1. Vector Spaces and Linear Operators

1.1 Vectors

A vector is a quantity with magnitude and direction.
It has components with respect to particular axes.

e.g. $\underset{\sim}{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$ is a vector in 3-D space

$\underset{\sim}{u}$ is a column vector.

Examples of vector quantities:

displacement $\underset{\sim}{x}$, velocity $\underset{\sim}{v}$, acceleration $\underset{\sim}{a}$, force $\underset{\sim}{F}$.

Notation: use underline, $\underset{\sim}{u}$
or overline, $\vec{u}$
(or bold if typesetting)

Vectors can be added:

$$\underset{\sim}{u} + \underset{\sim}{v} = \begin{pmatrix} u_1 + v_1 \\ u_2 + v_2 \\ u_3 + v_3 \end{pmatrix}.$$

Vectors can be scaled:

$$\lambda \underset{\sim}{u} = \begin{pmatrix} \lambda u_1 \\ \lambda u_2 \\ \lambda u_3 \end{pmatrix}.$$

The set of vectors forms a <u>vector space</u> over real numbers.

$\underset{\sim}{u} \in \mathbb{R}^2$ (2-D), $\mathbb{R}^3$ (3-D), $\mathbb{R}^N$ (N-D) $\begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}$

or complex numbers

$u_i \in \mathbb{C}$ with $\lambda \in \mathbb{C}$.

1.2 Real Vector Spaces

A real vector space V is defined as a set $(\underset{\sim}{u}, \underset{\sim}{v}, \dots)$ of vectors that is closed under (i) addition and (ii) multiplication by a scalar:

i.e. If $\underset{\sim}{u} \in V$ and $\underset{\sim}{v} \in V \Rightarrow \underset{\sim}{u} + \underset{\sim}{v} \in V$

Also, If $\lambda \in \mathbb{R} \Rightarrow \lambda \underset{\sim}{u} \in V$

where V is a vector space.

It has the following properties:

(commutative): $\underset{\sim}{u} + \underset{\sim}{v} = \underset{\sim}{v} + \underset{\sim}{u}$

(associative): $(\underset{\sim}{v} + \underset{\sim}{u}) + \underset{\sim}{w} = \underset{\sim}{v} + (\underset{\sim}{u} + \underset{\sim}{w})$

(distributive): $\lambda(\underset{\sim}{v} + \underset{\sim}{w}) = \lambda \underset{\sim}{v} + \lambda \underset{\sim}{w}$

$$(\lambda + \mu)\underset{\sim}{v} = \lambda \underset{\sim}{v} + \mu \underset{\sim}{v}$$

$$\lambda(\mu \underset{\sim}{v}) = (\lambda\mu)\underset{\sim}{v}$$

$\exists$ a zero or null vector $\underset{\sim}{0} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$ such that $\underset{\sim}{v} + \underset{\sim}{0} = \underset{\sim}{v}$

$\exists$ an additive inverse $-\underset{\sim}{v}$ such that $\underset{\sim}{v} + (-\underset{\sim}{v}) = \underset{\sim}{0}$.

<u>Note</u>: The set of non-negative real numbers, $\mathbb{R}^+$ is <u>not</u> a vector space since there is no additive inverse.

We can extend this to the concept of a complex vector space by allowing $\lambda, \mu, u_i, v_i, w_i \in \mathbb{C}$.

Matrices $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ with $a, b, c, d \in \mathbb{R}$ also form a vector space because:

$$\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} + \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1+a_2 & b_1+b_2 \\ c_1+c_2 & d_1+d_2 \end{pmatrix}$$

$$\lambda \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \lambda a & \lambda b \\ \lambda c & \lambda d \end{pmatrix}$$

with zero $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ and inverse $\begin{pmatrix} -a & -b \\ -c & -d \end{pmatrix}$.

1.3 LINEAR INDEPENDENCE

$\underset{\sim}{u}_1$ + $\underset{\sim}{u}_2$ are linearly independent if

$$\lambda_1 \underset{\sim}{u}_1 + \lambda_2 \underset{\sim}{u}_2 = \underset{\sim}{0} \Rightarrow \lambda_1 = \lambda_2 = 0$$

for the 2-D case.

e.g. $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ are linearly independent

since $\lambda_1\begin{pmatrix}1\\0\end{pmatrix} + \lambda_2\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\lambda_1\\\lambda_2\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$ if

and only if (iff) $\lambda_1 = \lambda_2 = 0$.

But $\begin{pmatrix}1\\1\end{pmatrix}$ and $\begin{pmatrix}2\\2\end{pmatrix}$ are linearly dependent since

$$\lambda_1\begin{pmatrix}1\\1\end{pmatrix} + \lambda_2\begin{pmatrix}2\\2\end{pmatrix} = \begin{pmatrix}\lambda_1 + 2\lambda_2\\\lambda_1 + 2\lambda_2\end{pmatrix} = \underset{\sim}{0} \text{ for } \lambda_1 = -2\lambda_2.$$

For $\mathbb{R}^N$, $\underset{\sim}{u}_1, \dots, \underset{\sim}{u}_N$ are linearly independent if

$$\lambda_1\underset{\sim}{u}_1 + \lambda_2\underset{\sim}{u}_2 + \dots + \lambda_N\underset{\sim}{u}_N = \underset{\sim}{0}$$

$$\Rightarrow \lambda_1 = \lambda_2 = \dots = \lambda_N = 0$$

e.g. $\lambda_1\begin{pmatrix}1\\1\\1\end{pmatrix} + \lambda_2\begin{pmatrix}2\\1\\0\end{pmatrix} + \lambda_3\begin{pmatrix}-1\\0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$

$$\Rightarrow \begin{pmatrix}\lambda_1 + 2\lambda_2 - \lambda_3\\\lambda_1 + \lambda_2\\\lambda_1 + \lambda_3\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

$$\Rightarrow \lambda_3 = -\lambda_1, \quad \lambda_2 = -\lambda_1 \quad \Rightarrow \lambda_1 + 2\lambda_2 - \lambda_3 = 0$$

Hence this set of column vectors is linearly dependent since we don't need $\lambda_1 = \lambda_2 = \lambda_3 = 0$ (e.g. we could have $\lambda_1 = 1$, $\lambda_2 = -1$, $\lambda_3 = -1$)

1.4 BASES AND DIMENSIONALITY

If all vectors in the vector space V are linear combinations of the form

$$\underset{\sim}{u} = a_1 \underset{\sim}{e}_1 + a_2 \underset{\sim}{e}_2 + \dots + a_N \underset{\sim}{e}_N$$

for $a_i \in \mathbb{R}$, then the set of vectors $\{\underset{\sim}{e}_1, \dots, \underset{\sim}{e}_N\}$ span V and form a basis for V.

The dimension of V is the number of basis vectors, N.

e.g. In $\mathbb{R}^2$, $\begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ (dimension 2)

In $\mathbb{R}^3$, $\begin{pmatrix} a \\ b \\ c \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + c \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ (dimension 3)

Basis vectors are not unique since

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{a+b}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{a-b}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and so $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ are basis vectors.

In the case of 2×2 matrices,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + b \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + c \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + d \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

forming a vector space of dimension 4.

$a + ib$ (where $a, b \in \mathbb{R}$) is a vector space over $\mathbb{R}^2$ with basis $\{1, i\}$. The set $\{1, \lambda i\}$ is also a basis because $a + \frac{b}{\lambda}(i\lambda) = a + ib$.

