Linear Operators and Matrices
ChE641, IIT Kanpur

Part - 4

Linear operators:

Defn. of a linear operator. $A(\lambda \underline{a} + \mu \underline{b}) = \lambda A \underline{a} + \mu A \underline{b}$

operator: $y = f(x)$

$\underline{y} = A \underline{x}$ ← 'input'

'output' — operator

$\underline{y} = A \underline{x}$ → how does this relation appear in a given basis

→ "Linear Transformation"

We have an orthonormal basis: $\{\underline{e}_i\}$ $i = 1 \dots N$ $\langle \underline{e}_i | \underline{e}_j \rangle = \delta_{ij}$

$\{\underline{e}_1, \underline{e}_2 \dots \underline{e}_N\}$: original basis

$\underline{e}_i' = A \underline{e}_i$ $1 \dots N$ (original basis)

$\underline{e}_i' = A \underline{e}_i$

What is the k^{th} component of $\underline{e}_i'$

$\underline{e}_i' = \sum_k \alpha_k^i \underline{e}_k$

N vectors $\underline{a} = \sum_k a_k \underline{e}_k$

$\langle \underline{e}_k | \underline{e}_i' \rangle = \langle \underline{e}_k | A \underline{e}_i \rangle = \alpha_k^i = A_{ki}$ → "Matrix"

$$A_{ij} \to \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{bmatrix} \to (N \times N) \text{ Square matrix.}$$

$\underline{y} = A\,\underline{x} \longrightarrow$ how this is represented in a given basis ?

$$\sum_{i=1}^{N} y_i\,\underline{e}_i = A \sum_{j=1}^{N} x_j\,\underline{e}_j \xrightarrow[\text{operator } A]{\text{linear}} = \sum_{j=1}^{N} x_j\, A\,\underline{e}_j$$

What is the k^{th} comp. y_k ??

Take inner pdt on both sides with $\underline{e}_k$.

$$\sum_i y_i \underbrace{\langle \underline{e}_k | \underline{e}_i \rangle}_{\delta_{ik}} = \sum_j x_j \overbrace{\langle \underline{e}_k | A\,\underline{e}_j \rangle}^{A_{kj}}$$

$$y_k = \sum A_{kj}\, x_j$$

$$\underline{y} = \overset{\text{lin. operator}}{A}\,\underline{x} \xrightarrow[\text{basis}]{\text{a given}} y_k = \sum_{j=1}^{N} A_{kj}\, x_j \qquad (k = 1 \cdots N)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2N} \\ \vdots & & & & \\ A_{N1} & \cdots & & \cdots & A_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

The linear operator A, when expressed in a given basis, takes the form of an $(N \times N)$ matrix

a vector $\longrightarrow$ column vector in a basis.

Properties of linear operators.

$$(A + B)\,\underline{x} = A\,\underline{x} + B\,\underline{x}$$

$$(\lambda A)\,\underline{x} = \lambda (A\,\underline{x})$$

$$(A B)\,\underline{x} = A (B\,\underline{x})$$

$$\boxed{AB \neq BA}$$

Not commutative

MN

lin operators.

$$\underline{v}'' = (M\,N)\underline{v}$$

$$N\underline{v} = \underline{v}'$$

$$\underline{v}'' = M(N\underline{v})$$

$$\underline{v}'' = M\cdot\underline{v}' = (M\,N)\underline{v}$$

$$\langle \underline{e}_i | \underline{v}'' \rangle = \langle \underline{e}_i | M\,\underline{v}' \rangle$$

