

# Linear Algebra - Part 6: Special Square Matrices, Orthonormal basis

ChE641, IIT Kanpur

Diagonal matrix

(Square matrices)

$(N \times N)$

$$\underline{A} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}$$

$\alpha, \beta, \gamma = 1$

$$\rightarrow \underline{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\underline{A} = \text{diag}(A_{11}, A_{22}, A_{33}, \dots, A_{NN})$$

$$\underline{A}^{-1} = \text{diag}\left(\frac{1}{A_{11}}, \frac{1}{A_{22}}, \dots, \frac{1}{A_{NN}}\right)$$

If  $A$  and  $B$  are diagonal matrices, then  $AB = BA$  (Commute)

Lower and upper triangular matrices:

$$\begin{pmatrix} \circ & \circ & \circ \\ \neq 0 & \circ & \circ \\ & \circ & \circ \end{pmatrix}$$

Lower triangular matrix

$$\begin{pmatrix} \circ & \neq 0 & \\ \circ & \circ & \\ \circ & \circ & \circ \end{pmatrix}$$

upper triangular matrix

If  $\underline{A}$  is lower/upper triangular, then

$$\boxed{\det \underline{A} = A_{11} A_{22} A_{33} \dots A_{NN}}$$

Symmetric:

$$\underline{A} \rightarrow A_{ij}$$

$$\underline{A}^T = A_{ji}$$

$$\underline{A} = \underline{A}^T$$

$$A_{ij} = A_{ji}$$

$$A_{12} = A_{21}$$

$$A_{13} = A_{31}$$

$$A_{23} = A_{32}$$

$$\begin{matrix} & A_{12} & & \\ A_{21} & \begin{pmatrix} 2 & 1 & 4 \\ 1 & 3 & 5 \\ 4 & 5 & 6 \end{pmatrix} & & \end{matrix}$$

Skew (or) Anti Symmetric:

$$\underline{A} = -\underline{A}^T$$

$$A_{ij} = -A_{ji}$$

zeros in the diagonal

$$\begin{matrix} & A_{12} & A_{13} & \\ A_{21} & \begin{pmatrix} 0 & 1 & 4 \\ -1 & 0 & 5 \\ -4 & -5 & 0 \end{pmatrix} & & \end{matrix}$$

$$A_{11} = -A_{11} \rightarrow A_{11} = 0$$

$$A_{22} = -A_{22} \rightarrow A_{22} = 0$$

$$A_{NN} = -A_{NN} \rightarrow A_{NN} = 0$$

$$\text{If } A = \pm A^T$$

$$(A^{-1})^T = (A^T)^{-1} = \pm A^{-1}$$

antisymmetric

$$A = A^T$$

$$(A^T)^{-1} = A^{-1}$$

$$A = -A^T$$

$$(A^T)^{-1} = -A^{-1}$$

Any  $N \times N$  matrix  $A = \underbrace{\frac{1}{2}(A + A^T)}_{\text{Symmetric}} + \underbrace{\frac{1}{2}(A - A^T)}_{\text{antisymmetric}}$

$$A = \frac{A + A^T}{2} + \frac{A - A^T}{2}$$

Symmetric

Orthogonal Matrices.

$A$  is orthogonal:

$$(A^{-1})^T = (A^T)^{-1} = (A^{-1})^{-1}$$

$$A^T = A^{-1}$$

if  $A$  is orthogonal,  
so is its inverse!!