The set $\{1, i\}$ is linearly independent on $\mathbb{R}$ but $\{1, i\}$ is linearly dependent on $\mathbb{C}$

1.5 INDEX NOTATION

We can express some equations in a more compact form using index notation:

e.g. $\sum_{i=1}^{n} i = 1 + 2 + \dots + n \quad \left(= \frac{1}{2} n(n+1) \right)$

$$\sum_{i=1}^{n} i^2 = 1 + 4 + \dots + n^2 \quad \left(= \frac{1}{6} n(n+1)(2n+1) \right)$$

(proof by induction)

So we can write a vector $\underset{\sim}{u}$ as

$$\underset{\sim}{u} = \sum_i u_i \underset{\sim}{e}_i$$

where the $\underset{\sim}{e}_i$ are the basis vectors.

This can be used to simplify matrix multiplication.

1.6 MATRICES

A_{ij} is an array of numbers, i = row, j = column.

We can multiply a $N \times L$ matrix by a $L \times M$ matrix to obtain a $N \times M$ matrix, where

$$(AB)_{ij} = \sum_{k=1}^{L} A_{ik} B_{kj}$$

i.e. ith row multiplies jth column.

<u>Note</u>: $AB \neq BA$

e.g. $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$, $B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$

$$\Rightarrow AB = \begin{pmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{pmatrix}$$

<u>Transpose of a matrix</u>: $(A^T)_{ij} = A_{ji}$ (i.e. interchange rows & columns)

<u>Complex conjugate</u>: $(A^*)_{ij} = (A_{ij})^*$ (i.e. $i \to -i$)

<u>Hermitian conjugate</u>: $(A^\dagger)_{ij} = (A_{ji})^*$ (complex conj. of transpose)

e.g. If $A = \begin{pmatrix} 1 & i \\ 0 & 2 \end{pmatrix}$

$$\Rightarrow A^T = \begin{pmatrix} 1 & 0 \\ i & 2 \end{pmatrix}, \quad A^* = \begin{pmatrix} 1 & -i \\ 0 & 2 \end{pmatrix}, \quad A^\dagger = \begin{pmatrix} 1 & 0 \\ -i & 2 \end{pmatrix}$$

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

<u>PROOF</u> : $(AB)^T_{ij} = (AB)_{ji} = \sum_k A_{jk} B_{ki}$

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

$$= (B^T A^T)_{ij}$$

$$\Rightarrow \quad (AB)^T = B^T A^T$$

Similarly $(AB)^{\dagger} = B^{\dagger} A^{\dagger}$.

1.7 <u>INNER PRODUCT</u>

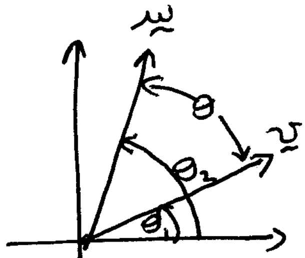
Given $\underset{\sim}{v}, \underset{\sim}{w} \in V$, the inner product $(\underset{\sim}{v}, \underset{\sim}{w})$, a scalar, has the following properties :

$$(\underset{\sim}{v}, \underset{\sim}{w}) = (\underset{\sim}{w}, \underset{\sim}{v})$$

$$(\underset{\sim}{v}, \lambda \underset{\sim}{w} + \mu \underset{\sim}{u}) = \lambda (\underset{\sim}{v}, \underset{\sim}{w}) + \mu (\underset{\sim}{v}, \underset{\sim}{u})$$

$$(\underset{\sim}{v}, \underset{\sim}{v}) \geqslant 0$$

$$(\underset{\sim}{v}, \underset{\sim}{v}) = 0 \text{ iff } \underset{\sim}{v} = \underset{\sim}{0}.$$



In $\mathbb{R}^2$ this is the usual scalar product,

$$\underset{\sim}{v} \cdot \underset{\sim}{w} = |\underset{\sim}{v}||\underset{\sim}{w}| \cos\theta = |\underset{\sim}{v}||\underset{\sim}{w}| (\cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2)$$

$$= v_1 w_1 + v_2 w_2 \quad \text{where } v_1 = |\underset{\sim}{v}|\cos\theta_1, \; v_2 = |\underset{\sim}{v}|\sin\theta_1,$$
$$w_1 = |\underset{\sim}{w}|\cos\theta_2, \; w_2 = |\underset{\sim}{w}|\sin\theta_2$$

This can be generalised to $\mathbb{R}^N$:

$$\underset{\sim}{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix}, \quad \underset{\sim}{w} = \begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix}$$

$$\Rightarrow \quad (\underset{\sim}{v}, \underset{\sim}{w}) = \sum_{i=1}^{N} v_i w_i .$$

We can also write

$$(\underset{\sim}{v}, \underset{\sim}{w}) = v^T w = (v_1 \; \cdots \; v_N) \begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix}$$

where v^T is the transpose of $\underset{\sim}{v}$, i.e. a row vector.

Note that

$$(\underset{\sim}{v}, \underset{\sim}{v}) = \sum_i v_i^2 \geqslant 0$$

and that

$$(\underset{\sim}{v}, \underset{\sim}{v}) = 0 \text{ iff } v_i = 0 \;\; \forall i \;\; (\Rightarrow \underset{\sim}{v} = \underset{\sim}{0})$$

V is called a "positive inner product space" or a "inner product space with positive semi-definite norm."

We have

$$(\underset{\sim}{v}, \underset{\sim}{w}) = \sum_i v_i w_i = \sum_i w_i v_i = (\underset{\sim}{w}, \underset{\sim}{v}) \text{ as required}$$

$$(\underset{\sim}{v}, \lambda \underset{\sim}{w} + \mu \underset{\sim}{u}) = \sum_i v_i (\lambda w_i + \mu u_i) = \sum_i (\lambda v_i w_i + \mu v_i u_i)$$

$$= \lambda (\underset{\sim}{v}, \underset{\sim}{w}) + \mu (\underset{\sim}{v}, \underset{\sim}{u}), \text{ as required, using } \lambda \underset{\sim}{v} = \begin{pmatrix} \lambda v_1 \\ \vdots \\ \lambda v_N \end{pmatrix}$$

This can be generalised to $\mathbb{C}^N$ by requiring

$$(\underset{\sim}{v}, \underset{\sim}{w}) = (\underset{\sim}{w}, \underset{\sim}{v})^*$$

$$(\underset{\sim}{v}, \lambda \underset{\sim}{w}) = \lambda (\underset{\sim}{v}, \underset{\sim}{w})$$

$$(\underset{\sim}{v}, \lambda \underset{\sim}{w} + \mu \underset{\sim}{u}) = \lambda (\underset{\sim}{v}, \underset{\sim}{w}) + \mu (\underset{\sim}{v}, \underset{\sim}{u})$$

Then

$$(\lambda \underset{\sim}{v}, \underset{\sim}{w}) = (\underset{\sim}{w}, \lambda \underset{\sim}{v})^* = \lambda^* (\underset{\sim}{w}, \underset{\sim}{v})^* = \lambda^* (\underset{\sim}{v}, \underset{\sim}{w})$$

So multiplying the first entry by λ produces a λ^*, but multiplying the second entry by λ produces a λ.

Hence $\quad (\lambda \underset{\sim}{v}, \mu \underset{\sim}{w}) = \lambda^* \mu \, (\underset{\sim}{v}, \underset{\sim}{w})$

This requires

$$(\underset{\sim}{v}, \underset{\sim}{w}) = \sum_i v_i^* w_i = v^\dagger w$$

$$= (v_1 \ldots v_N)^* \begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix}$$ in matrix notation.

This is a natural generalisation of the real case.

