

Chapter 3 Matrices and Vectors 矩陣與向量

§ 3-1 Matrices 矩陣

令 m 與 n 為正整數，一個大小(size)或「階數 order」為 $m \times n$ 的矩陣是一個數字 A_{ij} 的有序集合(ordered set)其中 $1 \leq i \leq m, 1 \leq j \leq n$ ，長相如下：

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{pmatrix}$$

矩陣內的數字 A_{ij} 稱為第「 i 列(橫)、第 j 行(直)」的「矩陣元素 matrix element」，若 $m = n$ 則 A 稱為「方陣 square matrix」。下列 3-1 表列出矩陣 A 相關的矩陣

matrix	elements	example
A	A_{ij}	$\begin{pmatrix} 1 & i \\ 1+i & 2 \end{pmatrix}$
\tilde{A} (or A^T) Transpose of A (倒置)	$(\tilde{A})_{ij} = A_{ji}$	$\begin{pmatrix} 1 & 1+i \\ i & 2 \end{pmatrix}$
A^* Complex conjugate of A (複數共軛)	$(A^*)_{ij} = (A_{ij})^*$	$\begin{pmatrix} 1 & -i \\ 1-i & 2 \end{pmatrix}$
$A^+ \equiv (\tilde{A})^*$ Hermitian conjugate of A (厄密共軛)	$(A^+)_{ij} = (\tilde{A}_{ji})^* = A_{ji}^*$	$\begin{pmatrix} 1 & 1-i \\ -i & 2 \end{pmatrix}$

* Hermitian conjugate $A^+ = (A^T)^* = (A^*)^T$

pf. $(A^*)_{ij}^T = (A^*)_{ji} = (A_{ji})^* = (\tilde{A}_{ij})^* = \tilde{A}_{ij}^*$, q.e.d.

* 對於矩陣 A , 若存在矩陣 A^{-1} 使得

$$A^{-1}A = AA^{-1} = 1 = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

A^{-1} 稱為 A 的反矩陣(inverse). 上式中的「1」矩陣稱為「單位矩陣 unit matrix」, 其元素除了對角線上的元素全為 1 之外其餘元素全為 0。此處引進一個符號

$$\text{Kronecher delta: } \delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}, \text{ 即 } 1_{ij} = \delta_{ij} \circ$$

可以證明任何方陣 A 乘以相同大小的單位矩陣 1 等於 A 自己, 即

$$1A = A1 = A$$

pf. $(1 \cdot A)_{ij} = \sum_k 1_{ik} A_{kj} = \sum_k \delta_{ik} A_{kj} = A_{ij}$ (因為所有 $k \neq i$ 的項都為 0)。又

$$(A \cdot 1)_{ij} = \sum_k A_{ik} 1_{kj} = \sum_k A_{ik} \delta_{kj} = A_{ij}$$
 (因為所有 $k \neq j$ 的項都為 0)

* 矩陣的相等: $A = B \Leftrightarrow A_{ij} = B_{ij}$, 即各對應元素皆相等。

* 若 A 與 B 為相同的 n 階方陣則定義運算如下

$$(\lambda A)_{ij} = \lambda A_{ij}, \quad \lambda = \text{const.} \quad (3-1)$$

$$(A + B)_{ij} = A_{ij} + B_{ij} \quad (3-2)$$

$$(AB)_{ij} = \sum_{k=1}^n A_{ik} B_{kj} \quad (3-3)$$

$$\begin{pmatrix} (AB)_{11} & (AB)_{12} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & (AB)_{ij} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ A_{i1} & A_{i2} & \dots & A_{in} \\ A_{n1} & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} B_{11} & \dots & B_{1j} & B_{1n} \\ B_{21} & \dots & B_{2j} & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & B_{nj} & \dots \end{pmatrix}$$

(3-3) 全寫出來就是 $\sum_{k=1}^n A_{ik} B_{kj} = A_{i1} B_{1j} + A_{i2} B_{2j} + \dots + A_{in} B_{nj} \circ$

若 $C = AB$, $C_{ij} = \sum_{k=1}^n A_{ik} B_{kj}$

ex. $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} ax+by \\ cx+dy \end{pmatrix}$

ex. $\begin{pmatrix} 2 & 5 & 8 \\ 1 & 2 & 3 \\ 3 & 6 & 9 \end{pmatrix} \begin{pmatrix} 1 & 0 & 2 \\ 0 & 8 & 1 \\ 4 & 7 & 5 \end{pmatrix} = \begin{pmatrix} 2 \cdot 1 + 5 \cdot 0 + 8 \cdot 4 & 2 \cdot 0 + 5 \cdot 8 + 8 \cdot 7 & 3 \cdot 1 + 6 \cdot 0 + 9 \cdot 4 \\ 1 \cdot 1 + 2 \cdot 0 + 3 \cdot 4 & 1 \cdot 0 + 2 \cdot 8 + 3 \cdot 7 & 3 \cdot 0 + 6 \cdot 8 + 9 \cdot 7 \\ 3 \cdot 1 + 6 \cdot 0 + 9 \cdot 4 & 3 \cdot 0 + 6 \cdot 8 + 9 \cdot 7 & 3 \cdot 2 + 6 \cdot 1 + 9 \cdot 5 \end{pmatrix}$

注意，通常 $AB \neq BA$ ，例如

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \text{ but } \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$$

但是 $(AB)C = A(BC)$

pf.

$$((AB)C)_{ij} = \sum_k (AB)_{ik} C_{kj} = \sum_k \sum_t A_{it} B_{tk} C_{kj} = \sum_t A_{it} \sum_k B_{tk} C_{kj} = \sum_t A_{it} (BC)_{tj} = (A(BC))_{ij}$$

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

pf. $(AB)_{ij}^T = (AB)_{ji} = \sum_k A_{jk} B_{ki} = \sum_k A_{kj}^T B_{ik}^T = \sum_k B_{ik}^T A_{kj}^T = (B^T A^T)_{ij} \Rightarrow (AB)^T = B^T A^T$

