

Chapter 7 Symmetric Matrices & Singular Value Decompositions

Orthogonal matrices (正交矩陣)

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• 定義: $Q_{n \times n}$ orthogonal: $\{q_1, q_2, \dots, q_n\}$ orthonormal

• 定理: 下列 (1)-(5) 等價:

(1) Q orthogonal

(2) $Q^T Q = I_n$

(3) $Qx \cdot Qy = x \cdot y$ (保積)

(4) $\|Qx\| = \|x\|$ (保長)

(5) $\|Qx - Qy\| = \|x - y\|$ (保距)

証

(1) \Rightarrow (2)

$$\begin{bmatrix} q_1^T \\ q_2^T \\ q_3^T \end{bmatrix} \begin{bmatrix} q_1 & q_2 & q_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(2) \Rightarrow (3)

$$Qx \cdot Qy = x \cdot Q^T Q y = x \cdot y$$

(3) \Rightarrow (1)

$$q_i \cdot q_j = Q e_i \cdot Q e_j = e_i \cdot e_j = \delta_{ij}$$

(3) \Rightarrow (4)

$$\|Qx\|^2 = Qx \cdot Qx = x \cdot x = \|x\|^2$$

(4) \Rightarrow (5)

$$\|Qx - Qy\| = \|Q(x - y)\| = \|x - y\|$$

• Remarks $\begin{cases} \text{保長} \\ \text{保積} \end{cases} \Rightarrow \begin{cases} \text{保角} \\ \text{保面積} \end{cases}$ ($\cos \theta = \frac{x \cdot y}{\|x\| \|y\|}$) (4,5) \Rightarrow (3) $\begin{cases} \|Qx - Qy\|^2 = \|Qx\|^2 - 2Qx \cdot Qy + \|Qy\|^2 \\ \|x - y\|^2 = \|x\|^2 - 2x \cdot y + \|y\|^2 \end{cases}$

• 定理 Q : orthogonal ($Q^T Q = I_n$) 則

(1) $\det(Q) = \pm 1$

(Q 的列)

$$\because \det(Q^T) \det(Q) = 1$$

(2) $Q Q^T = I_n \Rightarrow \{q_1, \dots, q_n\}$ orthonormal

(3) $Q^{-1} = Q^T$ orthogonal

$$(Q^T)^T Q^T = I_n$$

(4) P, Q orthogonal $\Rightarrow PQ$ orthogonal

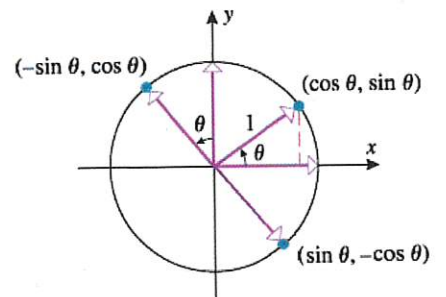
$$(PQ)^T P Q = Q^T P^T P Q = I_n$$

• 定理 $\begin{cases} O_n = \{A_{n \times n} \mid A^T A = I_n\} \\ SO_n = \{A_{n \times n} \mid A^T A = I_n, \det(A) = 1\} \end{cases}$ (general) orthogonal group
Special " "

• 定理 $Q \in O_2$

(1) $\det(Q) = 1, Q = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} = R_\theta: \begin{matrix} \text{Rot} \\ \text{Rot} \end{matrix} \begin{matrix} \parallel \\ \perp \end{matrix} \begin{matrix} x_\theta \\ y_\theta \end{matrix} \rightarrow \begin{matrix} x_{\theta+\varphi} \\ y_{\theta+\varphi} \end{matrix}$

(2) $\det(Q) = -1, Q = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix} = H_\theta: \begin{matrix} \text{Ref} \\ \text{Ref} \end{matrix} \begin{matrix} \parallel \\ \perp \end{matrix} \begin{matrix} x_\theta \\ y_\theta \end{matrix} \rightarrow \begin{matrix} x_{\theta-\varphi} \\ y_{\theta-\varphi} \end{matrix}$
(對 $L_{\theta/2}$ 作鏡射)



• 定理

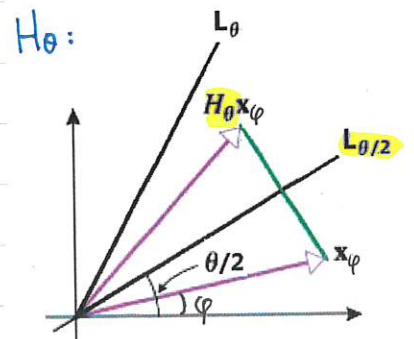
(1) $R_\alpha R_\beta = R_{\alpha+\beta} \quad \varphi \rightarrow \alpha + (\beta + \varphi)$

(2) $H_\alpha R_\beta = H_{\alpha-\beta} \quad \rightarrow \alpha - (\beta + \varphi)$

(3) $R_\alpha H_\beta = H_{\alpha+\beta} \quad \rightarrow \alpha + (\beta - \varphi)$

(4) $H_\alpha H_\beta = R_{\alpha-\beta} \quad \rightarrow \alpha - (\beta - \varphi)$

$$\text{或 } \begin{bmatrix} \cos \alpha & \sin \alpha \\ \sin \alpha & -\cos \alpha \end{bmatrix} \begin{bmatrix} \cos \beta & \sin \beta \\ \sin \beta & -\cos \beta \end{bmatrix} = \begin{bmatrix} \cos(\alpha-\beta) & -\sin(\alpha-\beta) \\ \sin(\alpha-\beta) & \cos(\alpha-\beta) \end{bmatrix}$$



Symmetric Matrix & Spectral theorem

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• 定理1 (Spectral th) $A_{n \times n}$: symmetric ($A^T = A$)

(1) $\begin{cases} Ax = \lambda x \\ Ay = \mu y \end{cases} \quad \lambda \neq \mu \Rightarrow x \cdot y = 0$

(2) all eigenvalues $\in \mathbb{R}$

(3) $\begin{cases} \exists \text{ orthonormal eigenbasis } \{q_1, \dots, q_n\} \Leftrightarrow \\ \exists \text{ orthogonal } Q = [q_1 \dots q_n], Q^T A Q = Q^{-1} A Q = \Lambda \end{cases}$

(4) $A = Q \Lambda Q^T = [q_1 \ q_2 \ \dots \ q_n] \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_n \end{bmatrix} \begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_n^T \end{bmatrix}$
 $= \lambda_1 q_1 q_1^T + \lambda_2 q_2 q_2^T + \dots + \lambda_n q_n q_n^T$
 $= \lambda_1 P_1 + \lambda_2 P_2 + \dots + \lambda_n P_n$