For matrices, we define the inner product as $\mathrm{Tr}(A^\dagger B)$ where Tr is the <u>trace</u> of a matrix which is the sum of the matrix's diagonal elements. e.g. $\mathrm{Tr} A = \sum_i A_{ii}$

So, if $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ and $B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$ then

$$\mathrm{Tr}(A^\dagger B) = \mathrm{Tr} \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$= \mathrm{Tr} \begin{pmatrix} a_{11}^* b_{11} + a_{21}^* b_{21} & a_{11}^* b_{12} + a_{21}^* b_{22} \\ a_{12}^* b_{11} + a_{22}^* b_{21} & a_{12}^* b_{12} + a_{22}^* b_{22} \end{pmatrix}$$

$$= a_{11}^* b_{11} + a_{21}^* b_{21} + a_{12}^* b_{12} + a_{22}^* b_{22}$$

$$= \sum_i \sum_j a_{ij}^* b_{ij}$$

This is the natural generalisation of $\sum_i v_i^* w_i$.

Inner products are used in quantum mechanics. If

$$\Psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix} \quad \text{and} \quad \Phi = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}$$

where the ψ_i and ϕ_i are complex numbers, the inner product is

$$(\Phi, \Psi) = \phi_1^* \psi_1 + \cdots + \phi_N^* \psi_N .$$

In quantum mechanics $(\Psi, \Psi) = \sum_i \psi_i^* \psi_i$ gives the probability of state Ψ.

1.8 ORTHONORMAL BASIS

Two vectors are orthogonal if $(\underset{\sim}{u}, \underset{\sim}{v}) = 0$. A set of basis , $\{\underset{\sim}{e}_1, \ldots, \underset{\sim}{e}_N\}$ are orthogonal if

$\underset{\sim}{e}_i \cdot \underset{\sim}{e}_j = 0$ for $i \neq j$.

The unit vectors $\{\hat{e}_1, \ldots, \hat{e}_N\}$ form an <u>orthonormal basis</u> if

$$\hat{e}_1 \cdot \hat{e}_1 = \ldots = \hat{e}_N \cdot \hat{e}_N = 1$$

Then

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}$$

Here δ_{ij} is the Kronecker delta.

If we define $N_i \equiv (e_i, e_i)$ then $\hat{e}_i = \dfrac{e_i}{\sqrt{N_i}}$

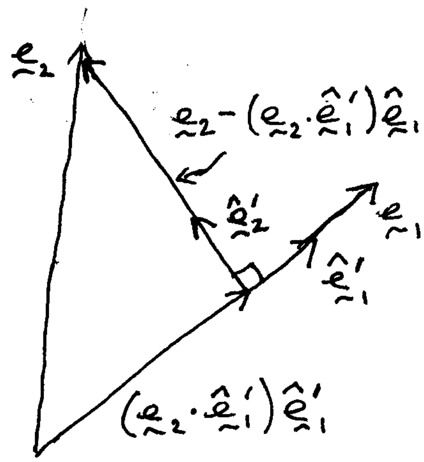
where $\sqrt{N_i}$ is the <u>norm</u> of the vector e_i.

We can use the Gram-Schmidt method to construct an orthonormal basis even if the set $\{e_i\}$ is not orthogonal.

e.g. Given the basis $\{e_1, e_2\}$ for $\mathbb{R}^2$

we define $$\hat{e}_1' = \frac{e_1}{\sqrt{e_1 \cdot e_1}}$$

and $$\hat{e}_2' = \frac{e_2 - (e_2 \cdot \hat{e}_1')\hat{e}_1'}{|e_2 - (e_2 \cdot \hat{e}_1')\hat{e}_1'|}$$



$$\Rightarrow \quad \hat{e}_1' \cdot \hat{e}_2' = 0 \quad \text{and} \quad \hat{e}_2' \cdot \hat{e}_2' = 1.$$

We can write any vector $\underset{\sim}{u}$ in terms of the orthonormal basis as

$$\underset{\sim}{u} = \sum_i u_i \hat{\underset{\sim}{e}}_i$$

Hence

$$(\hat{\underset{\sim}{e}}_k, \underset{\sim}{u}) = \left(\hat{\underset{\sim}{e}}_k, \sum_i u_i \hat{\underset{\sim}{e}}_i\right) = \sum_i \left(\hat{\underset{\sim}{e}}_k, u_i \hat{\underset{\sim}{e}}_i\right)$$

$$= \sum_i u_i \left(\hat{\underset{\sim}{e}}_k, \hat{\underset{\sim}{e}}_i\right) = \sum_i u_i \delta_{ik} = u_k$$

Similarly,

$$(\hat{\underset{\sim}{e}}_i, \underset{\sim}{u}) = u_i$$

and so

$$\underset{\sim}{u} = \sum_i \hat{\underset{\sim}{e}}_i (\hat{\underset{\sim}{e}}_i, \underset{\sim}{u})$$

Likewise,

$$(\underset{\sim}{u}, \hat{\underset{\sim}{e}}_k) = \sum_i \left(u_i \hat{\underset{\sim}{e}}_i, \hat{\underset{\sim}{e}}_k\right) = \sum_i u_i^* \left(\hat{\underset{\sim}{e}}_i, \hat{\underset{\sim}{e}}_k\right) = u_k^*$$

1.9. LINEAR OPERATORS AND MATRICES

A <u>linear operator</u> is a map A from V to V which takes vector $\underset{\sim}{v}$ into new vector $A\underset{\sim}{v}$ with the following properties:

$$A(\lambda \underset{\sim}{v} + \mu \underset{\sim}{w}) = \lambda (A\underset{\sim}{v}) + \mu (A\underset{\sim}{w})$$

$$(A+B)\underset{\sim}{v} = A\underset{\sim}{v} + B\underset{\sim}{v}$$

$$(\lambda A)\underset{\sim}{v} = \lambda (A\underset{\sim}{v})$$

$$(AB)\underset{\sim}{v} = A(B\underset{\sim}{v})$$

If A and B are linear operators then AB is a linear operator.

We can associate a matrix with A by considering its effect on basis vectors:

$$A\underset{\sim}{e}_i = \sum_j A_{ji}\underset{\sim}{e}_j \qquad \text{(summing over first index of } A\text{)}$$

We can distinguish between the operator $\hat{A}$ and the matrix A since the latter depends on the choice of basis (just as u_i is dependent on basis, although $\underset{\sim}{u}$ is not).

Then

$$(\hat{A}\hat{B})\underset{\sim}{e}_i = \hat{A}(\hat{B}\underset{\sim}{e}_i) = \hat{A}\left(\sum_j B_{ji}\underset{\sim}{e}_j\right)$$

$$= \sum_j B_{ji}\hat{A}\underset{\sim}{e}_j = \sum_j B_{ji}\sum_k A_{kj}\underset{\sim}{e}_k$$

$$= \sum_j\sum_k (B_{ji}A_{kj})\underset{\sim}{e}_k$$

$$= \sum_{j,k}(A_{kj}B_{ji})\underset{\sim}{e}_k$$

$$= \sum_k C_{ki}\underset{\sim}{e}_k \quad \text{where } C_{ki} = \sum_j A_{kj}B_{ji}$$

(matrix product)

Since

$$(\hat{\underset{\sim}{e}}_k, \hat{A}\hat{\underset{\sim}{e}}_i) = \left(\hat{\underset{\sim}{e}}_k, \sum_j A_{ji}\hat{\underset{\sim}{e}}_j\right)$$

$$= \sum_j A_{ji}(\hat{\underset{\sim}{e}}_k, \hat{\underset{\sim}{e}}_j) = \sum_j A_{ji}\delta_{kj} = A_{ki}$$

we have

$$\hat{A}\,\underset{\sim}{\hat{e}}_i = \sum_j \underset{\sim}{\hat{e}}_j \left(\underset{\sim}{\hat{e}}_j, \hat{A}\,\underset{\sim}{\hat{e}}_i\right)$$

because

$$\left(\underset{\sim}{\hat{e}}_j, \hat{A}\,\underset{\sim}{\hat{e}}_i\right) = A_{ji}$$

1.10 Summation Convention

The summation convention is that a repeated index is always summed, so we can omit the Σ sign.

e.g. $C_{ij} = A_{ik} B_{kj}$ for matrix multiplication.