* $(AB)^{-1} = B^{-1} A^{-1}$

$$\left. \begin{array}{l} \because (B^{-1} A^{-1}) \cdot (AB) = B^{-1} A^{-1} AB = B^{-1} B = 1 \\ \text{and } (AB) \cdot (B^{-1} A^{-1}) = AB B^{-1} A^{-1} = AA^{-1} = 1 \end{array} \right\} \Rightarrow B^{-1} A^{-1} = (AB)^{-1}$$

* 矩陣 A 的行列式 (determinant) $\det A$

每一個 n 階的方陣 A 都對應一個數字稱為 A 的行列式。

2x2 矩陣行列式的定義如下：

$$\text{if } A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow \det A = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - cb.$$

3 階方陣的行列式定義如下：

* The Levi-Civita symbol ε_{ijk}

考慮 {i, j, k} 為 {1, 2, 3} 3 個正整數的有序排列(permutation)集合, 這樣的集合共有 $3! = 6$ 個: {1,2,3}, {1,3,2}, {2,1,3}, {2,3,1}, {3,1,2}, {3,2,1}.

定義「交換數 number of inversion」為 $\{i, j, k\}$ 經相鄰數字左、右交換而成 $\{1, 2, 3\}$ 的總交換數。定義 Levi-Civita 符號 ε_{ijk}

$$\varepsilon_{ijk} = \begin{cases} +1, & \text{if number of inversion of } \{i, j, k\} \rightarrow \{1, 2, 3\} = \text{even.} \\ -1, & \text{if number of inversion of } \{i, j, k\} \rightarrow \{1, 2, 3\} = \text{odd} \end{cases}$$

$$\therefore \begin{cases} \varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \\ \varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1 \end{cases}$$

且 $\varepsilon_{ijk} = 0$ 如果任二腳標相等，i.e., $\varepsilon_{112} = \varepsilon_{131} = \varepsilon_{212} = \dots = 0$

* 一個 3 階矩陣 A 的「行列式」 $\det A$ 定義為

$$\det A = \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} = \sum_{\text{all } \{i, j, k\}} \delta_{ijk} A_{1i} A_{2j} A_{3k}$$

$$\det A = \sum \varepsilon_{ijk} A_{1i} A_{2j} A_{3k} = A_{11}A_{22}A_{33} + A_{13}A_{23}A_{32} + A_{12}A_{23}A_{31} - A_{13}A_{22}A_{31} - A_{12}A_{21}A_{33} - A_{11}A_{23}A_{32}$$

有一種簡單的 3×3 矩陣行列式的算法：

$$\text{ex. } A = \begin{vmatrix} 1 & 2 & 3 \\ -1 & 3 & 0 \\ 2 & -4 & 5 \end{vmatrix} = \begin{vmatrix} 1 & 2 & 3 & 1 & 2 \\ -1 & 3 & 0 & -1 & 3 \\ 2 & -4 & 5 & 2 & -4 \end{vmatrix} = 15 + 0 + 12 - 18 - 0 + 10 = 19$$

$$= 1 \cdot \begin{vmatrix} 3 & 0 \\ -4 & 5 \end{vmatrix} - 2 \cdot \begin{vmatrix} -1 & 0 \\ 2 & 5 \end{vmatrix} + 3 \cdot \begin{vmatrix} -1 & 3 \\ 2 & -4 \end{vmatrix} = 15 - 2(-5) + 3(4 - 6) = 15 + 10 - 6 = 19$$

另有一個 3 階方陣行列式的算法：

$$\det A = \sum_{j=1}^3 (-1)^{i+j} A'_{ij}, \quad \text{對任何一列 } i.$$

其中 A'_{ij} 為「cofactor of element A_{ij} 」

$$A'_{ij} = \det(\text{原方陣 } A \text{ 去掉第 } i \text{ 列及第 } j \text{ 行剩下的 } n-1 \text{ 階方陣})$$

* 行列式為 0 的方陣稱為「singular matrix」。若一方陣行列式非 0 則為「nonsingular」。

* 由「行列式」的定義可推出下列性質：

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

2. 若 A 任何行或列全為 0 則 $\det A = 0$ 。例如 $\begin{vmatrix} 2 & 0 & 3 \\ 1 & 0 & 1 \\ -1 & 0 & 4 \end{vmatrix} = 0$ 。

3. $\begin{vmatrix} \gamma a & \gamma b & \gamma c \\ d & e & f \\ g & h & i \end{vmatrix} = \gamma \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix}$ 。例如 $\begin{vmatrix} -6 & 3 & -9 \\ 2 & 1 & 0 \\ 1 & 1 & 2 \end{vmatrix} = -3 \begin{vmatrix} 2 & -1 & 3 \\ 2 & 1 & 0 \\ 1 & 1 & 2 \end{vmatrix}$ 。

4. A 任二行（或列）互換後所得的方陣的行列式 = $-\det A$ 。例如

$$\begin{vmatrix} 1 & -1 & 3 \\ 0 & 4 & 1 \\ 2 & 2 & 5 \end{vmatrix} = - \begin{vmatrix} 2 & 2 & 5 \\ 0 & 4 & 1 \\ 1 & -1 & 3 \end{vmatrix}。$$

5. 若 A 的任二行（或列）的元素全等，則 $\det A = 0$ 。例如

$$\begin{vmatrix} 2 & 1 & 2 \\ 1 & -4 & 1 \\ 3 & 5 & 3 \end{vmatrix} = 0。$$

6. $\det A$ 可經由某行（或列）的「拆解」而成 2 個方陣行列式的和。

例如

$$\begin{vmatrix} 1 & 2+3 & 3 \\ 0 & 1-4 & 5 \\ 2 & -2+0 & 6 \end{vmatrix} = \begin{vmatrix} 1 & 2 & 3 \\ 0 & 1 & 5 \\ 2 & -2 & 6 \end{vmatrix} + \begin{vmatrix} 1 & 3 & 3 \\ 0 & -4 & 5 \\ 2 & 0 & 6 \end{vmatrix}。$$