$$\begin{aligned} (A^{-1})^T &= (A^T)^{-1} \\ \downarrow & \\ B^T &= B^{-1} \end{aligned}$$

$$\begin{aligned} A^T &= A^{-1} \\ \Rightarrow (A^{-1})^T &= (A^T)^{-1} = A \end{aligned}$$

$$A^T = A^{-1}$$

$$A^T A = A^{-1} A$$

$$A^T A = I$$

$$\det(A^T A) = 1$$

$$\det A^T = \det A$$

$$\det(A^T) \det(A) = 1$$

$$(\det A)^2 = 1$$

$$\text{or } \det A = \pm 1$$

← orthogonal matrices

Orthogonal matrix:

let  $\underline{A}$ : orthogonal

$\underline{y} \in \text{real vector space}$

$$\underline{y} = \underline{A} \cdot \underline{x} \quad \left| \quad \underline{y}^T = \underline{x}^T \underline{A}^T$$

$$\begin{aligned} \langle \underline{y} | \underline{y} \rangle &= \underline{y}^T \underline{y} \\ &= \underline{x}^T \underline{A}^T \underline{A} \underline{x} \\ &= \underline{x}^T (\underline{A}^T \underline{A}) \underline{x} \end{aligned}$$

$\underline{y} = \underline{A} \underline{x}$  ← orthogonal

↑  
norm of  $|\underline{y}|$   
is not  
necessarily  $= |\underline{x}|$

$$\underline{y}^T \underline{y} = \underline{x}^T \underline{x}$$

$\langle \underline{y} | \underline{y} \rangle = \langle \underline{x} | \underline{x} \rangle$

$\underline{y} = \underline{A} \underline{x}$   
"pure rotation"  
↑  
orthogonal transform

Hermitian Matrix:

$$\underline{A} = \underline{A}^\dagger$$

Anti-Hermitian:  $\underline{A} = -\underline{A}^\dagger$

$$\underline{A} = \frac{1}{2} (\underline{A} + \underline{A}^\dagger) + \frac{1}{2} (\underline{A} - \underline{A}^\dagger)$$

Analogue of orthogonal matrix → "Unitary matrix"

$$\underline{A}^\dagger = \underline{A}^{-1}$$

$$\det(\underline{A}^\dagger \underline{A}) = \det(\underline{A}^\dagger) \det(\underline{A})$$

$$\det(\underline{A}^\dagger \underline{A}) = \left( \text{Abs.}(|\underline{A}^*| |\underline{A}|) \right)^2 = |\underline{A}|^* |\underline{A}|$$

$\det \underline{A} = \underline{\text{unit moduls}}$

Normal Matrices:

$$\underline{A} \underline{A}^\dagger = \underline{A}^\dagger \underline{A}$$

— A normal matrix  $\underline{A}$  commutes with its Hermitian conjugate.

examples: (1) Hermitian (symmetric)  
(2) unitary (orthogonal)

$$\underline{A} = \underline{A}^T \rightarrow \text{symmetric}$$

"Self-adjoint" ←  $\underline{A} = \underline{A}^\dagger \rightarrow \underline{\text{Hermitian matrix}}$

# Basis sets in a normed linear vector space

$$\underline{x} \in E_N$$

$E_N$ : N-dim Vec. space

$$\underline{x} = \sum_{i=1}^N x_i \underline{e}_i$$

$$\underline{e}_i = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i^{\text{th}} \text{ row}$$

$$\underline{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix} \quad \underline{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \end{bmatrix}$$

$\uparrow$

$\{\underline{e}_1, \underline{e}_2, \underline{e}_3, \dots, \underline{e}_N\} \rightarrow$  basis set in  $E_N$

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} = x_1 \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} + x_2 \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix} + \dots + x_N \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$\langle \underline{e}_i | \underline{e}_j \rangle = \delta_{ij} \quad \underline{e}_i^+ \underline{e}_j$$

$\rightarrow$  orthonormal basis

Can also use any set of L.I. vectors as a basis in  $E_N$ .

$$\underline{x} = \sum_{i=1}^N \alpha_i \underline{x}_i$$

$\{\underline{x}_i\} \rightarrow$  L.I.

$$\underline{x} = \underline{X} \cdot \underline{\alpha}$$

$$\underline{X}^{-1} \cdot \underline{x} = (\underline{X}^{-1} \underline{X}) \cdot \underline{\alpha}$$

$$\underline{\alpha} = \underline{X}^{-1} \cdot \underline{x}$$

$$\begin{bmatrix} \underline{\alpha} \\ \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix} \quad \begin{bmatrix} | & | & \dots & | \\ \underline{x}_1 & \underline{x}_2 & \dots & \underline{x}_N \\ | & | & \dots & | \end{bmatrix} = \underline{X}$$

$\swarrow$   
square

$\underline{X}^{-1}$  exists

# Gram-Schmidt Orthogonalization

$\{\underline{z}_1, \underline{z}_2, \underline{z}_3, \dots, \underline{z}_N\}$  : L.I. vectors

Can we

a set of  $N$  orthonormal vectors??

