Computing eigenvalues & eigenvectors :

Let V be an n-dimensional complex vector space & A be a general linear operator on V. We would like to find all the Eigenvectors & Eigenvalues of A

$$A|\alpha\rangle = \lambda_\alpha |\alpha\rangle$$

Rewrite, in orthonormal basis $\{|e_i\rangle\}$, as

$$A = A_{ij}|e_i\rangle\langle e_j| \quad ; \quad |\alpha\rangle = \alpha_k |e_k\rangle$$

$$0 = (A - \lambda_\alpha \mathbb{1})|\alpha\rangle = (A_{ij} - \lambda_\alpha \delta_{ij})|e_i\rangle\langle e_j| \cdot \alpha_k |e_k\rangle$$

$$= (A_{ij} - \lambda_\alpha \delta_{ij})|e_i\rangle \alpha_k \delta_{jk} = \left\{(A_{ij} - \lambda_\alpha \delta_{ij})\alpha_j\right\}\underbrace{|e_i\rangle}$$

$$\Rightarrow \quad 0 = \sum_{j=1}^{n}(A_{ij} - \lambda_\alpha \delta_{ij})\alpha_j \quad \forall \; i = 1, 2, \ldots n$$

n homogeneous linear equations in n variables $(\alpha_1, \alpha_2, \ldots \alpha_n)$.

$\longrightarrow$ Solution exists only when

$$0 = \underbrace{\det\left[A_{ij} - \lambda_\alpha \delta_{ij}\right]}_{\substack{\text{order } n \text{ polynomial in } \lambda_\alpha \\ \text{"Characteristic polynomial" of } A.}} \equiv \det(A - \lambda_\alpha \mathbb{1})$$

Solve to get n eigenvalues of the matrix/Op. A.

✱ **Hamilton-Cayley theorem:** Let $\varphi(\lambda) = \det(A - \lambda\mathbb{1})$ be the characteristic polynomial of an $n \times n$ matrix A (or equivalently a linear operator on n dimensional vector space) then

$$\boxed{\varphi(A) = 0}$$

{ R.H.S is 0 matrix or the 0 operator

Ex.: Show this for "diagonalizable" matrices (operators).

i.e. $A = U D_A U^{-1}$ with $D_A = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$

Quick review of determinant & Inverse of matrices: $\{A_{ij}\}$

$$\det(A) = \frac{1}{n!}\epsilon^{i_1 i_2 \cdots i_n}\epsilon^{j_1 j_2 \cdots j_n} A_{i_1 j_1} A_{i_2 j_2} \cdots A_{i_n j_n}$$
$$= \epsilon^{j_1 j_2 \cdots j_n} A_{1 j_1} A_{2 j_2} \cdots A_{n j_n}$$
$$= A_{1 j_1} \cdot C_{1 j_1}$$

$\epsilon^{i_1 i_2 \cdots i_n}$ is
1. Completely antisymmetric under interchange of any two indicies.
2. $\epsilon^{123\cdots n} = +1$

$C_{1j} = \epsilon^{j j_2 \cdots j_n} A_{2j_2} A_{3j_3} \cdots A_{nj_n}$ is the Cofactor of A_{1j}

More generally $\boxed{C_{1j} = \frac{1}{(n-1)!}\epsilon^{1 i_2 i_3 \cdots i_{n-1}}\epsilon^{j j_2 \cdots j_n} A_{i_2 j_2} A_{i_3 j_3} \cdots A_{i_n j_n}}$

1. $A_{ij} C_{1j} = 0$ if $i \neq 1$
   More generally, $A_{ik} C_{jk} = \begin{cases} 0 & \text{if } i \neq l \\ \det(A) & \text{if } i = j \end{cases}$

Ex. Argue 1, 2, 3 using the antisymmetry of $\epsilon^{j_1 j_2 \cdots j_n}$

2. If $A_{ij} = \alpha A_{ik}$ or $A_{ij} = \alpha A_{kj}$ $\{\alpha \in \mathbb{C}\}$
   then $\text{Det}(A) = 0$

3. If $A_{ij} = \alpha A_{kj} + \beta A_{mj}$ $\forall\ j = 1, 2, \cdots n$; $\alpha, \beta \in \mathbb{C}$
   then $\text{Det}(A) = 0$

★ More generally, $\det(A) = 0$ if all the rows (or columns) are not linearly independent.

i.e. $A_{ij}\alpha_j = 0$ $(\beta_i A_{ij} = 0)$ has a non trivial solution

or equivalently $A.\alpha = 0$ (or $\beta^T . A = 0$)

i.e. A has a non-trivial Kernal (vectors mapped to 0-vector)

Lets see the above expression of det & Cofactor in a 3x3 example.

$$\det(A) = \det\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = a_{11}\overbrace{\left(a_{22}a_{33} - a_{32}a_{23}\right)}^{C_{11}} + a_{12}\overbrace{\left(-a_{21}a_{33} + a_{31}a_{23}\right)}^{C_{12}}$$
$$+ a_{13}\underbrace{\left(a_{21}a_{32} - a_{31}a_{22}\right)}_{C_{13}}$$