Here k is a dummy index (since we can use any letter), while i and j are free indices (which must match on both sides of the equation).

A repeated index cannot appear more than twice.

e.g. $(ABC)\,\underset{\sim}{e}_i = \cancel{\sum_j} D_{ji}\,\underset{\sim}{e}_j$ with $D_{ji} = \cancel{\sum_k}\cancel{\sum_l} A_{jk} B_{kl} C_{li}$

where both k and l are summed.

1.11 Identity Operator

The general identity operator, I, is defined as

$$I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} ; \quad \Rightarrow I\,\underset{\sim}{e}_i = \sum_j I_{ji}\,\underset{\sim}{e}_j = \sum_j \delta_{ji}\,\underset{\sim}{e}_j = \underset{\sim}{e}_i$$

1.12 PERMUTATION OPERATOR

Consider the permutation operator, $\hat{P}$, with the properties:

$$\hat{P}\underset{\sim}{e}_1 = \underset{\sim}{e}_2 \,, \quad \hat{P}\underset{\sim}{e}_2 = \underset{\sim}{e}_3 \quad \text{and} \quad \hat{P}\underset{\sim}{e}_3 = \underset{\sim}{e}_1$$

Using the fact that

$$\hat{P}\underset{\sim}{e}_i = \sum_j P_{ji}\underset{\sim}{e}_j$$

gives the following equations:

$$P_{11}\underset{\sim}{e}_1 + P_{21}\underset{\sim}{e}_2 + P_{31}\underset{\sim}{e}_3 = \underset{\sim}{e}_2 \implies P_{11} = 0,\ P_{21} = 1,\ P_{31} = 0$$

$$P_{12}\underset{\sim}{e}_1 + P_{22}\underset{\sim}{e}_2 + P_{32}\underset{\sim}{e}_3 = \underset{\sim}{e}_3 \implies P_{12} = 0,\ P_{22} = 0,\ P_{32} = 1$$

$$P_{13}\underset{\sim}{e}_1 + P_{23}\underset{\sim}{e}_2 + P_{33}\underset{\sim}{e}_3 = \underset{\sim}{e}_1 \implies P_{13} = 1,\ P_{23} = 0,\ P_{33} = 0$$

Hence $\hat{P}$ is represented by the matrix $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$.

1.13 BASIS CHANGE

The same vector $\underset{\sim}{u}$ can be represented by different bases in different ways:

$$\underset{\sim}{u} = \sum_i u_i \underset{\sim}{e}_i = \sum_i u'_i \underset{\sim}{e}'_i$$

i.e. the same vector but different components.

Similarly for matrices:

$$\hat{A}\underset{\sim}{e}_i = \sum_j A_{ji}\underset{\sim}{e}_j \,, \quad \hat{A}\underset{\sim}{e}'_i = \sum_j A'_{ji}\underset{\sim}{e}'_j$$

i.e. the same operator but different components.

Let us assume that there is a change of basis such that

$$\underset{\sim}{e}_i' = \sum_j S_{ji} \underset{\sim}{e}_j \quad \text{and} \quad \underset{\sim}{e}_i = \sum_j T_{ji} \underset{\sim}{e}_j'$$

Then $\underset{\sim}{e}_i' = \sum_j S_{ji} \sum_k T_{kj} \underset{\sim}{e}_k' = \sum_j \sum_k T_{kj} S_{ji} \underset{\sim}{e}_k'$

$$\Rightarrow \quad T_{kj} S_{ji} = \delta_{ki}$$

$$\Rightarrow \quad TS = I = ST$$

Therefore T is the inverse of S.

Also $\hat{A} \underset{\sim}{e}_i = \sum_j A_{ji} \underset{\sim}{e}_j$ and so $\hat{A} \underset{\sim}{e}_i'$ can be expressed in two ways:

(i) $\hat{A} \underset{\sim}{e}_i' = \sum_j A_{ji}' \underset{\sim}{e}_j' = \sum_k \sum_j A_{ji}' S_{kj} \underset{\sim}{e}_k$

(ii) $\hat{A} \underset{\sim}{e}_i' = \sum_j \hat{A} S_{ji} \underset{\sim}{e}_j = \sum_j \sum_k S_{ji} A_{kj} \underset{\sim}{e}_k$

Therefore $$\sum_j A_{kj} S_{ji} = \sum_j A_{ji}' S_{kj}$$

$$\Rightarrow \quad (AS)_{ki} = (SA')_{ki}$$

$$\Rightarrow \quad A' = S^{-1} A S$$

This is called a <u>similarity</u> <u>transformation</u> and shows how matrix representation changes for different basis even though the operator $\hat{A}$ is the same.

How do vector components change under $\hat{S}$?

$$\underset{\sim}{u} = \sum_i u_i \underset{\sim}{e}_i = \sum_i u_i' \sum_j S_{ji} \underset{\sim}{e}_j = \sum_i \sum_j S_{ij} u_j' \underset{\sim}{e}_i$$

where we have interchanged i and j.

$$\Rightarrow \qquad u_i = \sum_j S_{ij} u_j' \qquad \text{(summing over second index of } S\text{)}$$

In matrix form

$$\begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} S_{11} & \cdots & S_{1N} \\ \vdots & \ddots & \vdots \\ S_{N1} & \cdots & S_{NN} \end{pmatrix} \begin{pmatrix} u_1' \\ \vdots \\ u_N' \end{pmatrix}$$

We can represent the basis transformation

$$\underset{\sim}{e}_i' = \sum_j S_{ji} \underset{\sim}{e}_j = \sum_j \underset{\sim}{e}_j S_{ji}$$

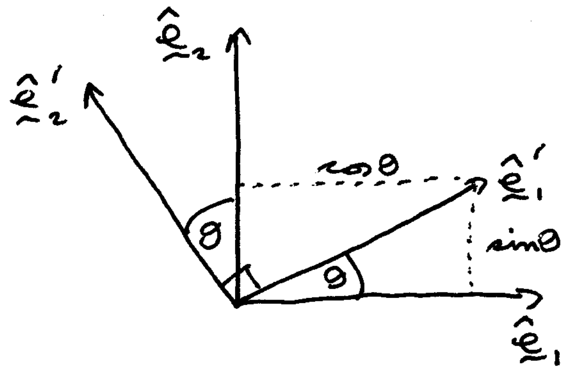
in matrix form by regarding $\underset{\sim}{e}_j$ as a row:

$$\left(e_1' \cdots e_N'\right) = \left(e_1 \cdots e_N\right) \begin{pmatrix} S_{11} & \cdots & S_{1N} \\ \vdots & \ddots & \vdots \\ S_{N1} & \cdots & S_{NN} \end{pmatrix}$$

Note: The basis index is distinct from the component index. Each basis has components $(\underset{\sim}{e}_j)_i$.

