c}_1 = C\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$

III. D. (Continued)

4. <u>Degenerate eigenvalue</u>, $\lambda_2 = \lambda_3 = +1$

a. $-c_1 + c_3 = 0$

$0 = 0$

$c_1 - c_3 = 0$

$\boxed{\begin{array}{l} c_1 = c_3 \\ c_2 \text{ has any value} \end{array}}$ → Corresponds to eigenvectors on a 2D manifold.

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

c. Chose $\boxed{\lambda_2 = +1 \quad \underset{\sim}{c}_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \qquad \lambda_3 = +1 \quad \underset{\sim}{c}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}$

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