証 (1) $\lambda(x \cdot y) = Ax \cdot y = x \cdot A^T y = x \cdot Ay = \mu(x \cdot y)$

(2) $\begin{cases} Ax = \lambda x \\ \lambda \in \mathbb{C}, x \neq 0 \end{cases} \Rightarrow \begin{cases} Ax = \lambda x \\ A\bar{x} = \bar{\lambda}\bar{x} \end{cases} \xrightarrow{(\cdot)^T_x} \begin{cases} \bar{x}^T Ax = \lambda \bar{x}^T x \\ \bar{x}^T A^T x = \bar{\lambda} \bar{x}^T x \end{cases} \xrightarrow{x \neq 0} \lambda = \bar{\lambda} \in \mathbb{R}$

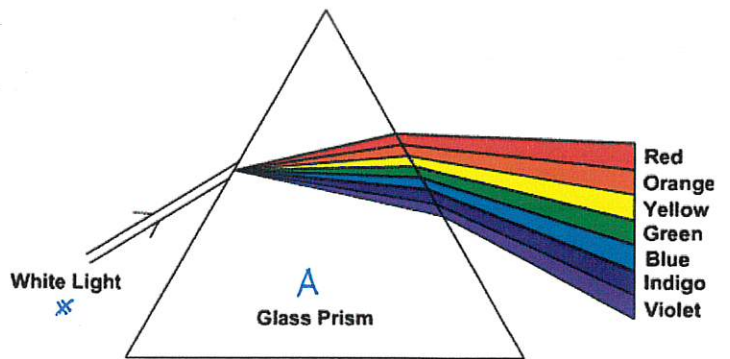
(3) $\begin{cases} \text{取 } q_1, \|q_1\| = 1, Aq_1 = \lambda_1 q_1 \\ \text{Span}(q_1)^\perp \text{ 的 orthonormal basis } \{v_2, \dots, v_n\} \Rightarrow \{q_1, v_2, \dots, v_n\}: \mathbb{R}^n \text{ 的 orthonormal basis} \end{cases}$
 $\Rightarrow A \sim B = \begin{bmatrix} \lambda_1 & * & \dots & * \\ 0 & & & \\ \vdots & & & \\ 0 & & & C \end{bmatrix} = Q^T A Q \xrightarrow{B^T = B} \begin{cases} * = 0 \\ C: \text{对称} \end{cases} \xrightarrow{\text{induction}} \begin{cases} \exists \text{ Span}(q_1)^\perp \text{ 的 orthonormal basis } \\ \{q_2, \dots, q_n\} \end{cases}$
 $\Rightarrow \{q_1, \dots, q_n\} \mathbb{R}^n \text{ orthonormal eigenbasis} \Rightarrow A \sim \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_n \end{bmatrix} \quad Cq_i = \lambda_i q_i \quad 2 \leq i \leq n$

• 定理2 A : symmetric $\Leftrightarrow A = Q \Lambda Q^T, Q^T Q = I_n$

• Remarks (Spectral decomposition)

$A = \lambda_1 q_1 q_1^T + \lambda_2 q_2 q_2^T + \dots + \lambda_n q_n q_n^T, \quad x = c_1 q_1 + c_2 q_2 + \dots + c_n q_n, \quad q_i^T q_j = q_i \cdot q_j$
 $= \lambda_1 P_1 + \lambda_2 P_2 + \dots + \lambda_n P_n$

$A: \begin{matrix} x \\ \parallel \\ \lambda_1 q_1 q_1^T \\ + \\ \lambda_2 q_2 q_2^T \\ + \\ \vdots \\ + \\ \lambda_n q_n q_n^T \end{matrix} \longrightarrow \begin{matrix} Ax \\ \parallel \\ \lambda_1 c_1 q_1 \\ + \\ \lambda_2 c_2 q_2 \\ + \\ \vdots \\ + \\ \lambda_n c_n q_n \end{matrix}$



$\begin{cases} A: \text{棱镜} \\ x: \text{白光} \end{cases} \quad \begin{cases} q_1, \dots, q_n \text{ 有色光} \\ \lambda_1, \dots, \lambda_n \text{ 折射率} \end{cases}$

Example 1 $A = \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix}$, $P_A(t) = t^2 + t - 6 = 0$

$$\begin{cases} \lambda_1 = 2, & v_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}, & q_{11} = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \\ \lambda_2 = -3, & v_2 = \begin{bmatrix} -1 \\ 2 \end{bmatrix}, & q_{12} = \frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ 2 \end{bmatrix} \end{cases} \quad Q = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix}$$

(i) $Q^T A Q = \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix}$

(ii) $A = Q \Lambda Q^T = \lambda_1 q_{11} q_{11}^T + \lambda_2 q_{12} q_{12}^T$
 $= \frac{2}{5} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \end{bmatrix} + \frac{-3}{5} \begin{bmatrix} -1 \\ 2 \end{bmatrix} \begin{bmatrix} -1 & 2 \end{bmatrix}$
 $= \frac{2}{5} \begin{bmatrix} 4 & 2 \\ 2 & 1 \end{bmatrix} + \frac{-3}{5} \begin{bmatrix} 1 & -2 \\ -2 & 4 \end{bmatrix} = 2P_1 - 3P_2$

註 $A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$, $b \neq 0 \Rightarrow \lambda_1 \neq \lambda_2$

$$P_A(t) = t^2 - (a+c)t + (ac-b^2) = 0$$

$$\begin{cases} \lambda_1, & v_1 = \begin{bmatrix} b \\ \lambda_1 - a \end{bmatrix} \\ \lambda_2, & v_2 = \begin{bmatrix} b \\ \lambda_2 - a \end{bmatrix} \end{cases} \quad v_1 \cdot v_2 = 0$$

$$A v_1 = \begin{bmatrix} b \lambda_1 \\ b^2 + c \lambda_1 - ac \end{bmatrix} = \begin{bmatrix} b \lambda_1 \\ \lambda_1^2 - a \lambda_1 \end{bmatrix} = \lambda_1 v_1$$