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

$$\underline{v}' = N\underline{v}$$

$$v_i'' = \sum_{j=1}^{N} M_{ij}\, v_j'$$

$$v_j' = \sum_{k=1}^{N} N_{jk}\, v_k$$

$$v_i'' = \sum_{j}^{} M_{ij} \sum_k N_{jk}\, v_k$$

$$v_i'' = \sum_j \sum_k (M_{ij} N_{jk}) v_k$$

$$\underline{v}'' = (MN)\,\underline{v}$$

$$v_i'' = \sum_k (MN)_{ik}\, v_k$$

$$\boxed{(MN)_{ik} = \sum_j M_{ij}\, N_{jk}}$$

Matrix Multiplication

$$(MN)_{11} = \sum_{j=1}^{N} M_{1j} N_{j1}$$

$$= M_{11}N_{11} + M_{12}N_{21} + M_{13}N_{31} + \dots M_{1N}N_{N1}$$

$$\begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1N} \\ \vdots & & & \\ M_{N1} & M_{N2} & \cdots & M_{NN} \end{pmatrix} \begin{pmatrix} N_{11} & N_{12} & \cdots & N_{1N} \\ \vdots & & & \\ N_{N1} & \cdots & \cdots & N_{NN} \end{pmatrix}$$

$$(A+B)_{ij} = A_{ij} + B_{ij}$$

$$(\lambda A)_{ij} = \lambda A_{ij}$$

$$(AB)_{ij} = \sum_k A_{ik} B_{kj}$$

$$A + B = B + A$$

$$AB \neq BA.$$

Identity matrix $\underline{\underline{I}}$ $\qquad$ $\underline{\underline{I}} \cdot \underline{\underline{A}} = \underline{\underline{A}}$

$N \times N$

Null matrix $\underline{\underline{0}}$ $\qquad$ $\underline{\underline{0}} + \underline{\underline{A}} = \underline{\underline{A}}$

<u>Transpose</u>:

$$\underline{\underline{A}} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & & & \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix}$$

$\underline{\underline{A}} : M \times N$

$\underline{\underline{A}}^T : N \times M$

$$\underline{\underline{A}}^T = \begin{pmatrix} A_{11} & A_{21} & \cdots & A_{N1} \\ A_{12} & A_{22} & & \vdots \\ \vdots & \vdots & & \vdots \\ A_{1N} & A_{2N} & & A_{NN} \end{pmatrix}$$

<u>Prove</u>:

$(AB)^T = B^T A^T$

A_{ij}

$(A^T)_{ij} = A_{ji}$

<u>Proof</u>:

$$(AB)^T_{ij} = (AB)_{ji}$$

$$= \sum_k{}' A_{jk} B_{ki}$$

$$\boxed{(AB)^T = B^T A^T}$$

$$= \sum_k{}' (A^T)_{kj} (B^T)_{ik}$$

$$(AB)^T_{ij} = \sum_k B^T_{ik} A^T_{kj} = (B^T A^T)_{ij}$$

Index Notation. (Einstein Convention)

Complex conjugate $\underline{\underline{A}}^*$ $\qquad$ $(A^*)_{ij} = (A_{ij})^*$

If a matrix has only real elements: $\underline{\underline{A}} = \underline{\underline{A}}^*$ $\qquad$ $A^\dagger$ A dagger

$\underline{\underline{A}} \to \underline{\underline{A}}^T_{ij} = A_{ji}$

A_{ij}

<u>Heremetian conjugate</u>

$$A^\dagger = (A^*)^T = (A^T)^*$$

if A is real $A^\dagger \to A^T$.

$(AB)^T = B^T A^T$

$(A\ B \ldots G)^\dagger = G^\dagger \ldots B^\dagger A^\dagger$

can prove

$\underline{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$ $\underline{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}$.

$\langle \underline{a} | \underline{b} \rangle = \sum_{i=1}^{N} a_i^* b_i$ ✓

$= a_1^* b_1 + a_2^* b_2 + \ldots + a_N^* b_N$

$\langle \underline{a} | \underline{b} \rangle = (a_1^* \ a_2^* \ldots a_N^*) \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}$

$(1 \times \cancel{N) \ (N} \times 1)$

$= 1 \times 1$

$$\boxed{\text{Trace } \underline{\underline{A}} = \sum_{i=1}^{N} A_{ii}}$$

a scalar

$Tr(A \pm B) = Tr A \pm Tr B$

$Tr(AB) = Tr(BA)$

$Tr(A^T) = Tr A$ $\quad Tr A^\dagger = (Tr A)^*$