Similarity Transformation and Diagonalization of Matrices
ChE641, IIT Kanpur

Module - 9

$\underline{A}$ → lin operator → N-dim basis → $\underline{\underline{A}}$

$$\left(\begin{matrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{matrix} \right)$$

$\{\underline{e}_i\}$ → original basis orthonormal

$i = 1 \cdots N$

New basis: $\{\underline{e}'_i\}$ $\quad i = 1 \cdots N$

N-dim $\quad \{\underline{e}_i\}$ → $\underline{a} = \sum a_i \underline{e}_i$

$$\boxed{\underline{e}'_j = \sum_{i=1}^{N} S_{ij}\, \underline{e}_i}$$

$j = 1 \cdots N$

$$\langle \underline{e}_k | \underline{e}'_j \rangle = \sum_{i=1}^{N} S_{ij} \underbrace{\langle \underline{e}_k | \underline{e}_i \rangle}_{\delta_{ki}}$$

$$= \sum_i S_{ij}\, \delta_{ki}$$

Transformation Matrix $\underline{\underline{S}}$

$$\langle \underline{e}_k | \underline{e}'_j \rangle = S_{kj}$$

$S_{kj} \rightarrow \left[\quad \right]$

$$\underline{x} = \sum_i \underbrace{x_i}_{\text{Origin}} \underline{e}_i$$

$$= \sum_j \underbrace{x'_j}_{\text{new}} \underline{e}'_j$$

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

$$\sum_i x_i \underline{e}_i = \sum_j x'_j \sum_i S_{ij} \underline{e}_i$$

$$\sum_{i=1}^{N} \underline{e}_i x_i = \sum_i \underline{e}_i \left\{ \sum_j S_{ij} x'_j \right\}$$

$i = 1 \cdots N$

$$x_i = \sum_j S_{ij} x'_j$$

$$\begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = \underline{\underline{S}} \cdot \begin{bmatrix} x'_1 \\ \vdots \\ x'_N \end{bmatrix}$$

$$\boxed{\underline{x} = \underline{\underline{S}} \cdot \underline{x}'}$$

$$\boxed{\underline{x}' = \underline{\underline{S}}^{-1} \cdot \underline{x}}$$

$$\underline{y} = \underline{\underline{A}}\,\underline{x}$$

$$\underline{\underline{S}}\,\underline{y}' = \underline{\underline{A}}\,\underline{\underline{S}}\,\underline{x}'$$

$$\underbrace{\underline{\underline{S}}^{-1}\underline{\underline{S}}}_{\underline{\underline{I}}}\,\underline{y}' = \underline{\underline{S}}^{-1}\underline{\underline{A}}\,\underline{\underline{S}}\,\underline{x}'$$

$$\underline{\underline{I}}\cdot\underline{y}' = \underline{y}'$$

$$\underline{y}' = \underbrace{\boxed{\underline{\underline{S}}^{-1}\underline{\underline{A}}\,\underline{\underline{S}}}}_{\underline{\underline{A}}'}\,\underline{x}'$$

$$\underline{y}' = \underline{\underline{A}}'\,\underline{x}'$$

$$\boxed{\underline{\underline{A}}' = \underline{\underline{S}}^{-1}\underline{\underline{A}}\,\underline{\underline{S}}}$$

$$\underline{y} = \underline{\underline{A}}\,\underline{x}$$

$$\underline{y}' = \underline{\underline{A}}'\,\underline{x}'$$

$$\boxed{\underline{x}' = \underline{\underline{S}}^{-1}\underline{x}}$$

Special transformation: $\underline{\underline{A}}' \rightarrow$ Diagonal form

New basis $\rightarrow$ eigenvectors of $\underline{\underline{A}}$ $\rightarrow$ then $\underline{\underline{A}}' \rightarrow$ diagonal

original basis: $\{\underline{e}_i\}$ $i = 1\cdots N$

New basis: $\{\underline{x}^j\}$ $j = 1\cdots N$ $\qquad \underline{\underline{A}}\,\underline{x}^j = \lambda_j\,\underline{x}^j$

$$\underline{x}^j = \sum_{i=1}^{N} S_{ij}\,\underline{e}_i \qquad S_{ij} = \langle \underline{e}_i | \underline{x}^j \rangle$$