1.14 ROTATION OPERATOR

For $V = \mathbb{R}^2$ the rotation of Cartesian axes corresponds to



$$\hat{\underset{\sim}{e}}'_1 = \cos\theta\, \hat{\underset{\sim}{e}}_1 + \sin\theta\, \hat{\underset{\sim}{e}}_2$$

$$\hat{\underset{\sim}{e}}'_2 = -\sin\theta\, \hat{\underset{\sim}{e}}_1 + \cos\theta\, \hat{\underset{\sim}{e}}_2$$

where $\{\hat{\underset{\sim}{e}}_1, \hat{\underset{\sim}{e}}_2\}$ and $\{\hat{\underset{\sim}{e}}'_1, \hat{\underset{\sim}{e}}'_2\}$ are orthonormal bases.

Therefore the rotation operator, $\hat{R}$ is given by

$$\hat{R}\hat{\underset{\sim}{e}}_1 = R_{11}\hat{\underset{\sim}{e}}_1 + R_{21}\hat{\underset{\sim}{e}}_2 \quad \Rightarrow \quad R_{11} = \cos\theta,\ R_{21} = \sin\theta$$

$$\hat{R}\hat{\underset{\sim}{e}}_2 = R_{12}\hat{\underset{\sim}{e}}_1 + R_{22}\hat{\underset{\sim}{e}}_2 \quad \Rightarrow \quad R_{12} = -\sin\theta,\ R_{22} = \cos\theta$$

$$\Rightarrow \quad R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

<u>Check</u>: $$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$$

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$$

For a vector $\underset{\sim}{v}$,

$$\hat{R}\underset{\sim}{v} = \hat{R}\left(\sum_i v_i \hat{\underset{\sim}{e}}_i\right) = \sum_i v_i \hat{R}\hat{\underset{\sim}{e}}_i = \sum_i v_i \sum_j R_{ji}\hat{\underset{\sim}{e}}_j$$

$$= \sum_i \sum_j \left(R_{ji} v_i \right) \underset{\sim}{\hat{e}}_j$$

But $$\hat{R} \underset{\sim}{v} = \sum_j \left(\hat{R} v_j \right) \underset{\sim}{\hat{e}}_j$$

and so $$\left(\hat{R} \underset{\sim}{v} \right)_j = \sum_i R_{ji} v_i$$ (summing over second index)

note: $$R R^T = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = R^T R$$

Also, $|R| = \det R = 1$, corresponding to orthogonal matrix (i.e. R^T is inverse of R).

Generalising to $V = \mathbb{R}^N$, rotations are still described by orthogonal matrices with $R R^T = I$.

Then

$$\left(\hat{R} \underset{\sim}{v}, \hat{R} \underset{\sim}{w} \right) = \sum_i \sum_j \sum_k \left(R_{ij} v_j , R_{ik} w_k \right)$$

$$= \sum_i \sum_j \sum_k R_{ij} R_{ik} v_j w_k$$

$$= \sum_i \sum_j \sum_k \left(R^T \right)_{ji} R_{ik} v_j w_k$$

$$= \sum_{j,k} \delta_{jk} v_j w_k$$

$$= \left(\underset{\sim}{v}, \underset{\sim}{w} \right).$$

Also
$$(\hat{R}\underset{\sim}{v}, \hat{R}\underset{\sim}{v}) = (\underset{\sim}{v}, \underset{\sim}{v}).$$

Therefore lengths and angles are preserved under rotation since
$$(\underset{\sim}{v}, \underset{\sim}{w}) = \underset{\sim}{v} \cdot \underset{\sim}{w} = |\underset{\sim}{v}||\underset{\sim}{w}|\cos\theta$$
where $|\underset{\sim}{v}| = \sqrt{\underset{\sim}{v}\cdot\underset{\sim}{v}}$ and $|\underset{\sim}{w}| = \sqrt{\underset{\sim}{w}\cdot\underset{\sim}{w}}$.

Generalising to $V = \mathbb{C}^N$ gives the concept of a <u>unitary</u> <u>matrix</u> which satisfies
$$UU^{\dagger} = I = U^{\dagger}U \implies U^{\dagger} = U^{-1} \implies \hat{U}^{\dagger} = \hat{U}^{-1}$$
(distinguishing between the matrix U and the operator $\hat{U}$)

U^{-1} is also unitary since $(U^{-1})^{\dagger} = (U^{T})^{-1} = (U^{-1})^{-1}$.

Also, if we take the determinant
$$|U^{\dagger}U| = |U^{\dagger}||U| = |U^{*}||U| = 1$$
and so the unitary matrix has unit modulus – this is the natural generalisation of $|R| = 1$.

The orthonormal bases $\{\hat{\underset{\sim}{e}}_i\}$ and $\{\hat{\underset{\sim}{e}}_i'\}$ are related by a unitary matrix.

<u>PROOF</u> $\hat{\underset{\sim}{e}}_i' = \sum_j U_{ji}\hat{\underset{\sim}{e}}_j$
$$\implies (\hat{\underset{\sim}{e}}_i', \hat{\underset{\sim}{e}}_j') = \sum_k\sum_l U_{ki}^{*}U_{lj}(\hat{\underset{\sim}{e}}_k, \hat{\underset{\sim}{e}}_l)$$
$$= \sum_{k,l} U_{ki}^{*}U_{lj}\delta_{kl}$$

$$= \sum_k U_{ki}^* U_{kj} = (U^\dagger U)_{ij} = \delta_{ij}$$

Also, $\underset{\sim}{y} = \hat{U}\underset{\sim}{x} \Rightarrow Y^\dagger Y = X^\dagger U^\dagger U X = X^\dagger X$

(matrix notation)

which means that the norm is unchanged.

1.15 Hermitian Operators

The Hermitian conjugate of linear operator is defined by

$$(\underset{\sim}{w}, \hat{A}\underset{\sim}{v}) = (\hat{A}^\dagger \underset{\sim}{w}, \underset{\sim}{v})$$

$$\left(\text{cf. } (\underset{\sim}{w}, \lambda\underset{\sim}{v}) = \lambda(\underset{\sim}{w}, \underset{\sim}{v}) = (\lambda^* \underset{\sim}{w}, \underset{\sim}{v})\right)$$

An operator is Hermitian if

$$\hat{A} = \hat{A}^\dagger \Rightarrow (\underset{\sim}{w}, \hat{A}\underset{\sim}{v}) = (\hat{A}\underset{\sim}{w}, \underset{\sim}{v})$$

Then the matrix A is also Hermitian, $A_{ij} = A_{ji}^*$

PROOF

$$A_{ji} = (\hat{\underset{\sim}{e}}_j, \hat{A}\hat{\underset{\sim}{e}}_i) = (\hat{A}\hat{\underset{\sim}{e}}_j, \hat{\underset{\sim}{e}}_i) = \sum_k (A_{kj}\hat{\underset{\sim}{e}}_k, \hat{\underset{\sim}{e}}_i)$$

$$= \sum_k A_{kj}^* (\hat{\underset{\sim}{e}}_k, \hat{\underset{\sim}{e}}_i) = \sum_k A_{kj}^* \delta_{ki} = A_{ij}^*$$

$$\Rightarrow A = A^\dagger$$

1.16 EIGENVECTORS

Eigenvectors are vectors $\underset{\sim}{v}$ which satisfy the equation

$$A\underset{\sim}{v} = \lambda \underset{\sim}{v}$$

where λ is an eigenvalue of A.

$$\Rightarrow \quad \sum_j A_{ij} v_j = \lambda v_i$$

The eigenvalue equation, $A\underset{\sim}{v} = \lambda\underset{\sim}{v}$, can be written

$$(A - \lambda I)\underset{\sim}{v} = \underset{\sim}{0}$$

$$\Rightarrow \begin{pmatrix} A_{11} - \lambda & A_{12} \\ A_{21} & A_{22} - \lambda \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{for 2-D.}$$

$$\Rightarrow \det(A - \lambda I) = 0$$

which gives the characteristic polynomial for λ of degree N for $V = \mathbb{C}^N$.