Example 2 $A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$, $P_A(t) = -t^3 + 2t^2 + t - 2 = -(t+1)(t-1)(t-2)$

$$\begin{cases} \lambda_1 = -1, & v_1 = \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}, & q_{11} = \frac{1}{\sqrt{6}} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} \\ \lambda_2 = 1, & v_2 = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}, & q_{12} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \\ \lambda_3 = 2, & v_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, & q_{13} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \end{cases} \quad Q = \begin{bmatrix} \frac{-2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \end{bmatrix}$$

$$Q^T A Q = \begin{bmatrix} -1 & & \\ & 1 & \\ & & 2 \end{bmatrix}$$

Example 3 $A = \begin{bmatrix} 5 & -4 & -2 \\ -4 & 5 & -2 \\ -2 & -2 & 8 \end{bmatrix}$, $P_A(t) = -t^3 + 18t^2 - 81t = -t(t-9)^2$ (重根沒問題)

$$\begin{cases} \lambda_1 = 0, & v_1 = \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix} & q_{11} = \frac{1}{3} \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix} \\ \lambda_2 = 9, & A - 9I = \begin{bmatrix} -4 & -4 & -2 \\ -4 & -4 & -2 \\ -2 & -2 & -1 \end{bmatrix}, & \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y - \frac{1}{2}z \\ y \\ z \end{bmatrix} \\ & v_2 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}, & v_3 = \begin{bmatrix} -1 \\ 0 \\ 2 \end{bmatrix} & q_{12} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \\ & w_3 = v_3 - \frac{v_3 \cdot v_2}{\|v_2\|^2} v_2 = \begin{bmatrix} -1 \\ 0 \\ 2 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ 2 \end{bmatrix} \parallel \begin{bmatrix} -1 \\ -1 \\ 4 \end{bmatrix} & q_{13} = \frac{1}{3\sqrt{2}} \begin{bmatrix} -1 \\ -1 \\ 4 \end{bmatrix} \end{cases}$$

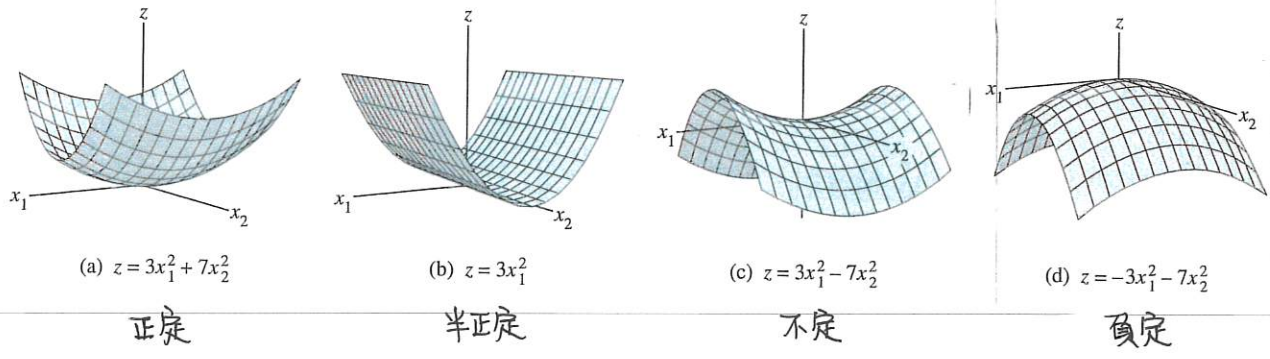
$$Q = \begin{bmatrix} \frac{2}{3} & \frac{-1}{\sqrt{2}} & \frac{-1}{3\sqrt{2}} \\ \frac{2}{3} & \frac{1}{\sqrt{2}} & \frac{-1}{3\sqrt{2}} \\ \frac{1}{3} & 0 & \frac{4}{3\sqrt{2}} \end{bmatrix}, \quad Q^T A Q = \begin{bmatrix} 0 & & \\ & 9 & \\ & & 9 \end{bmatrix}$$

$A_{n \times n}$ 对稱 $\Rightarrow \exists Q = [q_1 \dots q_n], Q^T A Q = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}, \{q_1, \dots, q_n\}$ orthonormal, $A q_i = \lambda_i q_i$

• 定理 1 (Principal axes) $F(x) = x^T A x \xrightarrow{x = Qy} y^T \Lambda y$: q_i 主軸
 $F(x_1, \dots, x_n) = \sum_{i=1}^n a_{ii} x_i^2 + 2 \sum_{i < j} a_{ij} x_i x_j = \lambda_1 y_1^2 + \dots + \lambda_n y_n^2$ (新座標系)

• 定理 2 Quadratic form: $F(x) = x^T A x$

$F(x)$ 或 A 為:	當	判別法: 所有特徵值 λ_i
正定 (positive definite)	$F(x) > 0, \forall x \neq 0$	全部為正
負定 (negative definite)	$F(x) < 0, \forall x \neq 0$	全部為負
不定 (indefinite)	$F(x)$ 有正有負, $\forall x \neq 0$	有正有負
半正定 (semi-positive definite)	$F(x) \geq 0, \forall x \in \mathbf{R}^n$	全部 ≥ 0
半負定 (semi-negative definite)	$F(x) \leq 0, \forall x \in \mathbf{R}^n$	全部 ≤ 0



• 定理 3 (Constraint optimization)

$F(x) = x^T A x, \|x\|=1$, 則 $\begin{cases} M = \lambda_1 \text{ at } q_1 \\ m = \lambda_n \text{ at } q_n \end{cases}$
 $(\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n)$

• 定理 4 $F(x) = x^T A x$, 則 $\max \{F(x) \mid \|x\|=1, x^T q_1 = 0\} = \lambda_2$ at q_2
 $x^T A x \xrightarrow{x = Qy} y^T \Lambda y = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \dots + \lambda_n y_n^2 = \lambda_2 y_2^2 + \dots + \lambda_n y_n^2$ $M = \lambda_2$ at q_2
 $\|x\|=1 \Rightarrow \|y\|=1 \Rightarrow y_1^2 + y_2^2 + \dots + y_n^2 = 1$ $y_2^2 + \dots + y_n^2 = 1$
 $x^T q_1 = 0 \Rightarrow y^T e_1 = 0 \Rightarrow [y_1 \dots y_n] \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = y_1 = 0$

• 定理 5 $F(x) = x^T A x$, 則 $\max \{F(x) \mid \|x\|=1, x^T q_1 = x^T q_2 = \dots = x^T q_{k-1} = 0\} = \lambda_k$ at q_k

• 定理 6 (Principal component analysis)

$X_{d \times n}$: data matrix, $\frac{1}{n} X^T X$: eigen values $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$

$\Rightarrow \begin{cases} 1st \text{ PC at } q_1 \\ 2nd \text{ " " } q_2 \\ dth \text{ " " } q_d \end{cases}$

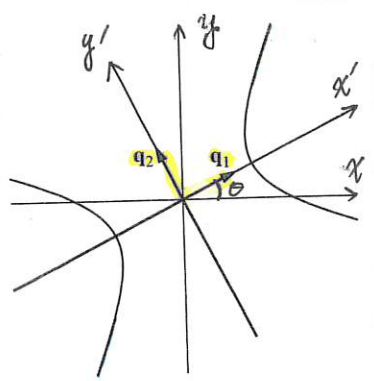
Quadratic Form (= 二次式)

$$\begin{cases} F(x, y) = [x \ y] \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = ax^2 + 2bxy + cy^2 \\ F(x) = x^T A x = y^T Q^T A Q y \quad \text{消除} \\ = y^T \Lambda y = \lambda_1 x'^2 + \lambda_2 y'^2 \end{cases}$$