$$\left(\underline{x}^{(1)}\ \underline{x}^{(2)} \cdots\cdots \underline{x}^{(N)}\right) \rightarrow \begin{array}{ccccc} S_{11} & S_{12(2)} & & S_{1N(N)} & \\ \left[\begin{matrix} x_1^{(1)} \\ x_2^{(1)} \\ \vdots \\ x_N^{(1)} \end{matrix}\right. & \begin{matrix} x_1^{(2)} \\ x_2^{(2)} \\ \vdots \\ x_N^{(2)} \end{matrix} & \cdots\cdots & \left.\begin{matrix} x_1^{(N)} \\ \vdots \\ \vdots \\ x_N^{(N)} \end{matrix}\right] & \underline{\underline{S}} \end{array}$$

Transformation:

$$\underline{\underline{S}} = \begin{bmatrix} \uparrow & \uparrow & & \uparrow \\ \underline{x}^{(1)} & \underline{x}^{(2)} & \cdots\cdots & \underline{x}^{(N)} \\ \downarrow & \downarrow & & \downarrow \end{bmatrix}$$

$$S_{ij} = (\underline{x}^j)_i \qquad (\underline{\underline{A}}')_{ij} = \left(S^{-1} A\, S\right)_{ij} = \sum_k \sum_l \left(S^{-1}\right)_{ik} A_{kl}\, S_{lj}$$

$$= \sum_k \sum_l \left(S^{-1}\right)_{ik} A_{kl}\, (\underline{x}^j)_l$$

$$= \sum_k \left(S^{-1}\right)_{ik} \lambda_j\, (\underline{x}^j)_k$$

$$\underline{\underline{A}}' = \sum_k \lambda_j \left(S^{-1}\right)_{ik} \left(S\right)_{kj}$$

$$(\underline{\underline{A}}')_{ij} = \lambda_j\,\delta_{ij} \longleftarrow$$

$$\underline{\underline{A}}' = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & \cdots \\ 0 & \lambda_2 & 0 & 0 & \cdots \\ 0 & 0 & \lambda_3 & 0 & \cdots \\ & & & \ddots & \\ & & & & \lambda_N \end{bmatrix}$$

$\downarrow$

purely diagonal.

"eigen basis"

Diagonalization of a Matrix

Example.

$$\underline{\underline{A}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

$$(\underline{\underline{A}} - \lambda \underline{\underline{I}}) = \begin{pmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{pmatrix}$$

$$\det(\underline{\underline{A}} - \lambda \underline{\underline{I}}) = 0$$

$$\longrightarrow (2-\lambda)^2 - 1 = 0$$

$$\longrightarrow \lambda^2 - 4\lambda + 4 - 1 = 0$$

$$\lambda^2 - 4\lambda + 3 = 0 \longrightarrow \lambda_1 = 1, \quad \lambda_2 = 3$$

eig vectors

$$(\underline{\underline{A}} - \lambda \underline{\underline{I}})\underline{x} = 0$$

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1^{(1)} \\ x_2^{(1)} \end{pmatrix} = 0$$

$$x_1^{(1)} + x_2^{(1)} = 0 \longrightarrow x_1^{(1)} = -x_2^{(1)}$$

$$\longrightarrow (\underline{x}^{(1)})^T \cdot \underline{x}^{(1)} = 1$$

$$\underline{x}^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

normalized.

$$|\underline{x}^{(1)}| = \sqrt{1^2 + 1^2} = \sqrt{2}$$

$$\underline{x}^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

eig vecs: $\underline{x}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$; $\underline{x}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

original basis vects $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$

$$\underline{x}^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{-1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}$$

$$\underline{x}^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}$$

$$\underline{\underline{A}} = \begin{pmatrix}2 & 1\\1 & 2\end{pmatrix} \qquad \underline{\underline{A}}' = \underline{\underline{S}}^{-1}\,\underline{\underline{A}}\,\underline{\underline{S}}$$

$$\underline{\underline{S}} = \begin{pmatrix}\underline{x}^{(1)} & \underline{x}^{(2)}\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}$$

$$\underline{\underline{S}} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\-1 & 1\end{pmatrix} \longrightarrow \text{Find } \underline{\underline{S}}^{-1}$$