Each solution λ_i gives the associated eigenvector $\underset{\sim}{v}^i$ (as distinct from the component v_i).

Note that since $A(\mu\underset{\sim}{v}) = \lambda(\mu\underset{\sim}{v})$ also satisfies the eigenvalue equation, eigenvectors can be normalised.

e.g. $$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0$$

$$\Rightarrow \lambda^2 - 1 = 0 \quad \Rightarrow \lambda = \pm 1$$

$$\lambda = 1 \Rightarrow \begin{pmatrix} v_2 \\ v_1 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = v_2 \Rightarrow \underset{\sim}{v}^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

(normalised)

$$\lambda = -1 \Rightarrow \begin{pmatrix} v_2 \\ v_1 \end{pmatrix} = -\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = -v_2 \Rightarrow \underset{\sim}{v}^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Similarly $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ gives $\begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm 1$

$$\lambda = 1 \Rightarrow \begin{pmatrix} -i v_2 \\ i v_1 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = -i v_2 \Rightarrow \underset{\sim}{v}^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\lambda = -1 \Rightarrow \begin{pmatrix} -i v_2 \\ i v_1 \end{pmatrix} = -\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = i v_2 \Rightarrow \underset{\sim}{v}^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Similarly $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ gives $\begin{vmatrix} -\lambda & 1 \\ -1 & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm i$ (complex)

$$\lambda = i \Rightarrow \begin{pmatrix} v_2 \\ -v_1 \end{pmatrix} = \begin{pmatrix} i v_1 \\ i v_2 \end{pmatrix} \Rightarrow v_1 = -i v_2 \Rightarrow \underset{\sim}{v}^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\lambda = -i \Rightarrow \begin{pmatrix} v_2 \\ -v_1 \end{pmatrix} = \begin{pmatrix} -i v_1 \\ -i v_2 \end{pmatrix} \Rightarrow v_1 = i v_2 \Rightarrow \underset{\sim}{v}^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

These examples illustrate a general rule - eigenvalues for a Hermitian matrix are real $(A_{ij}^* = A_{ji})$

PROOF $\quad (\underset{\sim}{v}, \hat{A}\underset{\sim}{v}) = (\hat{A}\underset{\sim}{v}, \underset{\sim}{v}) \Rightarrow \lambda(\underset{\sim}{v}, \underset{\sim}{v}) = \lambda^*(\underset{\sim}{v}, \underset{\sim}{v})$

$$\Rightarrow \lambda = \lambda^*$$

Eigenvectors for different eigenvalues are orthogonal

PROOF $\quad \hat{A}\underset{\sim}{v} = \lambda \underset{\sim}{v}, \; \hat{A}\underset{\sim}{w} = \mu \underset{\sim}{w} \Rightarrow (\underset{\sim}{w}, A\underset{\sim}{v}) = \lambda(\underset{\sim}{w}, \underset{\sim}{v})$

$$(A\underset{\sim}{w}, \underset{\sim}{v}) = \mu^*(\underset{\sim}{w}, \underset{\sim}{v}) = \mu(\underset{\sim}{w}, \underset{\sim}{v})$$

$$\Rightarrow (\underset{\sim}{w}, \underset{\sim}{v}) = 0 \text{ since } \lambda \neq \mu .$$

For a Hermitian matrix, H, one can construct a diagonal matrix from the eigenvalues,

$$D = \begin{pmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \lambda_N \end{pmatrix}$$

and a unitary matrix whose columns are the normalised eigenvectors

$$U = \begin{pmatrix} v_1^{(1)} & v_1^{(2)} & \dots & v_1^{(N)} \\ v_2^{(1)} & v_2^{(2)} & \dots & v_2^{(N)} \\ \vdots & \vdots & \ddots & \vdots \\ v_N^{(1)} & v_N^{(2)} & \dots & v_N^{(N)} \end{pmatrix}$$

Then $\quad H = UDU^{\dagger}$ and $H^{-1} = UD^{-1}U^{\dagger}$.

<u>PROOF</u> :

$$(U^{-1}HU)_{ij} = \sum_k \sum_l (U^{-1})_{ik} H_{kl} U_{lj} = \sum_{k,l} (U^{-1})_{ik} H_{kl} (v^j)_l$$

$$= \sum_k (U^{-1})_{ik} \lambda_j (v^j)_k \quad (\text{no } j \text{ sum})$$

$$= \sum_k \lambda_j (U^{-1})_{ik} U_{kj} = \lambda_j \delta_{ij} \quad (\text{no } j \text{ sum})$$

$$= D_{ij}$$

Hence $\qquad U^{-1}HU = D \Rightarrow H = UDU^{\dagger}$

Unitary and Hermitian matrices are related by the exponential function.

If H is Hermitian $\Rightarrow e^{H}$ is also Hermitian

(Also, if H is skew Hermitian, i.e. $H^{\dagger} = -H$, then e^{H} is unitary.)

1.17 LINK WITH QUANTUM MECHANICS

Observations in quantum mechanics are associated with Hermitian operators because the observed value is the eigenvalue and this must be real.

We can write the quantum state of a system as $|\underset{\sim}{u}\rangle$, which is a column vector with complex entries. Then $\langle \underset{\sim}{u}|$ is the complex conjugate row vector and

$$(\underset{\sim}{v}, \underset{\sim}{w}) = (|\underset{\sim}{v}\rangle, |\underset{\sim}{w}\rangle) = \langle \underset{\sim}{v} | \underset{\sim}{w}\rangle$$

Also

$$|\lambda \underset{\sim}{v}\rangle = \lambda |\underset{\sim}{v}\rangle, \quad \langle \lambda \underset{\sim}{v}| = \lambda^{*}\langle \underset{\sim}{v}|$$

We can write

$$|\hat{\underset{\sim}{e}}_i\rangle = |i\rangle$$

and

$$\sum_i \langle i | i \rangle = N \text{ but } \sum_i |i\rangle\langle i| = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

$$+ \cdots = I$$

1.18 GENERALISED INNER PRODUCT

For the generalised inner product we have to give up the concept that $(\underset{\sim}{v}, \underset{\sim}{v}) = 0 \Rightarrow \underset{\sim}{v} = \underset{\sim}{0}$.

In special relativity, $\delta_{ij} \rightarrow \eta_{\mu\nu}$ where $\mu = 0, 1, 2, 3$

and $\eta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$.

The 4-D distance is $(\underset{\sim}{x}, \underset{\sim}{x}) = \sum_{\mu,\nu} \eta_{\mu\nu} x^\mu x^\nu$

where $x^\mu = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$ and the Lorentz transformation

obeys $L^T \eta L = \eta$.

1.19 VECTOR SPACE OF FUNCTIONS

Well-behaved functions $f(x)$ on the interval $a \leq x \leq b$ form an infinite-dimensional vector space since

$$(f+g)(x) = f(x) + g(x)$$

$$(\lambda f)(x) = \lambda f(x)$$

$$f+g = g+f$$

$$(f+g)+h = f+(g+h)$$

$$\lambda(f+g) = \lambda f + \lambda g$$

$$\lambda(\mu f) = (\lambda\mu) f$$

$$(\lambda + \mu) f = \lambda f + \mu f$$

$\exists$ a null vector such that $f = 0 + f$

$\exists$ a vector $-f$ such that $f + (-f) = 0$.

Functions can be real (e.g. $ax + b$ with $a, b \in \mathbb{R}$) or complex (e.g. e^{itx} with $t \in \mathbb{R}$).