7. 某行（或列）加上另一行（或列）的 c 倍後，新方陣的行列式不變。例如

$$\begin{vmatrix} 2 & -1 & 0 \\ 1 & 2 & -3 \\ 4 & 5 & 6 \end{vmatrix} = \begin{vmatrix} 4 & 3 & -6 \\ 1 & 2 & -3 \\ 4 & 5 & 6 \end{vmatrix} : \text{右邊的行列式爲左邊的第一列加上第二}$$

列 $\times 2$ 。

* A 的反矩陣 A^{-1}

$$(A^{-1})_{ij} = \frac{\text{cofactor of } A_{ji}}{\det A}, \text{ i.e., if } \det A = 0, A^{-1} \text{ 不存在。其中}$$

cofactor of $A_{ji} = (-1)^{j+i} \det(A \text{ 去掉第 } j \text{ 列與第 } i \text{ 行後剩下的 } n-1 \text{ 階矩陣})$

ex. $A = \begin{pmatrix} 1 & i \\ 1+i & 2 \end{pmatrix} \Rightarrow \det A = 2 - (i-1) = 3-i \neq 0 \Rightarrow A^{-1} = \frac{1}{3-i} \begin{pmatrix} 1 & -i \\ -1-i & 1 \end{pmatrix}$

check: $AA^{-1} = \frac{1}{3-i} \begin{pmatrix} 2-i+1 & -i+i \\ 2+2i-2-2i & -i+1+2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $A^{-1}A = 1$.

Ex. $A = \begin{pmatrix} 1 & 0 & 3 \\ 2 & 0 & 0 \\ 2 & 2 & 1 \end{pmatrix} \Rightarrow \det A = 12 \Rightarrow A^{-1} = \frac{1}{12} \begin{pmatrix} 0 & 6 & 0 \\ -2 & -5 & 6 \\ 4 & -2 & 0 \end{pmatrix}$

Check: $AA^{-1} = \frac{1}{12} \begin{pmatrix} 12 & 6-6 & 0 \\ 0 & 12 & 0 \\ -4+4 & 12-10-2 & 12 \end{pmatrix} = 1 = A^{-1}A$.

Ex. 非齊次聯立方程組的解

$$\begin{cases} ax + by + cz = \alpha \\ dx + ey + fz = \beta \\ gx + hy + lz = \gamma \end{cases} \Rightarrow \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & l \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \equiv A \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

上式兩邊 $\times A^{-1} \Rightarrow A^{-1}A \begin{pmatrix} x \\ y \\ z \end{pmatrix} = A^{-1} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \Rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = A^{-1} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$ ，只要 $\det A \neq 0$ 。

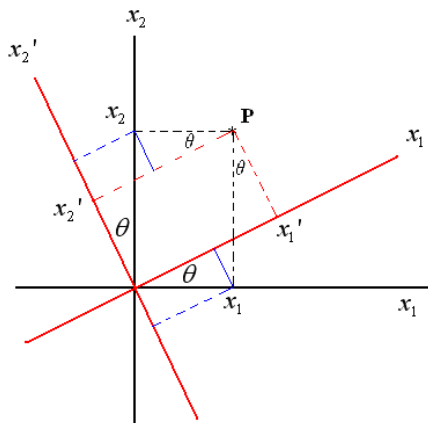
但是如果是齊次方程式 $\alpha = \beta = \gamma = 0$

$$\Rightarrow A \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \text{if } A^{-1} \text{ 存在} \Rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = A^{-1} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow x = y = z = 0$$

就只剩全 0 的「自明解 trivial solution」。所以齊次方程組要想有 nontrivial solution，那麼方程組裡未知數係數所形成的矩陣的行列式就不能為 0。

§ 3-2 座標轉換

考慮一個單純的座標旋轉。此處我們使用 (x_1, x_2) 而不用 (x, y) 來寫平面座標。考慮繞垂直於 x_1 與 x_2 軸且通過原點的軸



逆時針轉 θ 角，並定義轉完後的座標軸為 x'_1 與 x'_2 軸。若平面上一點P其座標在原座標系為 (x_1, x_2) ，在新座標系為 (x'_1, x'_2) 則可看出新舊座標之間的關係為

$$\begin{cases} x'_2 = -x_1 \sin \theta + x_2 \cos \theta & (3-1a) \\ = x_1 \cos(\frac{\pi}{2} + \theta) + x_2 \cos \theta & (3-1b) \\ x'_1 = x_1 \cos \theta + x_2 \sin \theta & (3-2a) \\ = x_1 \cos \theta + x_2 \cos(\frac{\pi}{2} - \theta) & (3-2b) \end{cases} \Rightarrow \begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

其中 $\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$ 稱為平面的「轉換或旋轉矩陣」。由(3-1b)與(3-2b)

可以看出若定義

$$\lambda_{ij} \equiv \cos(x'_i, x_j) = \cos(x'_i - \text{axis 與 } x_j - \text{axis 的夾角})$$

$$\Rightarrow \begin{cases} \lambda_{11} = \cos(x'_1, x_1) = \cos \theta \\ \lambda_{12} = \cos(x'_1, x_2) = \cos(\frac{\pi}{2} - \theta) = \sin \theta \\ \lambda_{21} = \cos(x'_2, x_1) = \cos(\frac{\pi}{2} + \theta) = -\sin \theta \\ \lambda_{22} = \cos(x'_2, x_2) = \cos \theta \end{cases}$$

這使得平面的座標旋轉可以重新寫為

$$\begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}。$$

或在 3D 空間

$$\begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\Rightarrow x'_1 = \lambda_{11}x_1 + \lambda_{12}x_2 + \lambda_{13}x_3 = \sum_{j=1}^3 \lambda_{1j}x_j$$

similar for x'_2 and x'_3 .