coeffs $\rightarrow \underline{x} \rightarrow$ original basis

coeff $\rightarrow \underline{x}' \rightarrow$ eig basis

$$\underline{x} = \underline{\underline{S}}\cdot\underline{x}'$$

$$\underline{x}' = \underline{\underline{S}}^{-1}\cdot\underline{x}$$

$$\underline{x} = x_1'\,\underline{x}^{(1)} + x_2'\,\underline{x}^{(2)}$$

$$\underline{\underline{A}}\cdot\underline{x} = x_1'\,\underline{\underline{A}}\,\underline{x}^{(1)} + x_2'\,\underline{\underline{A}}\,\underline{x}^{(2)}$$

$$= x_1'\,\lambda_1\,\underline{x}^{(1)} + x_2'\,\lambda_2\,\underline{x}^{(2)}$$

$$\underline{\underline{A}}\cdot\underline{x} = \begin{pmatrix}\underline{x}_1^{(1)} & \underline{x}^{(2)}\end{pmatrix}\underbrace{\begin{pmatrix}\lambda_1 & 0\\0 & \lambda_1\end{pmatrix}}_{\underline{\underline{\Lambda}}}\begin{pmatrix}x_1'\\x_2'\end{pmatrix}$$

$$\underline{\underline{A}}\cdot\underline{x} = \underline{\underline{S}}\cdot\underline{\underline{\Lambda}}\cdot\underline{x}'$$

$$\underline{\underline{A}}\,\underline{x} = \underline{\underline{S}}\cdot\underline{\underline{\Lambda}}\cdot\underline{\underline{S}}^{-1}\cdot\underline{x}' \qquad \underline{x}' = \underline{\underline{S}}^{-1}\cdot\underline{x}$$

$$\boxed{\underline{\underline{A}} = \underline{\underline{S}}\cdot\underline{\underline{\Lambda}}\cdot\underline{\underline{S}}^{-1}}$$

Diagonalization.

$$\boxed{\underline{\underline{\Lambda}} = \underline{\underline{S}}^{-1}\cdot\underline{\underline{A}}\cdot\underline{\underline{S}}} \rightarrow \begin{pmatrix}1 & 0\\0 & 3\end{pmatrix}$$

$\underline{\underline{S}}$ ✓ $\quad \underline{\underline{S}}^{-1}$

Spectral Resolution:

$$\underline{\underline{A}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \qquad \lambda_1 = 1, \quad \lambda_2 = 3$$

$$\underline{\underline{A}} = \sum_{i=1}^{N} \lambda_i \underbrace{\underline{x}^{(i)} \left(\underline{x}^{(i)}\right)^T}$$

$$\underline{x}^{(1)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$$

$$\left(\underline{x}^{(1)}\right)^T = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$$

$$\underline{x}^{(2)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

$$\left(\underline{x}^{(2)}\right)^T = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\underline{\underline{A}} = (1) \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} + (3). \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{-1}{2} \\ \frac{-1}{2} & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{3}{2} & \frac{3}{2} \\ \frac{3}{2} & \frac{3}{2} \end{pmatrix}$$

$$= \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Diagonalization:

$$\underline{\underline{A}} \cdot \underline{x}^{(i)} = \lambda_i \cdot \underline{x}^{(i)} \longrightarrow \lambda_i \quad i = 1 \dots N$$

$$(\text{orthogonal}) \quad \underline{x}^{(i)} \quad i = 1 \dots N$$

$$\underline{\underline{X}} = \begin{bmatrix} \uparrow & \uparrow & & \uparrow \\ \underline{x}_1 & \underline{x}_2 & \cdots & \underline{x}_N \\ \downarrow & \downarrow & & \downarrow \end{bmatrix}$$

$$\underline{\underline{A}} \cdot \underline{\underline{X}} = \underline{\underline{A}} \left[\underline{x}^{(1)} \dots \underline{x}^{(N)} \right] = \left[\underline{\underline{A}}\,\underline{x}^{(1)} \,\middle|\, \underline{\underline{A}}\,\underline{x}^{(2)} \,\middle|\, \cdots \,\middle|\, \underline{\underline{A}}\,\underline{x}^{(N)} \right]$$