For real cases:

space of lines in $\mathbb{R}^2$, $f = a_0 + a_1 x$, has dimension 2.

space of polynomials, $f = a_0 + a_1 x + \dots + a_D x^D$, has dimension $D+1$

Then $f + g = (a_0 + b_0) + (a_1 + b_1) x + \dots + (a_D + b_D) x^D$

We can define the inner product as

$$(f, g) = \int_a^b f(x) g(x) \, dx$$

$$\Rightarrow \quad (\lambda f, g) = \lambda (f, g) = (f, \lambda g)$$

and $(f, \lambda g + \mu h) = \lambda (f, g) + \mu (f, h)$.

The functions are orthogonal if $(f, g) = 0$.

For complex functions,

$$(f, g) = \int_a^b f^*(x) g(x) w(x) \, dx$$

where the weight function $w(x)$ is real and non-negative in the interval (a, b).

Then
$$(f, g)^* = (g, f)$$
$$(f, \lambda g) = \lambda (f, g)$$
$$(\lambda f, g) = \lambda^* (f, g)$$

The norm is defined as
$$\|f\| = (f, f)^{1/2} = \left[\int_a^b |f(x)|^2 w(x)\, dx \right]^{1/2}$$

and so the unit vector is
$$\hat{f} = \frac{f}{\|f\|} .$$

Also, $\exists$ a basis $\phi_n(x)$ on $a \le x \le b$ such that
$$f(x) = \sum_n c_n \phi_n(x)$$

Choose the orthonormal basis:
$$\int_a^b \hat{\phi}_i^*(x)\, \hat{\phi}_j(x)\, w(x)\, dx = \delta_{ij}$$

Then, with $f(x) = \sum_n c_n \hat{\phi}_n(x)$, we have
$$c_n = (\hat{\phi}_n, f) = \int_a^b \hat{\phi}_n^*(x)\, f(x)\, w(x)\, dx$$

In the case of a real function, $\phi_n(x) = x^n$ $(n = 0, 1, \dots)$, giving a Taylor series but these are not orthonormal. For polynomials, taking $w(x) = 1$, $-1 \le x \le 1$, we have
$$\hat{\phi}_0 = \frac{1}{\sqrt{2}}, \quad \hat{\phi}_1 = \sqrt{\frac{3}{2}}\, x, \quad \hat{\phi}_2 = \frac{5}{2\sqrt{2}} (3x^2 - 1)$$
corresponding to the Legendre polynomials.

1.20 FOURIER SERIES

The Dirichlet conditions for $f(x)$ to have a Fourier series are:

1. periodic
2. single-valued and continuous except for a finite number of discontinuities
3. finite number of maxima and minima within the period
4. integral of $|f(x)|$ over the period converges

Then

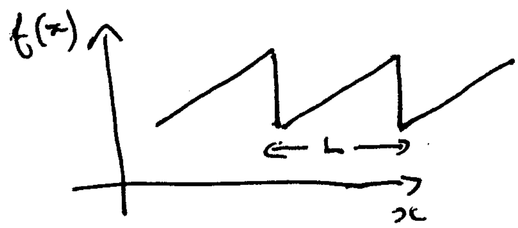
$$f(x) = \frac{1}{2}a_0 + \sum_{r=1}^{\infty}\left\{a_r \cos\frac{2\pi r x}{L} + b_r \sin\frac{2\pi r x}{L}\right\}$$

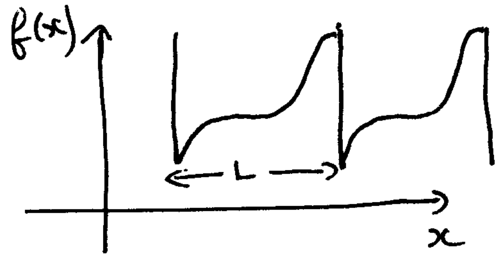
with
$$a_r = \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\cos\frac{2\pi r x}{L}\,dx$$

$$b_r = \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\sin\frac{2\pi r x}{L}\,dx$$

The factor of $\frac{1}{2}$ for a_0 gives $a_0 = \frac{2}{L}\int_{x_0}^{x_0+L} f(x)\,dx$

Usually take $x_0 = 0$ or $-\frac{L}{2}$.





Fourier series are easy to differentiate and integrate, with obvious physical significance (vibration of string, resonance, signal transmission in electric circuit).

Odd functions ($f(-x) = -f(x)$) are represented by Fourier sin series.

Even functions ($f(-x) = f(x)$) are represented by Fourier cosine series.

Because generally

$$f(x) = \frac{1}{2}\left[f(x) + f(-x)\right] + \frac{1}{2}\left[f(x) - f(-x)\right]$$

we will have a sine and cosine series.

We can combine these using complex numbers:

$$f(x) = \sum_{-\infty}^{\infty} c_r \exp \frac{2\pi i r x}{L}$$

with $$c_r = \frac{1}{L}\int_{x_0}^{x_0+L} f(x) . \exp\left(-\frac{2\pi i r x}{L}\right) dx .$$

It can be shown that

$$c_r = \frac{1}{2}(a_r - i b_r)$$

$$c_{-r} = \frac{1}{2}(a_r + i b_r)$$

We can also write the Fourier series as

$$f(x) = \frac{1}{2} a_0 + \sum_{k=1}^{\infty}\left(a_k e_k + \tilde{a}_k \tilde{e}_k\right)$$

with basis

$$e_k = \cos\frac{2\pi kx}{L}, \quad \tilde{e}_k = \sin\frac{2\pi kx}{L}$$

Then

$$e_k(x+L) = \cos\frac{2\pi kx}{L}\cos(2\pi k) - \sin\frac{2\pi kx}{L}\cancel{\sin(2\pi k)}$$

$$= e_k(x) \qquad \text{for } k = 0, 1, 2, \dots$$

Similarly

$$\tilde{e}_k(x+L) = \sin\frac{2\pi kx}{L}\cos(2\pi k) + \cos\frac{2\pi kx}{L}\cancel{\sin(2\pi k)}$$

$$= \tilde{e}_k(x) \qquad \text{for } k = 0, 1, 2, \dots$$

Hence

$$(e_k, e_l) = \int_{-L/2}^{L/2} \cos\frac{2\pi kx}{L}\cos\frac{2\pi lx}{L}\,dx$$

$$= \int_{-L/2}^{L/2} \frac{1}{2}\left\{\cos\frac{2\pi(k+l)x}{2L} + \cos\frac{2\pi(k-l)x}{2L}\right\}dx$$

$$= \frac{L}{\pi(k+l)}\sin\frac{\pi(k+l)}{2} + \frac{L}{\pi(k+l)}\sin\frac{\pi(k-l)}{2}$$

$$= N_k\delta_{kl} \quad \text{where } N_0 = L,\ N_k = \tfrac{1}{2}L \text{ for } k > 0$$

(note we have to go back to the integrand and treat those as special cases.)