所以可以寫出一個通式

$$x'_i = \sum_{j=1}^3 \lambda_{ij}x_j, \text{ for } i=1,2,3. \text{ 請特別注意 } i, j \text{ 的順序} \quad (3-14)$$

做為結論，3D 空間的旋轉矩陣可寫為 $\lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{pmatrix}$

其矩陣元素 $\lambda_{ij} = \cos(x'_i, x_j)$ 為 x'_i 軸在相對於 x_j 軸的「方向餘弦 directional cosine」。

Ex. 考慮值角座標系對 x_3 軸逆時針轉 90°

$$\Rightarrow \begin{cases} x'_1 = x_2 \\ x'_2 = -x_1 \\ x'_3 = x_3 \end{cases} \Rightarrow \text{非 0 矩陣元素為} \begin{cases} \cos(x'_1, x_2) = 1 = \lambda_{12} \\ \cos(x'_2, x_1) = -1 = \lambda_{21} \\ \cos(x'_3, x_3) = 1 = \lambda_{33} \end{cases}$$

$$\Rightarrow \lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

現考慮對 x_1 軸逆時針轉 90°

$$\Rightarrow \begin{cases} x'_1 - \text{axis} = x_1 \text{axis} \\ x'_2 = x_3 \\ x'_3 = -x_2 \end{cases} \Rightarrow \lambda_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

若定義向量

$$X = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad X' = \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix}$$

考慮兩次座標旋轉：先對 x_3 軸逆時針轉 90° 之後再對新的 x_1 軸逆時針轉 90°

$$\Rightarrow X' = \lambda_1 X, \text{ and } X'' = \lambda_2 X' = \lambda_2 \lambda_1 X \text{ 則}$$

$$\begin{pmatrix} x''_1 \\ x''_2 \\ x''_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_3 \\ x_1 \end{pmatrix}$$

然而若將這兩個座標旋轉的次序顛倒，結果

$$\lambda_1 \lambda_2 X = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_3 \\ -x_1 \\ -x_2 \end{pmatrix}$$

可以看出總旋轉矩陣 $\lambda_1 \lambda_2 \neq \lambda_2 \lambda_1$ 所以最終結果也不同。這也是矩陣乘法「不可交換性 non-commutability」的一個明顯的例子。本例子也清楚點出旋轉運動中角度變化「角位移」 $\Delta\theta$ 不是一個向量，因為不滿足向量加法的可交換性。

* 旋轉矩陣的性質

(1) 空間中過原點一直線與 x_1, x_2, x_3 軸的夾角分別為 α, β, γ ，則該直線的方向餘弦 directional cosine 滿足

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1 \quad (3-5)$$

證明 (3-5) 式如下：令 \vec{r} 為在直線上點 P 的位置向量

$$\Rightarrow \vec{r} = [r \cos \alpha, r \cos \beta, r \cos \gamma]$$

$$\begin{aligned} \vec{r} \cdot \vec{r} &= x^2 + y^2 + z^2 = (r \cos \alpha)^2 + (r \cos \beta)^2 + (r \cos \gamma)^2 = r^2 \\ \Rightarrow (\cos \alpha)^2 + (\cos \beta)^2 + (\cos \gamma)^2 &= 1. \end{aligned}$$

(2) 若過原點兩直線與 x_1, x_2, x_3 軸的夾角分別為 (α, β, γ) 與 $(\alpha', \beta', \gamma')$ ，而且兩直線間夾角為 θ ，則

$$\cos \theta = \cos \alpha \cos \alpha' + \cos \beta \cos \beta' + \cos \gamma \cos \gamma' \quad (3-6)$$

證明 (3-6) 式如下：兩直線上各選一點 P 與 P'，位置向量各為

$$\begin{aligned} \vec{r} &= [r \cos \alpha, r \cos \beta, r \cos \gamma], \quad \vec{r}' = [r' \cos \alpha', r' \cos \beta', r' \cos \gamma'] \\ \vec{r} \cdot \vec{r}' &= xx' + yy' + zz' \\ &= rr' \cos \alpha \cos \alpha' + rr' \cos \beta \cos \beta' + rr' \cos \gamma \cos \gamma' = rr' \cos \theta \\ \Rightarrow \cos \theta &= \cos \alpha \cos \alpha' + \cos \beta \cos \beta' + \cos \gamma \cos \gamma'. \end{aligned}$$

現考慮座標系 (x_1, x_2, x_3) 對一通過原點的任意軸做旋轉而成 $\Rightarrow (x'_1, x'_2, x'_3)$ ，而 $\lambda_{ij} = \cos(x'_i, x_j), j=1..3$ 。則為 x'_i 軸在原座標系 (x_1, x_2, x_3) 的方向餘弦。由 (3-5)，因 x'_1 軸方向餘弦可得

$$\lambda_{11}^2 + \lambda_{12}^2 + \lambda_{13}^2 = 1 \quad (3-7)$$

similarly, 由 x'_2 與 x'_3 可得 $\lambda_{21}^2 + \lambda_{22}^2 + \lambda_{23}^2 = 1$ 與 $\lambda_{31}^2 + \lambda_{32}^2 + \lambda_{33}^2 = 1$ ，連同上式可寫為

$$\sum_{j=1}^3 \lambda_{1j}^2 = \sum_j \lambda_{1j} \lambda_{1j} = 1 = \sum_j \lambda_{2j} \lambda_{2j} = \sum_j \lambda_{3j} \lambda_{3j} \quad (3-8)$$

$$\Rightarrow \sum_j \lambda_{ij} \lambda_{kj} = 1, \text{ if } i = k. \quad (3-9)$$

已知 x'_1 軸和 x'_2 在原座標系的方向餘弦分別為 $(\lambda_{11}, \lambda_{12}, \lambda_{13})$ 與 $(\lambda_{21}, \lambda_{22}, \lambda_{23})$ ，現由於 x'_1 與 x'_2 夾角為 90° ，所以可由 (3-6)

$$\Rightarrow \lambda_{11} \lambda_{21} + \lambda_{12} \lambda_{22} + \lambda_{13} \lambda_{23} = \cos \theta = \cos \frac{\pi}{2} = 0 \Rightarrow \sum_j \lambda_{1j} \lambda_{2j} = 0$$

由於 x'_1 與 x'_3 夾角為 90° 、 x'_2 與 x'_3 夾角亦為 90° ，所以

$$\sum_j \lambda_{1j} \lambda_{3j} = 0 = \sum_j \lambda_{2j} \lambda_{3j} = \sum_j \lambda_{1j} \lambda_{2j} \quad (3-10)$$

$$\Rightarrow \sum_j \lambda_{ij} \lambda_{kj} = 0, \text{ if } i \neq k. \quad (3-11)$$

