

5. Orthogonal Matrices and Subspaces

- 1. Orthogonal vectors x and y

$$\begin{array}{l} \text{(test)} \\ \boxed{x^T y = 0} \\ \boxed{\bar{x}^T y = 0} \end{array}$$

Pythagoras Law of right triangles: $\|x - y\|^2 = \|x\|^2 + \|y\|^2$

Law of cosines: $\|x - y\|^2 = \|x\|^2 + \|y\|^2 - 2\|x\|\|y\|\cos\theta$

$$\theta = 90^\circ \quad \checkmark$$

$$(x-y)^T(x-y) = \cancel{x^T x} + \cancel{y^T y} - \cancel{x^T y} - \cancel{y^T x} = \|x\|^2 + \|y\|^2 - 2\|x\|\|y\| \stackrel{!}{=} 0$$

- 2. Orthogonal basis for a subspace

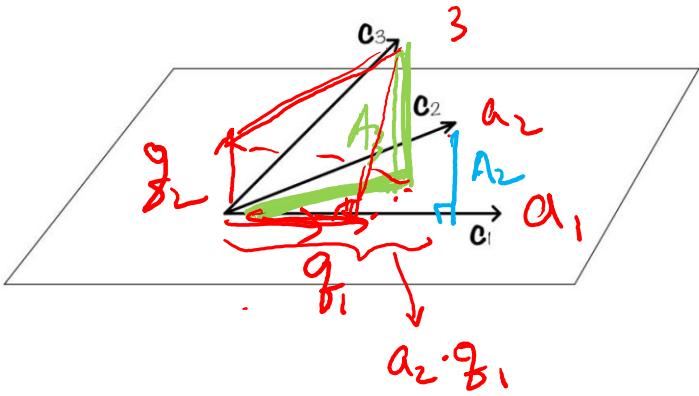
$$\text{orthogonal: } v_i^T v_j = 0 \xrightarrow{v_i / \|v_i\|} \text{orthonormal: } v_i^T v_i = 1$$

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad H_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix}$$

- Standard basis is orthogonal (even orthonormal) in \mathbb{R}^n (i, j, k in \mathbb{R}^3)
- ~~Hadamard matrices H_n containing orthogonal bases of \mathbb{R}^n~~
 - Are those orthogonal matrices?
- Every subspace of \mathbb{R}^n has an orthogonal basis: Gram-Schmidt idea
 - Two independent vectors a and b in the plane: $a^T c = 0$

$$H_8 = \begin{bmatrix} H_4 & H_4 \\ H_4 & -H_4 \end{bmatrix}$$

$$\underline{A_2 \perp q_1?} \quad A_2^T q_1 = 0 = [a_2 - (a_2^T q_1) q_1]^T \cdot q_1 \\ = A_2^T q_1 - (a_2^T q_1) \cdot q_1^T q_1$$



$$a_1 = \|a_1\| q_1$$

$$a_2 = (a_2^T q_1) q_1 + \|A_2\| q_2$$

$$a_3 = (\underbrace{a_3^T q_1}_{r_{13}}) q_1 + (\underbrace{a_3^T q_2}_{r_{23}}) q_2 + \|A_3\| q_3$$

$$q_1 = \frac{a_1}{\|a_1\|} \quad A_2 = a_2 - (\underbrace{a_2^T q_1}_{r_{12}}) q_1$$

$$q_2 = \frac{A_2}{\|A_2\|} \quad A_3 = a_3 \left[(\overbrace{a_3^T q_2}^{r_{23}}) q_2 + (\overbrace{a_3^T q_1}^{r_{13}}) q_1 \right]$$

$$q_3 = \frac{A_3}{\|A_3\|}$$

$$[a_1 \ a_2 \ a_3] = [q_1 \ q_2 \ q_3] \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{bmatrix}$$