Similarly

$$(\tilde{e}_k, \tilde{e}_l) = \int_{-L/2}^{L/2} \sin\frac{2\pi k x}{L} \sin\frac{2\pi l x}{L}\, dx$$

$$= \tilde{N}_k \delta_{kl} \text{ where } \tilde{N}_0 = 0,\ \tilde{N}_k = \tfrac{1}{2}L \text{ for } k > 0.$$

and

$$(e_k, \tilde{e}_l) = \int_{-L/2}^{L/2} \cos\frac{2\pi k x}{L} \sin\frac{2\pi l x}{L}\, dx$$

$$= 0 \text{ for all } k, l.$$

Thus $\{e_k, \tilde{e}_l\}$ are "nearly" orthonormal basis.

$$(e_s, f) = \tfrac{1}{2} a_0 (e_s, e_0) + \sum_{k=1}^{\infty} \left[a_k (e_s, e_k) + \cancel{\tilde{a}_k (e_s, \tilde{e}_k)} \right]$$

$$= \sum_{k=0}^{\infty} \tfrac{1}{2} L a_k \delta_{sk} = \tfrac{1}{2} L a_s$$

$$\Rightarrow \quad a_s = \frac{2}{L}(e_s, f) \qquad (s = 0, 1, \dots)$$

Also,

$$(\tilde{e}_s, f) = \sum_{k=1}^{\infty} \tilde{a}_k (\tilde{e}_s, \tilde{e}_k) = \tfrac{1}{2} L \tilde{a}_s$$

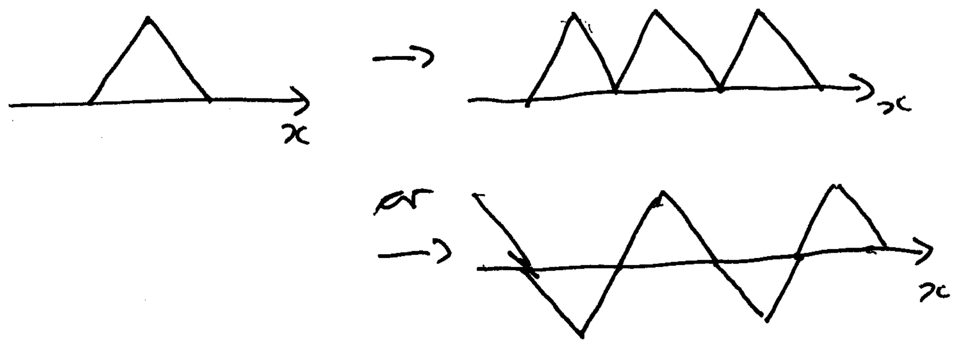
$$\Rightarrow \tilde{a}_s = \frac{2}{L}(\tilde{e}_s, f) \qquad (s = 1, 2, \dots)$$

cf. $$a_r = \frac{2}{L}\int_{x_0}^{x_0+L} f(x) \cos\frac{2\pi r x}{L}\, dx$$

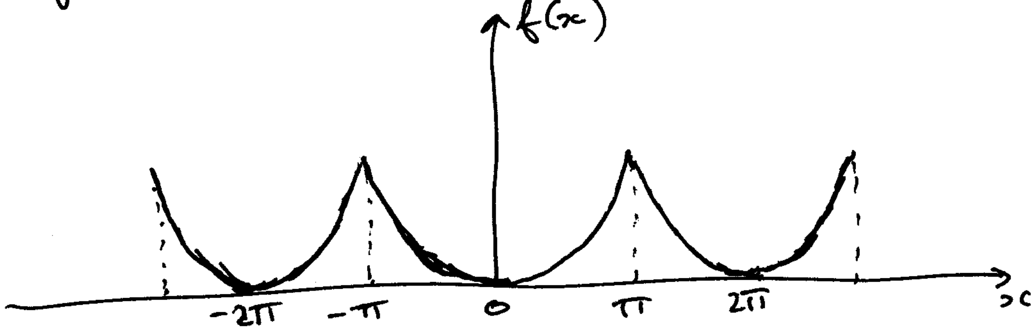
$$b_r = \frac{2}{L}\int_{x_0}^{x_0+L} f(x) \sin\frac{2\pi r x}{L}\, dx.$$

In the case of non-periodic functions we continue the function f outside the original range to make it periodic but continuous at the endpoints.

There are several ways of doing this:



e.g. $f(x) = x^2 \quad (-\pi \leq x \leq \pi)$ (even function)



$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} x^2 \cos(kx)\,dx = \frac{4}{k^2}(-1)^k$$

$$\tilde{a}_k = \frac{1}{\pi}\int_{-\pi}^{\pi} x^2 \sin(kx)\,dx = 0$$ (integrand is odd function)

1.21 ADJOINT, SELF-ADJOINT AND HERMITIAN OPERATORS

Let the operator $\mathcal{L}$ map f to another function, $\mathcal{L}f$.

The adjoint operator $\mathcal{L}^+$ is defined by

$$(\mathcal{L}^+ f, g) = (f, \mathcal{L}g)$$

i.e. $$\int_a^b f^*(x)\, \mathcal{L}\, g(x)\, w(x)\, dx$$

$$= \int_a^b \left[\mathcal{L}^\dagger f(x)\right]^* g(x)\, w(x)\, dx$$

plus boundary terms.

$\mathcal{L}$ is self-adjoint if $\mathcal{L} = \mathcal{L}^\dagger$.

$\mathcal{L}$ is Hermitian if the boundary terms vanish also.

The parity operator $(x \to -x)$ is Hermitian since

$$(f, Pg) = \int_{-L/2}^{L/2} f(x)\, g(-x)\, dx = -\int_{L/2}^{-L/2} f(-x)\, g(x)\, dx$$

$$= \int_{-L/2}^{L/2} f(-x)\, g(x)\, dx = (Pf, g).$$

Then $$(\tilde{e}_r, e_s) = 0$$

since $$(\tilde{e}_r, Pe_s) = (\tilde{e}_r, e_s) = (P\tilde{e}_r, e_s) = -(\tilde{e}_r, e_s)$$

using $e_s \sim \cos$ (even function), $\tilde{e}_r \sim \sin$ (odd function)

The derivative operator (d/dx) is nearly Hermitian

$$\left(f, \frac{d}{dx} g\right) = \int f^* \frac{dg}{dx}\, dx = \left[f^* g\right] - \int g \frac{df^*}{dx}\, dx$$

$$= -\left(\frac{d}{dx} f, g\right)$$

Hence $\left(\frac{d}{dx}\right)^{+} = -\frac{d}{dx}$.

But $\frac{d^2}{dx^2}$ is Hermitian since

$$\left(f, \frac{d^2 g}{dx^2}\right) = -\left(\frac{df}{dx}, \frac{dg}{dx}\right) = \left(\frac{d^2 f}{dx^2}, g\right)$$ and $i\frac{d}{dx}$ is Hermitian.

Then $(e_r, e_s) \propto \delta_{rs}$

since
$$\left(e_r, \frac{d^2 e_s}{dx^2}\right) = -\left(\frac{2\pi r}{L}\right)^2 (e_r, e_s)$$
$$= \left(\frac{d^2 e_r}{dx^2}, e_s\right)$$
$$= -\left(\frac{2\pi s}{L}\right)^2 (e_r, e_s)$$

$\Rightarrow (e_r, e_s) = 0$ unless $r = s$.

More generally $\mathcal{L}$ may be the <u>linear</u> differential operator $\frac{d}{dx}$, in which case the eigenfunctions $y_i(x)$ give solutions of the differential equation

$$\mathcal{L}\, y(x) = f(x)$$

with eigenvalues λ_i.

$$\mathcal{L}\, y_i = \lambda_i\, w(x)\, y_i \Rightarrow \int_a^b y_j^* \mathcal{L}\, y_i\, dx = \lambda_i \int_a^b y_j^* y_i\, w(x)\, dx.$$

If $\mathcal{L}$ is Hermitian,

$$\Rightarrow \int_a^b (\mathcal{L} y_j)^* y_i \, dx = \lambda_j^* \int_a^b y_j^* y_i \, w(x) \, dx \quad \text{is same.}$$

$i = j \Rightarrow \lambda_i$ real

$i \neq j \Rightarrow \int_a^b y_j^* y_i \, w(x) \, dx = 0 \quad \Rightarrow y_i, y_j$ orthogonal.