合併 (3-9) 與 (3-10) 與 kronecher delta，旋轉矩陣的元素有如下性質

$$\sum_j \lambda_{ij} \lambda_{kj} = \delta_{ik} \quad (3-12)$$

(3-12) 稱為旋轉矩陣元素的「正交條件 orthogonal condition」，是基於直角座標軸之間都是彼此正交（垂直）的。

一矩陣 A 被稱為「正交矩陣 orthogonal matrix」如果 $A^T = A^{-1}$ 。我們可以由 (3-12) 證明旋轉矩陣 λ 就是「正交矩陣」：

$$\text{pf. } \because (\lambda \lambda^T)_{ij} = \sum_k \lambda_{ik} \lambda_{kj}^T = \sum_k \lambda_{ik} \lambda_{jk} = \delta_{ij} = 1_{ij}$$

$$\text{且 } (\lambda^T \lambda)_{ij} = \delta_{ij} \Rightarrow \lambda \lambda^T = \lambda^T \lambda = 1 \Rightarrow \lambda^T = \lambda^{-1} \quad ((\lambda^T \lambda)_{ij} = \delta_{ij} \text{ 自己回去證明})$$

* 幾種特殊的矩陣

$$A = A^* \Leftrightarrow A: \text{real}$$

$$A^T = A \Leftrightarrow A: \text{symmetric}$$

$$A^T = -A \Leftrightarrow A: \text{antisymmetric}$$

$$A^+ = A \Leftrightarrow A: \text{Hermitian}$$

$$A^{-1} = A^T \Leftrightarrow A: \text{orthogonal}$$

$$A^{-1} = A^+ \Leftrightarrow A: \text{unitary}$$

$$A_{ij} = 0 \text{ if } i \neq j, \text{ or } A_{ij} = a_{ij} \delta_{ij} \Leftrightarrow A: \text{diagonal}$$

$$A^2 = A \Rightarrow (A^n = A) \Leftrightarrow A: \text{indepoten}$$

* 座標系統的 inversion : 透過原點的反射(reflection), 即所有 $x_i \rightarrow -x_i$ 。

$$\begin{cases} x'_1 = -x_1 \\ x'_2 = -x_2 \\ x'_3 = -x_3 \end{cases}$$

所以 inversion 矩陣為

$$\lambda_I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, (\lambda_I)_{ij} = -\delta_{ij} \Rightarrow \lambda_I^T = \lambda_I^{-1} \Rightarrow \lambda_I \text{ orthogonal.}$$

注意：座標 inversion 的動作是不能經由座標旋轉的組合形成！ i.e.,

$$\lambda_I \neq \lambda_R \lambda'_R \dots$$

其中 λ_R 表旋轉矩陣。可以證明 $\det \lambda_R = 1$ and $\det \lambda_I = -1$ ，所有的旋轉也稱為 proper rotation，而 inversion 則稱為 improper rotation。

座標旋轉在「純量」、「向量」的定義上是有意義的：考慮一個下列形式的座標轉換

$$x'_i = \sum_j \lambda_{ij} x_j \text{ with } \sum_j \lambda_{ij} \lambda_{kj} = \delta_{ik}$$

若一個量 φ 在這樣的座標轉換之下「不變」則 φ 為一純量，例如質量 $M(x', y', z') = M(x, y, z)$ 所以質量為一純量。若有一個量以集合 $\mathbf{A} = (A_1, A_2, A_3)$ 表現而當座標由 $\{x_i\} \xrightarrow{\lambda} \{x'_i\}$ 時 \mathbf{A} 的分量也做相同的轉換

$$A'_i = \sum_j \lambda_{ij} A_j \Rightarrow \bar{\mathbf{A}} = (A_1, A_2, A_3) \text{ is a vector.}$$

* 行列式的微分

$$A = A(x) \Rightarrow \det A = \sum \varepsilon_{ijk} A_{1i}(x) A_{2j}(x) A_{3k}(x)$$

$$\Rightarrow \frac{d}{dx} [\det A(x)] = \sum \varepsilon_{ijk} (A'_{1i} A_{2j} A_{3k} + A_{1i} A'_{2j} A_{3k} + A_{1i} A_{2j} A'_{3k})$$

$$\text{ex. } \frac{d}{dx} \begin{vmatrix} x & x^2 & x^3 \\ e^x & 1 & 0 \\ \sin x & 0 & 0 \end{vmatrix} = \begin{vmatrix} 1 & 2x & 3x^2 \\ e^x & 1 & 0 \\ \sin x & 0 & 0 \end{vmatrix} + \begin{vmatrix} x & x^2 & x^3 \\ e^x & 0 & 0 \\ \sin x & 0 & 0 \end{vmatrix} + \begin{vmatrix} x & x^2 & x^3 \\ e^x & 1 & 0 \\ \cos x & 0 & 0 \end{vmatrix}$$

§ 3-3 Eigenvalue problem 本徵值問題

一個任意的 $A_{3 \times 3}$ 矩陣可視為一個作用在任何一个 3×1 行向量

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

的「operator 算符」，作用如 $A\vec{v} = \vec{u}$ ，i.e., A 作用在 \vec{v} 後將 \vec{v} 變成 \vec{u} 。例如

$$\begin{pmatrix} 1 & 0 & 1 \\ 2 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \\ 1 \end{pmatrix}$$

* 對應於一個給定的矩陣 A ，有一組特別的向量 \vec{x} 具有一特性：

$$A\vec{x} = \lambda\vec{x}, \lambda \text{ 爲一常數}$$

$\Rightarrow \vec{x}$ 為矩陣 A 的「對應於「eigenvalue 本徵值」 λ 」的「本徵向量 eigenvector」。換言之，當矩陣 A 作用在自己的 eigenvector 時只會將 eigenvector 放大 λ 倍，而這個放大的倍數稱為 eigenvalue. 例如

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix} \text{ 就是矩陣 } A = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \text{ 的 eigenvector, } \therefore \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 2 \\ -2 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