A: 对稱
 $x = Qy$
 $Q^T A Q = \Lambda = \begin{bmatrix} \lambda_1 & \\ & \lambda_2 \end{bmatrix}$

Example 1 化簡二次曲線 $x^2 + 4xy - 2y^2 = 6$

$$\begin{aligned} [x \ y] \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} &= 6, \quad A = \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix}, \quad Q = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix} \\ x^T A x &= 6 \quad \left\{ \begin{aligned} Q^T A Q &= \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix} = \Lambda \\ x &= Qy \end{aligned} \right. \\ y^T Q^T A Q y &= 6 \\ y^T \Lambda y &= 6 \\ [x' \ y'] \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix} &= 6 \\ 2x'^2 - 3y'^2 &= 6 \quad \text{双曲線} \end{aligned}$$



$$\begin{cases} \cot 2\theta = \frac{a-c}{2b} = \frac{3}{4} \text{ (高中)} \\ \tan \theta = \frac{1}{2} \Rightarrow q_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \\ \tan 2\theta = \frac{2 \cdot \frac{1}{2}}{1 - \frac{1}{4}} = \frac{4}{3} \end{cases}$$

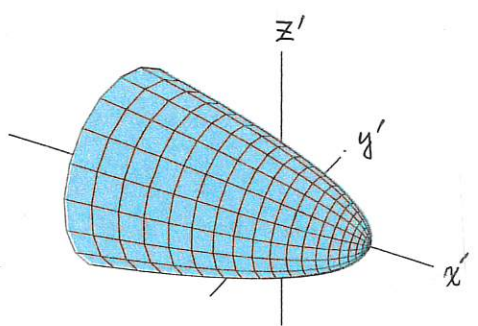
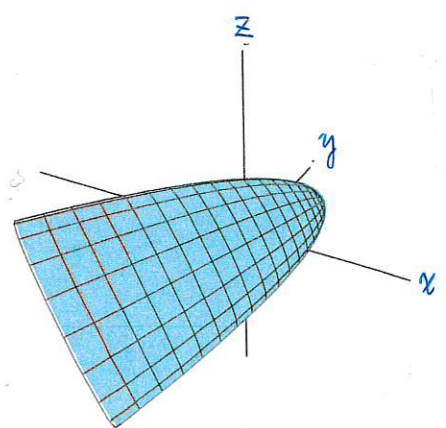
Example 2 $x^2 + 4xy - 2y^2 + 2x + 4y = 6$

$$\begin{aligned} [x \ y] \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + [2 \ 4] \begin{bmatrix} x \\ y \end{bmatrix} &= 6 \\ x^T A x + [2 \ 4] x &= 6 \\ y^T Q^T A Q y + [2 \ 4] Q y &= 6 \\ [x' \ y'] \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix} + [2 \ 4] \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x' \\ y' \end{bmatrix} &= 6 \\ 2x'^2 - 3y'^2 + \frac{8}{\sqrt{5}}x' + \frac{6}{\sqrt{5}}y' &= 6 \\ 2(x' + \frac{2}{\sqrt{5}})^2 - 3(y' - \frac{1}{\sqrt{5}})^2 &= 7 \quad \text{双曲線, 中心}(\frac{-2}{\sqrt{5}}, \frac{1}{\sqrt{5}}) \end{aligned}$$

$\begin{cases} \lambda_1, \lambda_2 > 0 & \text{橢圓} \\ < 0 & \text{双曲線} \\ = 0 & \text{拋物線} \end{cases}$

Example 3 $5x^2 + 5y^2 + 8z^2 - 8xy - 4yz - 4zx + 2x + 2y + z = 9$

$$\begin{aligned} [x \ y \ z] \begin{bmatrix} 5 & -4 & -2 \\ -4 & 5 & -2 \\ -2 & -2 & 8 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + [2 \ 2 \ 1] \begin{bmatrix} x \\ y \\ z \end{bmatrix} &= 9 \\ x^T A x + [2 \ 2 \ 1] x &= 9 \\ y^T Q^T A Q y + [2 \ 2 \ 1] Q y &= 9 \\ [x' \ y' \ z'] \begin{bmatrix} 9 & & \\ & 9 & \\ & & 9 \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} + [2 \ 2 \ 1] Q \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} &= 9 \\ 9y'^2 + 9z'^2 + 3x' &= 9 \\ x' = 3(1 - y'^2 - z'^2) & \text{(Paraboloid)} \end{aligned}$$



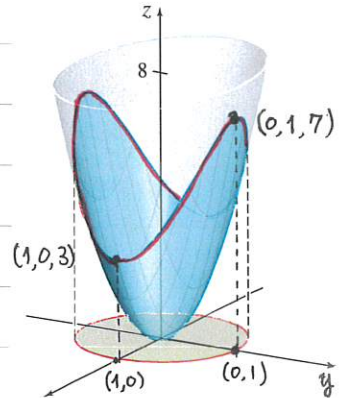
Constraint Optimization

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$$\text{求 } \begin{cases} F(x) = x^T A x \\ F(x, y) = [x \ y] \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = ax^2 + 2bxy + cy^2 \end{cases} \text{ 在 } \begin{cases} \|x\| = 1 \\ x^2 + y^2 = 1 \end{cases} \begin{matrix} \geq \text{極大值 } M \\ \leq \text{極小值 } m \end{matrix}$$

• Example 1 $F(x, y) = 3x^2 + 7y^2, \quad x^2 + y^2 = 1$ $\begin{cases} M = 7 \text{ at } \mathcal{E}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ m = 3 \text{ at } \mathcal{E}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{cases}$

$$3 = 3x^2 + 3y^2 \leq 3x^2 + 7y^2 \leq 7x^2 + 7y^2 = 7$$



• Example 2 $F(x, y) = 2x^2 - 3y^2, \quad x^2 + y^2 = 1$ $\begin{cases} M = 2 \text{ at } \mathcal{E}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ m = -3 \text{ at } \mathcal{E}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{cases}$

$$-3 = -3x^2 - 3y^2 \leq 2x^2 - 3y^2 \leq 2x^2 + 2y^2 = 2$$

• Example 3 $F(x, y) = x^2 + 4xy - 2y^2, \quad x^2 + y^2 = 1$ $\begin{cases} M = \lambda_1 = 2 \text{ at } \mathcal{q}_1 \\ m = \lambda_2 = -3 \text{ at } \mathcal{q}_2 \end{cases}$

$$\begin{cases} F(x) = x^T A x = x^2 + 4xy - 2y^2, & x^2 + y^2 = 1, & \|x\| = 1 & \{ \mathcal{q}_1, \mathcal{q}_2 \}, & \{ x^T A x \mid \|x\| = 1 \} \\ \parallel x = Qy, & & & & \\ F(y) = y^T \Lambda y = 2u^2 - 3v^2, & u^2 + v^2 = 1, & \|y\| = 1, & \{ \mathcal{e}_1, \mathcal{e}_2 \}, & \{ y^T \Lambda y \mid \|y\| = 1 \} \end{cases}$$

$$A = \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix} \begin{cases} \lambda_1 = 2 \\ \lambda_2 = -3 \end{cases} \quad Q = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix} \quad M = 2, m = -3$$