Inverse of a matrix : If $\det(A) \neq 0$ ★ $\boxed{(A^{-1})_{ij} = \dfrac{C_{ji}}{\det(A)}}$

$$(A^{-1})_{ij}\, A_{jk} = \frac{1}{\det(A)}\, C_{ji}\, A_{jk} = \frac{1}{\cancel{\det(A)}} \cdot \cancel{\det(A)}\, \delta_{ik} = \delta_{ik}$$

Example computation of Eigenvalues & Eigenvectors :

Let $A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 5 \\ 0 & 4 & 3 \end{pmatrix}$. The eigenvalues are determined from the characteristic equation

$$0 = \det(A - \lambda I_3) = \det\begin{pmatrix} 1-\lambda & 0 & 0 \\ 0 & 4-\lambda & 5 \\ 0 & 4 & 3-\lambda \end{pmatrix}$$
$$= (1-\lambda)\left((4-\lambda)(3-\lambda) - 20\right)$$
$$= (1-\lambda)(\lambda^2 - 7\lambda - 8) = (1-\lambda)(\lambda+1)(\lambda-8)$$
$$\Rightarrow \lambda = 1, -1, 8$$

To determine Eigenvector : Solve $A.\alpha = \lambda_\alpha \alpha$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 5 \\ 0 & 4 & 3 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 1\begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \left.\begin{array}{l} a = a \\ 4b + 5c = b \Rightarrow 3b = -5c \\ 4b + 3c = c \Rightarrow 4b = -2c \end{array}\right\} \Rightarrow b = c = 0 \; ; \quad \boxed{a\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 5 \\ 0 & 4 & 3 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = -1\begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{l} a = -a \Rightarrow a = 0 \\ 4b + 5c = -b \Rightarrow b = -c \\ 4b + 3c = -c \Rightarrow b = -c \end{array} \; ; \quad \boxed{c\begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 5 \\ 0 & 4 & 3 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 8\begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \left.\begin{array}{l} a = 8a \Rightarrow a = 0 \\ 4b + 5c = 8b \Rightarrow 5c = 4b \\ 4b + 3c = 8c \Rightarrow 4b = 5c \end{array}\right\} \Rightarrow c = \frac{4b}{5} \; ; \quad \boxed{b\begin{pmatrix} 0 \\ 1 \\ 4/5 \end{pmatrix}}$$

Diagonalization of Hermitian operators:

- Hermitian operators on an n-dimensional vector space have n real eigenvalues, some of which could be repeated.
- Eigenvectors corresponding to distinct Eigenvalues are always orthogonal.
- If an eigenvalue has degeneracy $\underline{m}$ then $\exists$ $\underline{m \text{ linearly independent eigenvectors}}$
  - We will not prove this formally but will see how this works in examples (in tutorial).
- Using Gram-Schmidt orthogonalization we can always construct orthonormal eigenvector in the m-dimensional Subspace as well.
- Thus, for Hermitian operators we have a set of n- orthonormal Eigenvectors which also form a Basis of V.

Q: What is the matrix representation of Hermitian operator H in the basis formed by its own orthonormal Eigenvectors?

Let $(\lambda_1, \lambda_2, \cdots \lambda_n)$ be the n eigenvalues &
$(|\alpha_1\rangle, |\alpha_2\rangle, \cdots |\alpha_n\rangle)$ be the corresponding orthonormal eigenvectors

i.e. $H|\alpha_i\rangle = \lambda_i|\alpha_i\rangle$ & $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$ $\quad i,j \in (1,2,\cdots n)$

The matrix elements of H in $\{|\alpha_i\rangle\}$ basis are then

$$H_{ij} = \langle\alpha_i|H|\alpha_j\rangle = \langle\alpha_i|\lambda_j|\alpha_j\rangle = \lambda_j\delta_{ij}$$

$$\equiv \begin{cases} \lambda_i & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases}$$

i.e. H is represented by a diagonal matrix in its own eigenvector basis (eigenbasis)

$$H \equiv \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & & \vdots \\ \vdots & & & \ddots & \\ 0 & 0 & \cdots & & \lambda_n \end{pmatrix} \quad \text{in } \{|\alpha_1\rangle, |\alpha_2\rangle, \cdots |\alpha_n\rangle\} \text{ basis.}$$

Comments :

- Note that the Eigenvalues of an operator do not depend on which basis we represent the operator in.

  ★ The equation $H|\alpha\rangle = \lambda_\alpha |\alpha\rangle$ is an abstract eqn independent of any basis!