$\underline{a}, \underline{b}, \underline{c}$

$$\underline{x}_1 = \underline{a}$$

$$\underline{x}_2 = \underline{b} - \frac{(\underline{b} \cdot \underline{x}_1)}{\|\underline{x}_1\| \|\underline{x}_1\|} \underline{x}_1$$

$$\underline{x}_1 \cdot \underline{x}_2 = 0$$

$$\underline{x}_1 \cdot \underline{x}_2 = \underline{b} \cdot \underline{x}_1 - \frac{(\underline{b} \cdot \underline{x}_1)(\underline{x}_1 \cdot \underline{x}_1)}{\|\underline{x}_1\|^2} = 0$$

$\{\underline{y}_1, \dots, \underline{y}_N\}$  orthogonal

$$\underline{y}_1 = \underline{z}_1$$

$$\underline{y}_2 = \underline{z}_2 - \frac{(\underline{y}_1^T \underline{z}_2)}{\|\underline{y}_1\|^2} \underline{y}_1$$

$$\underline{y}_3 = \underline{z}_3 - \frac{(\underline{y}_1^T \underline{z}_3)}{\|\underline{y}_1\|^2} \underline{y}_1 - \frac{(\underline{y}_2^T \underline{z}_3)}{\|\underline{y}_2\|^2} \underline{y}_2$$

$$\underline{y}_N = \underline{z}_N - \sum_{j=1}^{N-1} \frac{(\underline{y}_j^T \underline{z}_N)}{\|\underline{y}_j\|^2} \underline{y}_j$$

$$\underline{y}_1^T \underline{y}_2 = 0 \quad \underline{y}_1^T \underline{y}_3 = 0 \quad \underline{y}_2^T \underline{y}_3 = 0$$

$$\underline{y}_j^T \underline{y}_i = 0 \quad i \neq j$$

$$\underline{x}_i = \frac{\underline{y}_i}{\|\underline{y}_i\|} \quad i=1 \dots N$$

$$\underline{x}_i^T \underline{x}_j = \delta_{ij}$$

ortho-normal

If  $\{\underline{x}_1, \dots, \underline{x}_N\}$  form an orthonormal basis,

$$\underline{x} = \sum_{i=1}^N \alpha_i \underline{x}_i$$

$$\underline{x}_j^T \underline{x} = \sum_{i=1}^N \alpha_i \underline{x}_j^T \underline{x}_i$$

$$\alpha_i = \underline{x}_i^T \underline{x}$$

$$\underline{x}_j^T \underline{x} = \alpha_j$$

$$\underline{x} = \sum_i \alpha_i \underline{x}_i$$

$$= \sum_i \underline{x}_i \alpha_i$$

$$\underline{x} = \sum_i \underline{x}_i \underline{x}_i^T \underline{x}$$

$$\sum_i \underline{x}_i \underline{x}_i^T = \underline{I}$$

Resolution of the identity in a given orthonormal basis

If  $\{\underline{x}_1, \underline{x}_2, \dots, \underline{x}_N\}$  is a nonorthonormal, but LI.

$$\underline{x} = \sum_{i=1}^N \alpha_i \underline{x}_i$$

$$\underline{x}_i^T \underline{x}_j \neq \delta_{ij}$$

Find "Reciprocal basis"  $\rightarrow \{\underline{z}_1, \underline{z}_2, \dots, \underline{z}_N\}$  s.t.