• Example 4 $F(x, y) = 2x^2 + 12xy - 9y^2, \quad 4x^2 + 9y^2 = 36, \quad \begin{cases} x = 3u \\ y = 2v \end{cases} \quad \left(\frac{x^2}{9} + \frac{y^2}{4} = 1 \right)$

$$= 18(u^2 + 4uv - 2v^2), \quad u^2 + v^2 = 1,$$

$$\begin{cases} M = 2 \cdot 18 = 36 \text{ at } \begin{bmatrix} u \\ v \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix} \text{ or } \begin{bmatrix} x \\ y \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} 6 \\ 2 \end{bmatrix} \\ m = -3 \cdot 18 = -54 \text{ at } \begin{bmatrix} u \\ v \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ 2 \end{bmatrix} \text{ or } \begin{bmatrix} x \\ y \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} -3 \\ 4 \end{bmatrix} \end{cases}$$

• Example 5 $F(x, y, z) = 4x^2 + 9y^2 + 3z^2, \quad x^2 + y^2 + z^2 = 1$ $\begin{cases} M = 9 \text{ at } \mathcal{E}_2 = [0 \ 1 \ 0]^T \\ m = 3 \text{ at } \mathcal{E}_3 = [0 \ 0 \ 1]^T \end{cases}$

$$3 = 3x^2 + 3y^2 + 3z^2 \leq 4x^2 + 9y^2 + 3z^2 \leq 9x^2 + 9y^2 + 9z^2 = 9$$

• Example 6 $F(x, y, z) = x^T A x = 3x^2 + 3y^2 + 4z^2 + 4xy + 2yz + 2zx, \quad x^2 + y^2 + z^2 = \|x\|^2 = 1$

$$= y^T \Lambda y = 6u^2 + 3v^2 - w^2, \quad u^2 + v^2 + w^2 = \|y\|^2 = 1$$

$$A = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 3 & 1 \\ 1 & 1 & 4 \end{bmatrix}, \quad \begin{cases} \lambda_1 = 6 \\ \lambda_2 = 3 \\ \lambda_3 = -1 \end{cases} \quad Q = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} 6 \\ 3 \\ -1 \end{bmatrix}$$

$$\begin{cases} M = 6 = \lambda_1 = \max \lambda_i & y = \mathcal{E}_1, \quad x = \mathcal{q}_1 \\ \text{at} \\ m = -3 = \lambda_3 = \min \lambda_i & y = \mathcal{E}_3, \quad x = \mathcal{q}_3 \end{cases}$$

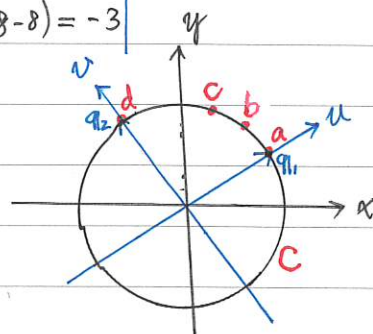
(1) $Q = [q_1, \dots, q_m]$ orthogonal: (i) $\{q_1, \dots, q_m\}$ orthonormal $\Leftrightarrow Q^T Q = I_m$

- \Rightarrow $\begin{cases} \text{(a) } \|Qx\| = \|x\| \quad (\text{保長}) \\ \text{(b) } Q^{-1} = Q^T \Rightarrow Q: \text{ nonsingular} \Rightarrow Q: 1-1, \text{ onto } (\mathbb{R}^n \rightarrow \mathbb{R}^n) \\ \text{(c) } (Q^T)^T Q^T = Q Q^T = I_m \Rightarrow Q^T: \text{ " } \Rightarrow Q^T: \text{ " } (\text{保長}) \\ \text{(d) } C = \{x \in \mathbb{R}^n \mid \|x\| = 1\} \xrightarrow[Q^T]{Q} C: 1-1 \ \& \ \text{onto} \end{cases}$

(2) $x^T A x = y^T Q^T A Q y = y^T \Lambda y$

$$\begin{cases} F(x) = [x, y] \begin{bmatrix} 1 & 2 \\ 2 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \xrightarrow[x=Qy]{} [u, v] \begin{bmatrix} 2 & 0 \\ 0 & -3 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = F(y) \\ F(x, y) = x^2 + 4xy - 2y^2 \xrightarrow{} 2u^2 - 3v^2 = F(u, v) \end{cases}$$

	$y = \begin{bmatrix} u \\ v \end{bmatrix}$	$F(u, v) = 2u^2 - 3v^2$	$x = \begin{bmatrix} x \\ y \end{bmatrix}$	$F(x, y) = x^2 + 4xy - 2y^2$	$x = Qy = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix}$
(a)	$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	2	$\frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}$	$\frac{1}{5}(4+8-2) = 2$	
(b)	$\frac{1}{5} \begin{bmatrix} 4 \\ 3 \end{bmatrix}$	$\frac{1}{25}(32-27) = \frac{1}{5}$	$\frac{1}{5\sqrt{5}} \begin{bmatrix} 5 \\ 10 \end{bmatrix}$	$\frac{1}{5}(1+8-8) = \frac{1}{5}$	
(c)	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\frac{1}{2}(2-3) = -\frac{1}{2}$	$\frac{1}{\sqrt{10}} \begin{bmatrix} 1 \\ 3 \end{bmatrix}$	$\frac{1}{10}(1+12-18) = -\frac{1}{2}$	
(d)	$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	-3	$\frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ 2 \end{bmatrix}$	$\frac{1}{5}(1-8-8) = -3$	



Principal Component Analysis (PCA) 主成分分析 (dimension reduction)