對應的「本徵值」與「本徵向量」是相互聯繫的；每一個 A 的本徵向量只對應一個本徵值，但是對於某些「本徵值」有可能一個「本徵值」有多於一個「本徵向量」與之對應。

給定一個矩陣，要如何計算其對應的本徵值與本徵向量？請見下列例子：

$$A = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \text{ 令 } \bar{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \Rightarrow \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\Rightarrow (A - \lambda I)\bar{x} = \begin{pmatrix} 1-\lambda & -1 \\ -1 & 1-\lambda \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

要避免 trivial solution $x_1 = x_2 = 0$ 則前面的矩陣行列式必須為 0

$$\Rightarrow \det(A - \lambda I) = \det \begin{pmatrix} 1-\lambda & -1 \\ -1 & 1-\lambda \end{pmatrix} = 0$$

$$\Rightarrow (1-\lambda)^2 - 1 = (1-\lambda-1)(1-\lambda+1) = -\lambda(2-\lambda) = 0$$

$$\Rightarrow \lambda = 0, 2 \equiv \lambda_1, \lambda_2$$

上式在解 λ 時所導入的方程式 $\det(A - \lambda I) = 0$ 叫做 secular equation (久期方程式)。

對於本徵值 $\lambda_1 = 0$, let $\bar{x}_1 = \begin{pmatrix} a \\ b \end{pmatrix}$

$$\Rightarrow \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0 \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{pmatrix} a-b \\ -a+b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow a = b \Rightarrow \text{let } a = 1 = b \Rightarrow \bar{x}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\text{check: } \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0 \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

長度 = 1 的向量稱做「歸一化的 normalized」向量。我們通常希望所得的本徵向量是歸一化的，歸一化的 \bar{x}_1 就是原 \bar{x}_1 將自己的長度除掉

$$\bar{x}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \Rightarrow |\bar{x}_1| = 1.$$

對於本徵值 $\lambda_2 = 2$, let $\bar{x}_2 = \begin{pmatrix} c \\ d \end{pmatrix}$

$$\Rightarrow \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = 2 \begin{pmatrix} c \\ d \end{pmatrix} \Rightarrow \begin{pmatrix} 1-2 & -1 \\ -1 & 1-2 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} -c-d \\ -c-d \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow c = -d \Rightarrow c = 1 \Rightarrow d = -1 \Rightarrow \bar{x}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{check: } \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 2 \\ -2 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\text{normalized } \bar{x}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \Rightarrow |\bar{x}_2| = 1.$$

所以， $A = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \Rightarrow \lambda_1 = 0, \bar{x}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \lambda_2 = 2, \bar{x}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$

Ex. Find eigenvalues for $A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix}$

$$\text{From } (A - \lambda I)\bar{x} = \begin{bmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -1 & 1 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -\lambda & 0 & 1 \\ 0 & -\lambda & 1 \\ 0 & -1 & 1-\lambda \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0$$

$$\Rightarrow \det \begin{pmatrix} -\lambda & 0 & 1 \\ 0 & -\lambda & 1 \\ 0 & -1 & 1-\lambda \end{pmatrix} = 0 = -\lambda \begin{vmatrix} -\lambda & 1 \\ -1 & 1-\lambda \end{vmatrix} + \begin{vmatrix} 0 & -\lambda \\ 0 & -1 \end{vmatrix} = -\lambda[-\lambda(1-\lambda)+1] = -\lambda[\lambda^2 - \lambda + 1]$$

$$\Rightarrow \lambda = 0, \frac{1 \pm \sqrt{1-4}}{2} = \frac{1 \pm \sqrt{3}i}{2}$$

這也讓我們看到一個「實矩陣」是可能有「複數」的本徵值。

* 由於解「本徵值」時要解一個久期方程式

$$\det \begin{pmatrix} a_{11} - \lambda & a_{12} & \dots \\ a_{21} & a_{22} - \lambda & \dots \\ \dots & \dots & \dots \end{pmatrix} = 0$$

所以對於一個 $n \times n$ 的矩陣最多可以解出 n 個複根，但是常會遇到重根的 case，那些重根的 λ 稱為「簡併的 degenerate」本徵值。如果 λ 是 m 重根，則 λ 為「 m 重簡併 m -fold degenerate」。「簡併的」本徵值所對應的本徵向量也稱為「簡併的本徵向量」。

Ex. Find eigenvalues and eigenvectors for $A = \begin{pmatrix} 1 & 1 \\ -1 & 3 \end{pmatrix}$

$$\text{Sol. } \det \begin{vmatrix} 1-\lambda & 1 \\ -1 & 3-\lambda \end{vmatrix} = 0 = (1-\lambda)(3-\lambda) + 1 = \lambda^2 - 4\lambda + 4 = (\lambda-2)^2 \Rightarrow \lambda_1 = \lambda_2 = 2$$

$$\begin{pmatrix} 1 & 1 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 2 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \Rightarrow \begin{pmatrix} 1-2 & 1 \\ -1 & 3-2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} x_1 - x_2 = 0 \\ -x_1 + x_2 = 0 \end{cases} \Rightarrow x_1 = x_2$$

$$\Rightarrow \bar{x}_1 = \bar{x}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\text{check: } \begin{pmatrix} 1 & 1 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

ex. Find eigenvalues and eigenvectors for $A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$

$$\text{Sol: } \Rightarrow \det \begin{vmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{vmatrix} = 0 = -\lambda \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 1 \\ 1 & -\lambda \end{vmatrix} + \begin{vmatrix} 1 & -\lambda \\ 1 & 1 \end{vmatrix}$$

$$= -\lambda(\lambda^2 - 1) + (\lambda + 1) + (1 + \lambda)$$

$$= -\lambda(\lambda - 1)(\lambda + 1) + 2(\lambda + 1)$$

$$= (\lambda + 1)[2 - \lambda^2 + \lambda]$$

$$= (\lambda + 1)(-\lambda + 2)(\lambda + 1)$$

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

$$\Rightarrow \lambda = 2, -1, -1 \equiv \lambda_1, \lambda_2, \lambda_3.$$

For 非簡併本徵值 $\lambda_1 = 2$

$$\begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{cases} -2x_1 + x_2 + x_3 = 0 & (1) \\ x_1 - 2x_2 + x_3 = 0 & (2) \\ x_1 + x_2 - 2x_3 = 0 & (3) \end{cases} \left. \begin{matrix} (1) \\ (2) \end{matrix} \right\} 2x_1 - x_2 - x_3 = 0$$

$$\left. \begin{matrix} (1) \\ (3) \end{matrix} \right\} 2x_1 - x_2 - x_3 = 0$$

$$(1) - (2) \Rightarrow -3x_1 + 3x_2 = 0 \Rightarrow x_1 = x_2 \therefore \text{choose } x_1 = 1 = x_2$$

$$\Rightarrow \bar{x}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \Rightarrow \bar{x}_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