$$= \left[\lambda_1 \underline{x}^{(1)} \,\middle|\, \lambda_2 \underline{x}^{(2)} \,\middle|\, \cdots \,\middle|\, \lambda_n \underline{x}^{N} \right]$$

$$\underline{\underline{A}}\,\underline{\underline{X}} = \underline{\underline{X}}\,\underline{\underline{\Lambda}} \qquad \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & \\ & 0 & \ddots & 0 & \\ & & & & \lambda_N \end{pmatrix}$$

$$\boxed{\underline{\underline{X}}^{-1} \underline{\underline{A}}\,\underline{\underline{X}} = \underline{\underline{\Lambda}}}$$

If $\underline{\underline{A}}$ is symmetric $\underline{\underline{A}}^T = \underline{\underline{A}} \longrightarrow N$ orthogonal eig vectors

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

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

$$\underline{\underline{X}} = [\underline{x}_1 \dots \underline{x}_N]$$

$$\underline{\underline{X}}^T = \begin{bmatrix} \underline{x}_1^T \\ \vdots \\ \underline{x}_N^T \end{bmatrix}$$

$$\underline{\underline{X}}^T \cdot \underline{\underline{X}} = \begin{bmatrix} \underline{x}_1^T \cdot \underline{x}_1 & \cancel{\underline{x}_1^T \underline{x}_2}\ 0 & \cdots & \cancel{\underline{x}_1^T \underline{x}_N}\ 0 \\ \cancel{\underline{x}_2^T \underline{x}_1}\ 0 & \underline{x}_2^T \underline{x}_2 & \cdots & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

1

$$\underline{\underline{X}}^T \cdot \underline{\underline{X}} = \underline{\underline{I}}$$

$$\boxed{\underline{\underline{X}}^T = \underline{\underline{X}}^{-1}} \longrightarrow \text{orthogonal matrices}$$

$\{\underline{e}_i\}$

orthogonal transformation

Normal Matrices — Hermitian / unitary

ODE's

$$\frac{d\underline{x}}{dt} = \underline{\underline{A}} \cdot \underline{x}$$

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Coupled

$$\frac{dx_1}{dt} = A_{11}x_1 + A_{12}x_2 + A_{13}x_3$$

$$\frac{dx_2}{dt} = A_{12}x_1 + A_{22}x_2 + \cdots$$

$$\underline{\underline{A}} = \underline{\underline{X}}\,\underline{\underline{\Lambda}}\,\underline{\underline{X}}^{-1}$$

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

$$\frac{d\underline{x}}{dt} = \underline{\underline{A}} \cdot \underline{x}$$

$$= \underline{\underline{X}} \cdot \underline{\underline{\Lambda}} \left(\underline{\underline{X}}^{T} \cdot \underline{x}\right) \quad \underline{y}$$

$$\underline{y} = \underline{\underline{X}}^{T} \cdot \underline{x} \qquad \boxed{\underline{y} = \underline{\underline{X}}^{-1} \cdot \underline{x}}$$

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

$$\frac{d\underline{x}}{dt} = \underline{\underline{X}} \cdot \underline{\underline{\Lambda}} \cdot \underline{y}$$

$$\frac{d}{dt}\left(\underline{\underline{X}}^{-1} \cdot \underline{x}\right) = \underbrace{\underline{\underline{X}}^{-1}\,\underline{\underline{X}}}_{\underline{\underline{I}}}\;\underline{\underline{\Lambda}}\;\underline{y}$$

$$\underline{\underline{\Lambda}} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

$$\frac{d\underline{y}}{dt} = \underline{\underline{\Lambda}} \cdot \underline{y}$$

$$\frac{d}{dt}\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

"Decoupled"

"Normal Modes"

$$\frac{dy_1}{dt} = \lambda_1 y_1 \qquad \frac{dy_2}{dt} = \lambda_2 y_2 \qquad \frac{dy_3}{dt} = \lambda_3 y_3$$

$$y_1 = y_1(0)\,e^{\lambda_1 t} \qquad y_2 = y_2(0)\,e^{\lambda_2 t} \qquad y_3 = y_3(0)\,e^{\lambda_3 t}$$