• data matrix $X = \begin{bmatrix} x_1 & x_2 & \dots & x_n \\ y_1 & y_2 & \dots & y_n \end{bmatrix}$ $X_1 = X$
 $X_2 = Y$

mean : $\mu_x = E(X) = \frac{1}{n} \sum_{i=1}^n x_i$
 variance : $\sigma_x^2 = \text{Var}(X) = \frac{1}{n} \sum_{i=1}^n (x_i - \mu_x)^2 = \frac{1}{n} \sum_{i=1}^n x_i^2 - \mu_x^2 = \frac{1}{n} X X^T - \text{Cov}(X, X)$
 covariance : $\sigma_{xy} = \text{Cov}(X, Y) = \frac{1}{n} \sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y) = \frac{1}{n} \sum_{i=1}^n x_i y_i = \frac{1}{n} X Y^T$

• Covariance matrix: $C = \begin{bmatrix} \sigma_x^2 & \sigma_{xy} \\ \sigma_{yx} & \sigma_y^2 \end{bmatrix} = \begin{bmatrix} \text{Cov}(X, X) & \text{Cov}(X, Y) \\ \text{Cov}(Y, X) & \text{Cov}(Y, Y) \end{bmatrix} = \frac{1}{n} \begin{bmatrix} X \\ Y \end{bmatrix} \begin{bmatrix} X^T & Y^T \end{bmatrix} = \frac{1}{n} X X^T$

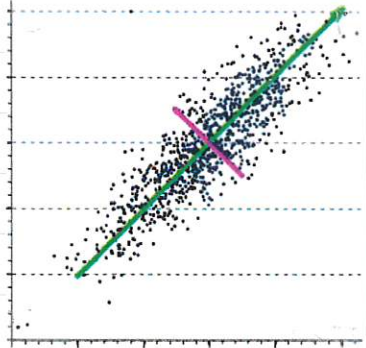
• $X_{d \times n}$ (去中心化), $C = \frac{1}{n} X X^T = \begin{bmatrix} \text{Cov}(x_1, x_1) & \text{Cov}(x_1, x_2) & \dots & \text{Cov}(x_1, x_d) \\ \text{Cov}(x_2, x_1) & \text{Cov}(x_2, x_2) & \dots & \text{Cov}(x_2, x_d) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(x_d, x_1) & \text{Cov}(x_d, x_2) & \dots & \text{Cov}(x_d, x_d) \end{bmatrix}_{d \times d}$

C : 对稱 \Rightarrow (1) $\exists \{q_1, \dots, q_d\}$ orthonormal, $C q_i = \lambda_i q_i, \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$
 (2) $\begin{cases} F(u) = u^T C u, \|u\| = 1 & \text{max} = \lambda_1 \text{ at } q_1 \\ \|u\| = 1, u^T q_1 = 0 & \text{max} = \lambda_2 \text{ at } q_2 \\ \|u\| = 1, \begin{cases} u^T q_1 = 0 \\ u^T q_2 = 0 \end{cases} & \text{max} = \lambda_3 \text{ at } q_3 \end{cases}$

Principal Component Analysis (PCA)

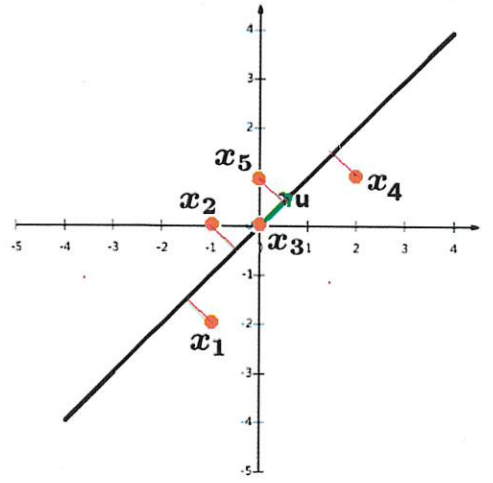
$$\text{Max}_{\|u\|=1} \frac{1}{n} \sum_{i=1}^n (x_i \cdot u)^2 = \text{Max}_{\|u\|=1} u^T \left(\frac{1}{n} \sum_{i=1}^n x_i x_i^T \right) u = \text{Max}_{\|u\|=1} u^T \left(\frac{1}{n} [x_1 \dots x_n] \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \right) u$$

$$= \text{Max}_{\|u\|=1} u^T \left(\frac{1}{n} X X^T \right) u = \text{Max}_{\|u\|=1} u^T C u$$



• 定理 1 data matrix $X_{d \times n}$ (去中心化), $C = \frac{1}{n} X X^T = Q \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_d \end{bmatrix} Q^T$

(1) $\begin{cases} \text{1st PC: } q_1, \lambda_1 \\ \text{2nd PC: } q_2, \lambda_2 \\ \vdots \\ \text{dth PC: } q_d, \lambda_d \end{cases} \quad \lambda_1 \geq \dots \geq \lambda_d$
 (2) $\begin{cases} \text{PCA 後 data: } Y = Q^T X \\ C' = \frac{1}{n} Y Y^T = \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_d \end{bmatrix} \end{cases}$



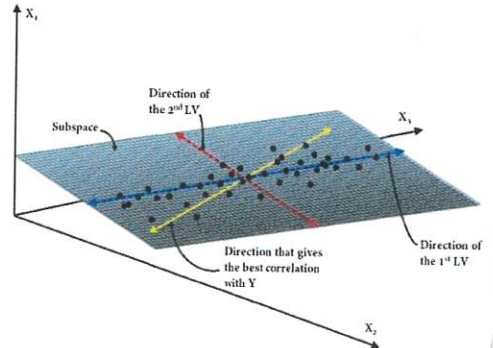
Example

LA: $\begin{bmatrix} 79 & 79 & 80 & 82 & 80 \end{bmatrix}$ $\xrightarrow{\text{去中心化}} X = \begin{bmatrix} -1 & -1 & 0 & 2 & 0 \\ -2 & 0 & 0 & 1 & 1 \end{bmatrix}$

ML: $\begin{bmatrix} 68 & 70 & 70 & 71 & 71 \end{bmatrix}$
 $C = \frac{1}{5} X X^T = \frac{1}{5} \begin{bmatrix} 6 & 4 \\ 4 & 6 \end{bmatrix}, \begin{cases} \lambda_1 = 2, q_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ \lambda_2 = \frac{2}{5}, q_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \end{cases}$

$\begin{cases} \text{1st PC: } q_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ \text{2nd PC: } q_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \end{cases} \quad Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, Q^T = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$

PCA 後 data: $\begin{cases} Y = Q^T X = \begin{bmatrix} -3 & -1 & 0 & 3 & 1 \\ -1 & 1 & 0 & -1 & 1 \end{bmatrix} : \frac{5}{6} (83\%) \\ C' = \frac{1}{5} Y Y^T = \begin{bmatrix} 2 & 0 \\ 0 & \frac{2}{5} \end{bmatrix} \end{cases}$