For 簡併本徵值 $\lambda_2 = \lambda_3 = -1$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow y_1 + y_2 + y_3 = 0$$

$$\Rightarrow \text{choose } y_1 = 1, y_2 = -1, y_3 = 0$$

$$\Rightarrow \bar{x}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \Rightarrow \bar{x}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

$$\text{or choose } y_1 = 1, y_2 = 0, y_3 = -1$$

$$\Rightarrow \bar{x}_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \Rightarrow \bar{x}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

總結：

$$\begin{cases} \lambda_1 = 2, \bar{x}_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}; \\ \lambda_2 = \lambda_3 = -1, \bar{x}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \bar{x}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \end{cases}$$

我們注意到 $\bar{x}_1 \cdot \bar{x}_2 = 0$ and $\bar{x}_1 \cdot \bar{x}_3 = 0$ 但是簡併本徵向量之間卻不彼此正交，不過我們可以透過所謂的「Gram-Schmit 過程」使得到一組相互正交的簡併本徵向量。

* 向量的內積(inner product, or, dot product) $\bar{a} \cdot \bar{b}$

考慮 2 個行向量

$$\bar{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}, \bar{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

定義 \bar{a}, \bar{b} 間的內積為

$$\bar{a} \cdot \bar{b} \equiv \bar{a}^+ \bar{b} = \begin{pmatrix} a_1^* & a_2^* & a_3^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \sum_i a_i^* b_i$$

* 2 個向量的內積若為 0, $\vec{a} \cdot \vec{b} = 0$, 稱向量 \vec{a}, \vec{b} 相互垂直 (正交 orthogonal)。

* Gram-Schmit 過程：一個將一組 n 個彼此不平行 (但不必彼此垂直) 的向量建構成一組 n 個彼此垂直向量的方法。先考慮一組 2 個不平行向量 $\{\vec{a}, \vec{b}; \vec{a} \neq c\vec{b}, c$ 為一常數 $\}$, 所以向量 \vec{b} 可以分解為平行與垂直 \vec{a} 的分量：

$$\begin{aligned}\vec{b} &= \vec{b}_{//} + \vec{b}_{\perp} \Rightarrow \vec{b}_{\perp} = \vec{b} - \vec{b}_{//} \\ \because \vec{b}_{//} &= (\vec{b} \cdot \hat{a})\hat{a} \\ \Rightarrow \vec{b}_{\perp} &= \vec{b} - (\vec{b} \cdot \hat{a})\hat{a} \\ \Rightarrow \{\vec{a}, \vec{b}_{\perp}\} &: \text{an orthogonal set.}\end{aligned}$$

上式中出現的 \hat{a} 為向量 \vec{a} 方向的「單位向量」 $\hat{a} = \frac{\vec{a}}{|\vec{a}|} = \frac{\vec{a}}{\sqrt{\vec{a} \cdot \vec{a}}}$ 。

再考慮 3 個不相互垂直的向量集合 $\{\vec{a}, \vec{b}', \vec{c}\}$, 我們可以先用 Gram-Schmit 由 \vec{b}' 建構 \vec{b} 使得 $\vec{a} \perp \vec{b}$, 於是 \vec{c} 可以分解為平行 \vec{a}, \vec{b} 的分量加上同時垂直於 \vec{a}, \vec{b} 的分量

$$\begin{aligned}\vec{c} &= \vec{c}_{\perp} + \vec{c}_a + \vec{c}_b \\ \Rightarrow \vec{c}_a &= (\vec{c} \cdot \hat{a})\hat{a}, \quad \vec{c}_b = (\vec{c} \cdot \hat{b})\hat{b} \\ \Rightarrow \vec{c}_{\perp} &= \vec{c} - \vec{c}_a - \vec{c}_b \Rightarrow \{\vec{a}, \vec{b}, \vec{c}_{\perp}\} \text{ an orthogonal set.}\end{aligned}$$

4 個以上的向量集合也模仿上面照章辦理。

Ex. 由 $\left\{ \vec{x}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \vec{x}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \vec{x}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right\}$ 建構一組正交集。

解：可以看出 $\vec{x}_1 \perp \vec{x}_2$

$$\begin{aligned}\bar{x}_{31} &\equiv (\bar{x}_3 \cdot \hat{x}_1)\hat{x}_1 = \frac{1}{2} \cdot 1 \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \\ \bar{x}_{32} &\equiv (\bar{x}_3 \cdot \hat{x}_2)\hat{x}_2 = \frac{1}{2} \cdot 1 \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \\ \Rightarrow \bar{x}_{3\perp} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} - \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - \frac{1}{2} - \frac{1}{2} \\ 0 - \frac{1}{2} + \frac{1}{2} \\ -1 - 0 - 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} \Rightarrow \bar{x}_{3\perp} \perp \bar{x}_1 \text{ and } \bar{x}_2\end{aligned}$$

* 定理：Hermitian 矩陣 A 的本徵值必全為實數，

i.e., if $A^+ = A$, and $A\bar{x} = \lambda\bar{x} \Rightarrow \lambda \in R$.