$$\underline{z}_i^T \underline{x}_j = \delta_{ij}$$

Geometry:

Three non-coplanar vectors  $\underline{a}, \underline{b}, \underline{c} \rightarrow \underline{b} \times \underline{c}$

$$\underline{\hat{a}} = \frac{\underline{b} \times \underline{c}}{\underline{a} \cdot (\underline{b} \times \underline{c})}$$

$$\underline{a} \cdot \underline{\hat{a}} = 1$$

$$\underline{b} \cdot \underline{\hat{b}} = 1$$

$$\underline{c} \cdot \underline{\hat{c}} = 1$$

$$\underline{a} \cdot \underline{\hat{b}} = \underline{a} \cdot \underline{\hat{c}} = \underline{c} \cdot \underline{\hat{a}} = \dots = 0$$

$$\underline{\hat{b}} = \frac{\underline{a} \times \underline{c}}{\underline{b} \cdot (\underline{a} \times \underline{c})}$$

$$\underline{\hat{c}} = \frac{\underline{a} \times \underline{b}}{\underline{c} \cdot (\underline{a} \times \underline{b})}$$

If we have a LI nonorthogonal basis  $\{\underline{x}_1, \underline{x}_2, \dots, \underline{x}_N\}$

$$\underline{x} = \sum_i \alpha_i \underline{x}_i$$

Assume reciprocal basis  $\{\underline{z}_i\}$

$$\underline{z}_j^T \underline{x} = \sum_i \alpha_i \delta_{ij}$$

$$\alpha_j = \underline{z}_j^T \underline{x}$$

$$\underline{x} = \sum \alpha_i \underline{x}_i$$

$$\underline{x} = \sum \underline{x}_i \alpha_i = \left( \sum \underline{x}_i \underline{z}_i^T \right) \underline{x}$$

$$\sum_i \underline{x}_i \underline{z}_i^T = \underline{I}$$

How do find the Reciprocal basis.

$$\{\underline{x}_1, \underline{x}_2, \dots, \underline{x}_N\} \rightarrow \underline{X} = \begin{bmatrix} | & | & & | \\ \underline{x}_1 & \underline{x}_2 & \dots & \underline{x}_N \\ | & | & & | \end{bmatrix}$$

$\underline{X}^{-1}$  exists

$$\underline{X}^{-1} \underline{X} = \underline{I}$$

define  $\underline{Z}^{\dagger} = \underline{X}^{-1}$

$$\text{or } \underline{Z} = (\underline{X}^{-1})^{\dagger}$$

$$\underline{Z}^{\dagger} = \begin{bmatrix} \underline{z}_1^{\dagger} \\ \underline{z}_2^{\dagger} \\ \vdots \\ \underline{z}_N^{\dagger} \end{bmatrix} = \underline{X}^{-1}$$

$$\underline{Z} = \begin{bmatrix} | & | & & | \\ \underline{z}_1 & \underline{z}_2 & \dots & \underline{z}_N \\ | & | & & | \end{bmatrix}$$

$$\underline{Z} = [\underline{z}_1 \dots \underline{z}_N]$$

$$\underline{Z}^{\dagger} \underline{X} = \begin{bmatrix} \underline{z}_1^{\dagger} \\ \underline{z}_2^{\dagger} \\ \vdots \\ \underline{z}_N^{\dagger} \end{bmatrix} [\underline{x}_1 \ \underline{x}_2 \ \dots \ \underline{x}_N] = \langle \underline{z}_i | \underline{x}_j \rangle = \underline{X}^{-1} \underline{X} = \underline{I}$$

$$\underline{z}_i^{\dagger} | \underline{x}_j = \delta_{ij}$$

$$\underline{z}_i^{\dagger} \underline{x}_j = \delta_{ij}$$

$$\langle \underline{z}_i | \underline{x}_j \rangle = \delta_{ij}$$

$$\underline{x} = \sum_{i=1}^N \alpha_i (\underline{x}_i)$$