Remarks

- (1) $\{q_1, q_2, \dots, q_d\}$ orthonormal
- (2) $\begin{cases} \lambda_1 + \lambda_2 + \dots + \lambda_d = \sigma_1^2 + \dots + \sigma_d^2 = \text{tr}(C) \\ Y_1, Y_2, \dots, Y_d \text{ 獨立} \end{cases}$

Singular value decomposition (SVD) 奇異值分解

No. _____
Date: / /

• $A_{m \times n}$, $\text{rank}(A) = r$

$A^T A$ 对稱 $\Rightarrow \exists \{v_1, v_2, \dots, v_r, v_{r+1}, \dots, v_n\}$ orthonormal eigenbasis

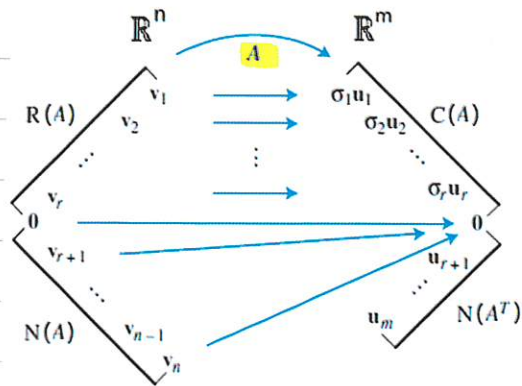
$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > 0 = \dots = 0$ eigen values : $A^T A v_i = \lambda_i v_i$
 \downarrow
 $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0 = \dots = 0$ singular " : $\sigma_i = \sqrt{\lambda_i}$

• 定理 1

(1) $\|A v_i\|^2 = \lambda_i \geq 0$, 令 $A v_i = \sigma_i u_i$, $\|u_i\| = 1$

(2) orthonormal bases ($\mathbb{R}^n : \mathcal{V} = \{v_1, \dots, v_n\}$)

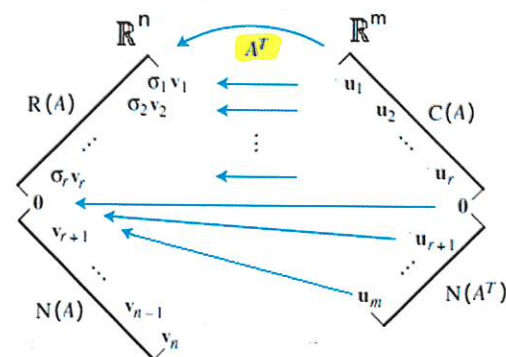
$\left\{ \begin{array}{l} R(A) : \{v_1, \dots, v_r\} \quad A v_i = \sigma_i u_i, \quad N(A) : \{v_{r+1}, \dots, v_n\} \\ C(A) : \{u_1, \dots, u_r\} \quad A^T u_i = \sigma_i v_i, \quad N(A^T) : \{u_{r+1}, \dots, u_m\} \end{array} \right.$
 $(\mathbb{R}^m : \mathcal{U} = \{u_1, \dots, u_m\})$



証

(1) $A v_i \cdot A v_j = v_i \cdot A^T A v_j = \lambda_j v_i \cdot v_j = \begin{cases} \lambda_i & i=j \\ 0 & i \neq j \end{cases}$

(2) $\left\{ \begin{array}{l} \{v_1, \dots, v_r\} \text{ } R(A) \text{ 基底} \Rightarrow \{A v_1, \dots, A v_r\} \text{ } C(A) \text{ 基底.} \\ A^T u_i = A^T (\frac{1}{\sigma_i} A v_i) = \frac{1}{\sigma_i} A^T A v_i = \sigma_i v_i \end{array} \right.$



• 定理 2 (SVD)

$$A_{m \times n} = \begin{bmatrix} u_1 & \dots & u_r & | & u_{r+1} & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & & & 0 \\ & \sigma_2 & & & & & \\ & & \ddots & & & & \\ & & & \sigma_r & & & \\ & & & & 0 & & \\ & & & & & 0 & \\ & & & & & & \ddots \\ & & & & & & & \sigma_n \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_r^T \\ \vdots \\ v_n^T \end{bmatrix}$$

$$= U_{m \times m} \Sigma_{m \times n} V_{n \times n}^T \quad \left\{ \begin{array}{l} U^T U = I_m \\ V^T V = I_n \end{array} \right.$$

$$= \underbrace{\sigma_1 u_1 v_1^T}_{\text{rank}=1} + \underbrace{\sigma_2 u_2 v_2^T}_{\text{rank}=2} + \dots + \underbrace{\sigma_r u_r v_r^T}_{\text{rank}=r}$$

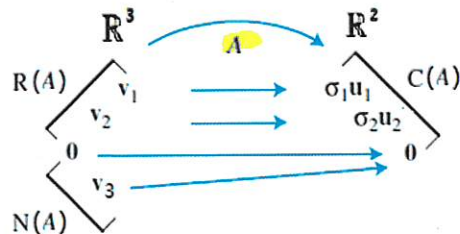
$$A^T = V \Sigma^T U^T$$

証: $A V = [A v_1 \dots A v_r \mid 0 \dots 0] = [\sigma_1 u_1 \dots \sigma_r u_r \mid 0 \dots 0] = U \Sigma$

• 定理 3 (Simplified SVD)

$$A_{m \times n} = [U_r \mid U_{n-r}] \begin{bmatrix} D_r & | & 0 \\ \hline 0 & | & 0 \end{bmatrix} \begin{bmatrix} V_r^T \\ \vdots \\ V_{n-r}^T \end{bmatrix}$$

$$= U_r D_r V_r^T$$



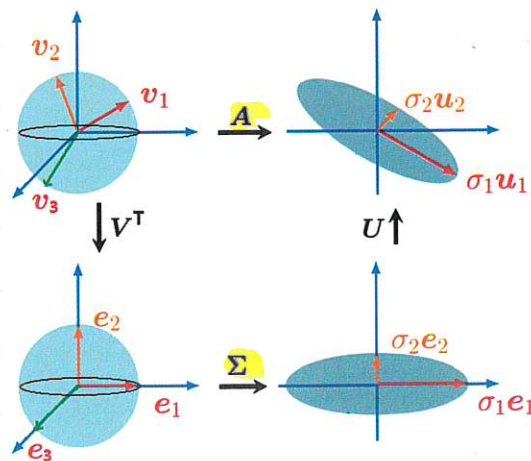
• Example

$$A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}, \quad A^T A = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$$