Pf. 先讓本徵向量 \bar{x} 為歸一化的向量： $|\bar{x}|^2 = \bar{x} \cdot \bar{x} = 1$

$$\begin{aligned}\text{for } A\bar{x} &= \lambda\bar{x} \Rightarrow (A\bar{x})^+ = (\lambda\bar{x})^+ \\ \Rightarrow \bar{x}^+ A^+ &= \lambda^* \bar{x}^+ \quad (\because (\lambda \cdot 1)^+ = \lambda^* \cdot 1) \\ \text{from } \bar{x} \cdot (A\bar{x}) &= \bar{x}^+ A\bar{x} = \bar{x}^+ (\lambda\bar{x}) = \lambda\bar{x} \cdot \bar{x} = \lambda \\ \text{also } \bar{x}^+ A\bar{x} &= (\bar{x}^+ A)\bar{x} = \lambda^* \bar{x}^+ \bar{x} = \lambda^* \bar{x} \cdot \bar{x} = \lambda^* \\ \therefore \lambda &= \lambda^* \Rightarrow \lambda \in R.\end{aligned}$$

* 定理：若 A 為 Hermitian 且 $\begin{cases} A\bar{x}_1 = \lambda_1\bar{x}_1 \\ A\bar{x}_2 = \lambda_2\bar{x}_2 \end{cases}$, $\lambda_1 \neq \lambda_2 \Rightarrow \bar{x}_1 \cdot \bar{x}_2 = 0$, i.e., $\bar{x}_1 \perp \bar{x}_2$

pf. 由 $A\bar{x}_1 = \lambda_1\bar{x}_1$

$$\begin{aligned}\Rightarrow \bar{x}_2 \cdot A\bar{x}_1 &= \lambda_1 \bar{x}_2 \cdot \bar{x}_1 \\ \text{also } \bar{x}_2 \cdot A\bar{x}_1 &= \bar{x}_2^+ A\bar{x}_1 = (\bar{x}_2^+ A)\bar{x}_1 = \lambda_2^* \bar{x}_2^+ \bar{x}_1 = \lambda_1 \bar{x}_2 \cdot \bar{x}_1 \\ \Rightarrow (\lambda_1 - \lambda_2^*) \bar{x}_2 \cdot \bar{x}_1 &= 0 \\ \Rightarrow \bar{x}_2 \cdot \bar{x}_1 &= 0 \quad (\because \lambda_1 \neq \lambda_2) \\ \therefore \bar{x}_2 &\perp \bar{x}_1\end{aligned}$$

習題

1. Evaluate the following determinants

$$(a) \begin{vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}, \quad (b) \begin{vmatrix} 1 & 2 & 0 \\ 3 & 1 & 2 \\ 0 & 3 & 1 \end{vmatrix}, \quad (c) \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{vmatrix}$$

2. Test the set of linear homogeneous equations

$$x + 3y + 3z = 0,$$

$$x - y + z = 0,$$

$$2x + y + 3z = 0,$$

to see if it possesses a nontrivial solution.

3. Given the pair of equations

$$x + 2y = 3,$$

$$2x + 4y = 6,$$

(a) Show that the determinant of the coefficients vanishes.

(b) Show that the numerator determinants (Eq. (3.18)) also vanish.

(c) Find at least two solutions.

4. (a) The matrix equation $A^2 = 0$ does not imply $A = 0$. Show that the most general 2×2 matrix whose square is zero may be written as

$$\begin{pmatrix} ab & b^2 \\ -a^2 & -ab \end{pmatrix},$$

where a and b are real or complex numbers.

(b) If $C = A + B$, in general

$$\det C \neq \det A + \det B.$$

Construct a specific numerical example to illustrate this inequality.

5. Given

$$K = \begin{pmatrix} 0 & 0 & i \\ -i & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},$$

show that

$$K^n = KKK \dots (n \text{ factors}) = 1$$

(with the proper choice of n , $n \neq 0$).

6. Show that $(AB)^\dagger = B^\dagger A^\dagger$.

7. Matrix C is *not* Hermitian. Show that $C + C^\dagger$ and $i(C - C^\dagger)$ are Hermitian. This means that a non-Hermitian matrix may be resolved into two Hermitian parts

$$C = \frac{1}{2}(C + C^\dagger) + \frac{1}{2i}i(C - C^\dagger).$$

This decomposition of a matrix into two Hermitian matrix parts parallels the decomposition of a complex number z into $x + iy$, where $x = (z + z^*)/2$ and $y = (z - z^*)/2i$.

8. Find the eigenvalues and orthonormal eigenvectors for the following matrices.

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad \text{ANS. } \lambda = 0, 1, 2.$$

$$A = \begin{pmatrix} 1 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad \text{ANS. } \lambda = -1, 0, 2.$$

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}. \quad \text{ANS. } \lambda = -1, 1, 2.$$

$$A = \begin{pmatrix} 1 & \sqrt{8} & 0 \\ \sqrt{8} & 1 & \sqrt{8} \\ 0 & \sqrt{8} & 1 \end{pmatrix}. \quad \text{ANS. } \lambda = -3, 1, 5.$$

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}. \quad \text{ANS. } \lambda = 0, 1, 2.$$

9. (a) Determine the eigenvalues and eigenvectors of

$$\begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}.$$

Note that the eigenvalues are degenerate for $\varepsilon = 0$ but the eigenvectors are orthogonal for all $\varepsilon \neq 0$ and $\varepsilon \rightarrow 0$.

- (b) Determine the eigenvalues and eigenvectors of

$$\begin{pmatrix} 1 & 1 \\ \varepsilon^2 & 1 \end{pmatrix}.$$

Note that the eigenvalues are degenerate for $\varepsilon = 0$ and for this (non-symmetric) matrix the eigenvectors ($\varepsilon = 0$) do *not* span the space.

- (c) Find the cosine of the angle between the two eigenvectors as a function of ε for $0 \leq \varepsilon \leq 1$.

10. Find the transformation matrix which rotates a rectangular coordinate system through an angle of 120° about an axis making equal angles with the original three coordinate axes

11. Let U be a unitary matrix and let x_1, x_2 be two eigenvectors of U belonging to the eigenvalues λ_1, λ_2 , respectively. Show that
- (a) $|\lambda_1| = |\lambda_2| = 1$
 - (b) If $\lambda_1 \neq \lambda_2$, $x_1^\dagger x_2 = 0$

12. Find the eigenvalues and normalized eigenvectors of the matrix

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Express your answers numerically (3 significant figures).