- The equation determining the Eigenvalues of H is invariant under arbitrary change of Basis.

$$\det(H - \lambda \mathbb{1}) = 0$$

change of Basis : $H \rightarrow \tilde{H} = U H U^{-1}$

where U is any invertible matrix (i.e. $\det(U) \neq 0$)

$$\Rightarrow \det(\tilde{H} - \lambda \mathbb{1}) = \det(U H U^{-1} - \lambda U U^{-1}) = \det(U.(H - \lambda \mathbb{1}).U^{-1})$$

$$= \cancel{\det(U)}. \det(H - \lambda \mathbb{1}) . \cancel{\det(U^{-1})}$$

$$= \det(H - \lambda \mathbb{1})$$

Simultaneous Diagonalization of two (or more) operators :

We have seen above that a Hermitian operation takes a nice and simple diagonal matrix form when expressed in the basis of its own eigenvectors

Now will discuss a general condition under which two operators, say H_1 & H_2, simultaneously take diagonal matrix form.

From our above discussion it already clear that this will happen when the two operators have same eigenvectors. But this can be made sure even without computing the Eigenvectors.

★ Two operators H_1 and H_2 takes simultaneous diagonal form (Simultaneously diagonalizable) iff the commutator of H_1 & H_2 vanishes

i.e. $[H_1, H_2] \equiv H_1 H_2 - H_2 H_1 = 0$

We will show this by showing that when $[H_1, H_2] = 0$ then H_1 & H_2 have same eigenvectors & vice versa.

① When H_1 & H_2 have same eigenvectors then they commute.

$\{|\alpha_i\rangle\}_{i=1,2,\dots n}$

$$H_1|\alpha_i\rangle = \lambda_{1i}|\alpha_i\rangle$$
$$H_2|\alpha_i\rangle = \lambda_{2i}|\alpha_i\rangle$$

$$[H_1, H_2]|\alpha\rangle = (H_1H_2 - H_2H_1)\, a_i|\alpha_i\rangle = a_i(H_1H_2 - H_2H_1)|\alpha_i\rangle$$
$$= a_i(\lambda_{1i}\lambda_{2i} - \lambda_{2i}\lambda_{1i})|\alpha_i\rangle = 0$$

② When $[H_1, H_2] = 0$, we can always find an orthonormal basis which form eigenvectors for both H_1 & H_2.

Let $\{|\alpha_i\rangle\}$ be an Eigenbasis for H_1 i.e.

$$H_1|\alpha_i\rangle = \lambda_{1i}|\alpha_i\rangle \quad \forall\ i = 1, 2, \dots n$$

$$\Rightarrow \quad 0 = (H_1H_2 - H_2H_1)|\alpha_i\rangle = H_1(H_2|\alpha_i\rangle) - \lambda_{1i}(H_2|\alpha_i\rangle)$$

i.e. $$H_1(H_2|\alpha_i\rangle) = \lambda_{1i}(H_2|\alpha_i\rangle)$$

$$\Rightarrow \quad H_2|\alpha_i\rangle = \lambda_{2i}|\alpha_i\rangle \quad \forall\ i = 1, 2, \dots n$$

when $\exists$ degeneracy:

$$H_1|\alpha\rangle = \lambda_1|\alpha\rangle \quad \Rightarrow H_1(a_1|\alpha\rangle + a_2|\tilde\alpha\rangle) = \lambda_1(a_1|\alpha\rangle + a_2|\tilde\alpha\rangle)$$
$$H_1|\tilde\alpha\rangle = \lambda_1|\tilde\alpha\rangle$$

$$\left.\begin{array}{l} H_1(H_2|\alpha\rangle) = \lambda_1(H_2|\alpha\rangle) \\ H_1(H_2|\tilde\alpha\rangle) = \lambda_1(H_2|\tilde\alpha\rangle) \end{array}\right\} \Rightarrow \left.\begin{array}{l} H_2|\alpha\rangle = a|\alpha\rangle + b|\tilde\alpha\rangle \\ H_2|\tilde\alpha\rangle = \tilde a|\alpha\rangle + \tilde b|\tilde\alpha\rangle \end{array}\right]$$

Thus in $\{|\alpha\rangle, |\tilde\alpha\rangle\}$ subspace, we have

$$H_1 \equiv \lambda_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \& \quad H_2 \equiv \begin{pmatrix} a & b \\ \tilde a & \tilde b \end{pmatrix}$$

Now, we simply diagonalize H_2 by changing basis to its eigenvectors in the $\{|\alpha\rangle, |\tilde{\alpha}\rangle\}$ subspace. Let $\{|\beta\rangle, |\tilde{\beta}\rangle\}$ be the orthonormal eigenvectors of H_2 i.e.

$$H_2|\beta\rangle = \lambda_2|\beta\rangle \quad \& \quad H_2|\tilde{\beta}\rangle = \tilde{\lambda}_2|\tilde{\beta}\rangle$$

Clearly $H_1|\beta\rangle = \lambda_1|\beta\rangle$ & $H_1|\tilde{\beta}\rangle = \lambda_1|\tilde{\beta}\rangle$ since $|\beta\rangle$ & $|\tilde{\beta}\rangle$ are vectors in the $\{|\alpha\rangle, |\tilde{\alpha}\rangle\}$ subspace.

Thus we have successfully diagonalized H_1 & H_2 simultaneously!