$$\left\{ \begin{array}{l} \lambda_1 = 360, \quad v_1 = \frac{1}{3} \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}, \quad A v_1 = \begin{bmatrix} 18 \\ 6 \end{bmatrix}, \quad \sigma_1 = 6\sqrt{10}, \quad u_1 = \frac{1}{\sqrt{10}} \begin{bmatrix} 3 \\ 1 \end{bmatrix} \\ \lambda_2 = 90, \quad v_2 = \frac{1}{3} \begin{bmatrix} -2 \\ 1 \\ 2 \end{bmatrix}, \quad A v_2 = \begin{bmatrix} 3 \\ -9 \end{bmatrix}, \quad \sigma_2 = 3\sqrt{10}, \quad u_2 = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 \\ -3 \end{bmatrix} \\ \lambda_3 = 0, \quad v_3 = \frac{1}{3} \begin{bmatrix} 2 \\ -2 \\ 1 \end{bmatrix}, \quad A v_3 = 0 \end{array} \right.$$

$$A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} = \frac{1}{\sqrt{10}} \begin{bmatrix} 3 & 1 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{bmatrix} \frac{1}{3} \begin{bmatrix} 1 & 2 & 2 \\ -2 & -1 & 2 \\ 2 & -2 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 6\sqrt{10} \\ 6\sqrt{10} \end{bmatrix} u = \begin{bmatrix} 24 \\ -12 \end{bmatrix} \leftarrow \begin{bmatrix} 6\sqrt{10} \cdot 1 \\ 3\sqrt{10} \cdot 2 \end{bmatrix} \leftarrow \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \leftarrow \frac{1}{3} \begin{bmatrix} -1 \\ -2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} v$$



- Remarks: (1) $A_{n \times n}$: nonsingular $\Leftrightarrow n$ non-zero singular values
- (2) $\begin{cases} A^T A v_i = \lambda_i v_i, & 1 \leq i \leq n \\ A A^T u_i = \lambda_i u_i, & 1 \leq i \leq m \end{cases}$ (或 $A^T A = V \begin{bmatrix} D_r^2 & 0 \\ 0 & 0 \end{bmatrix} V^T, D_r^2 = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_r \end{bmatrix}$)
(或 $A A^T = U \begin{bmatrix} D_r^2 & 0 \\ 0 & 0 \end{bmatrix} U^T, \quad \text{"}$)
(PCA: $A = X$)

• Image Compression

$$A = \underbrace{\sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_k u_k v_k^T + \dots + \sigma_r u_r v_r^T}_{\text{rank} = k}$$

rank: 1 1 1 1

保留影像比例 = $\frac{\sigma_1 + \sigma_2 + \dots + \sigma_k}{\sigma_1 + \sigma_2 + \dots + \sigma_r}$

SVD 壓縮後的效果



原圖

80%



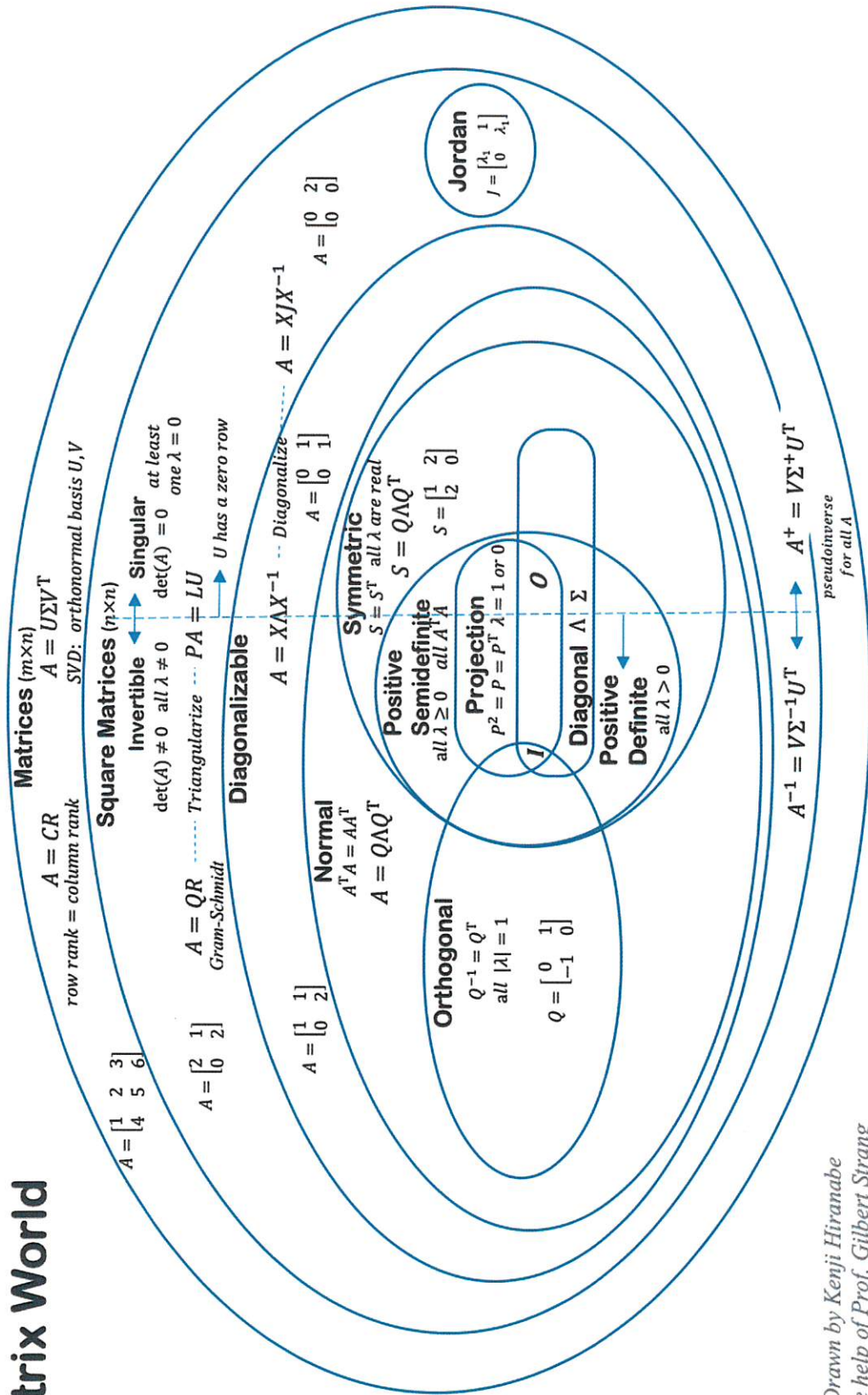
原圖

50%

70%

90%

Matrix World



(v1.3) Drawn by Kenji Hiranabe
 with the help of Prof. Gilbert Strang