$$A = QR$$

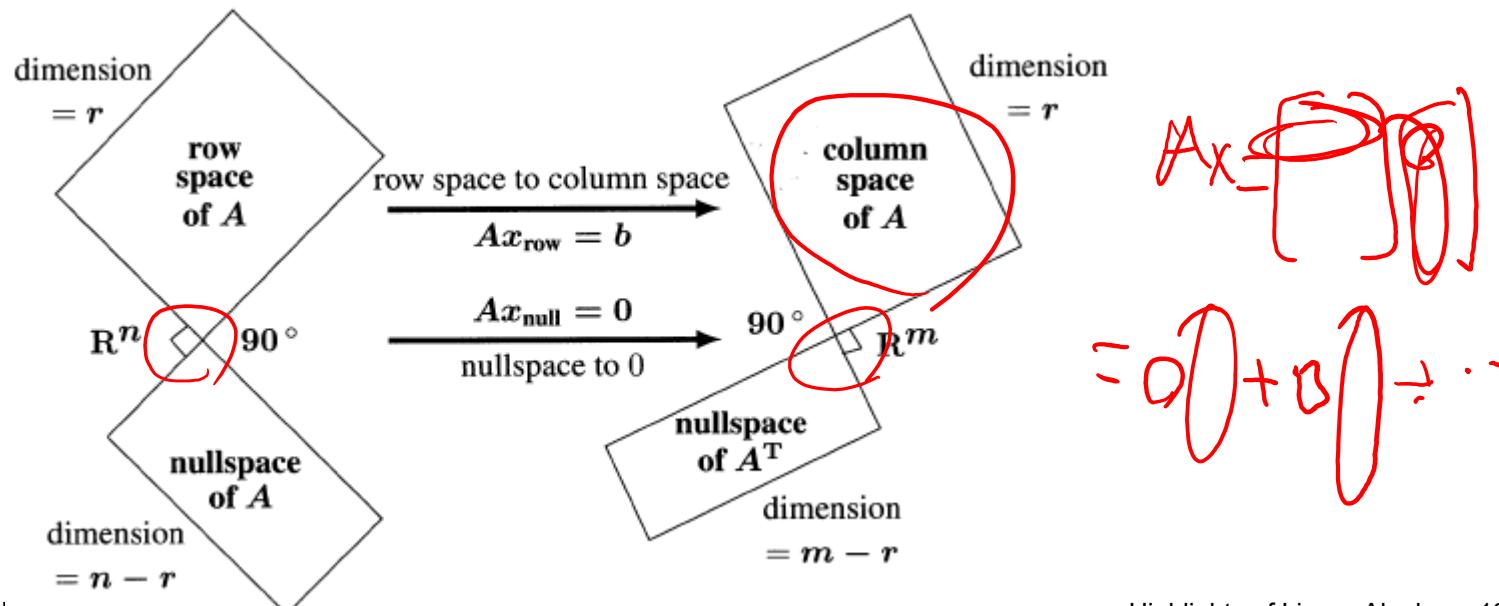
$$\underline{r_{ij} = q_i^T a_j}$$

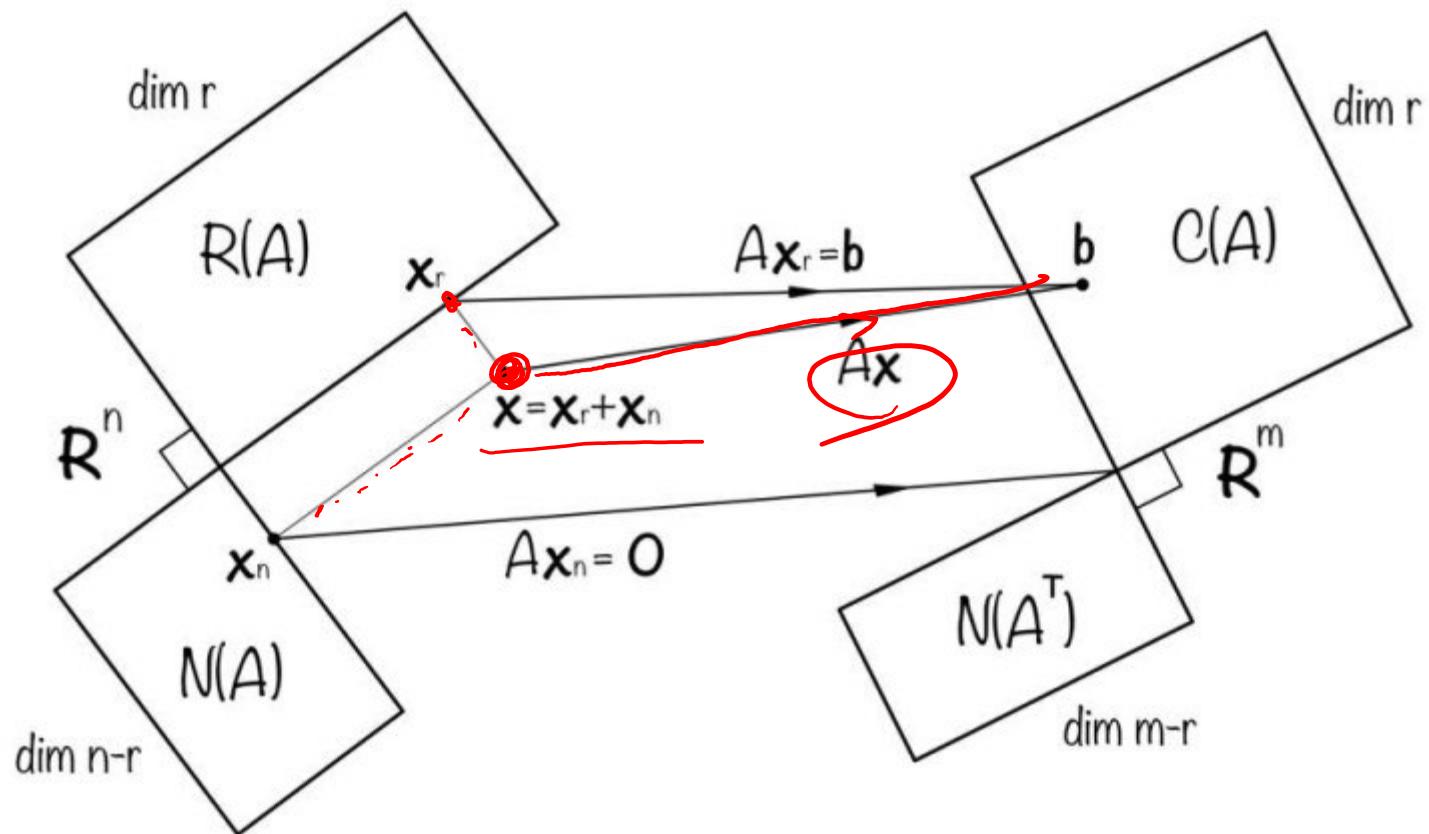
$$A = \begin{matrix} & n \\ \text{---} & \text{---} \\ m & \end{matrix}$$

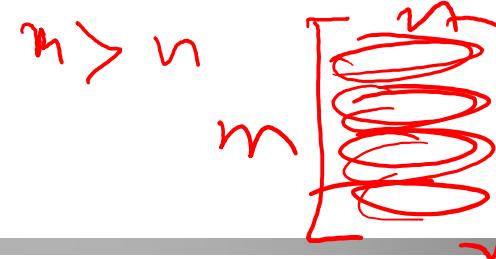
- 3. Orthogonal subspace R (row space) and N (null space)

- Ax=0: The row space of A is orthogonal to the nullspace of A
- A^Ty=0: The column space of A is orthogonal to the nullspace of A^T

$(Ax = 0 \text{ means each row } \cdot x = 0)$ \rightarrow $\begin{bmatrix} \text{row 1} \\ \vdots \\ \text{row } m \end{bmatrix} [x] = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}, A^T y = \begin{bmatrix} (\text{column 1})^T \\ \vdots \\ (\text{column } n)^T \end{bmatrix} [y] = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$







- 4. Tall thin matrices Q with orthonormal columns:

$Q^T Q \bar{Q} I$ multiplies any vector \mathbf{x} , the length of the vector does not change: $\|\mathbf{Qx}\| = \|\mathbf{x}\|$

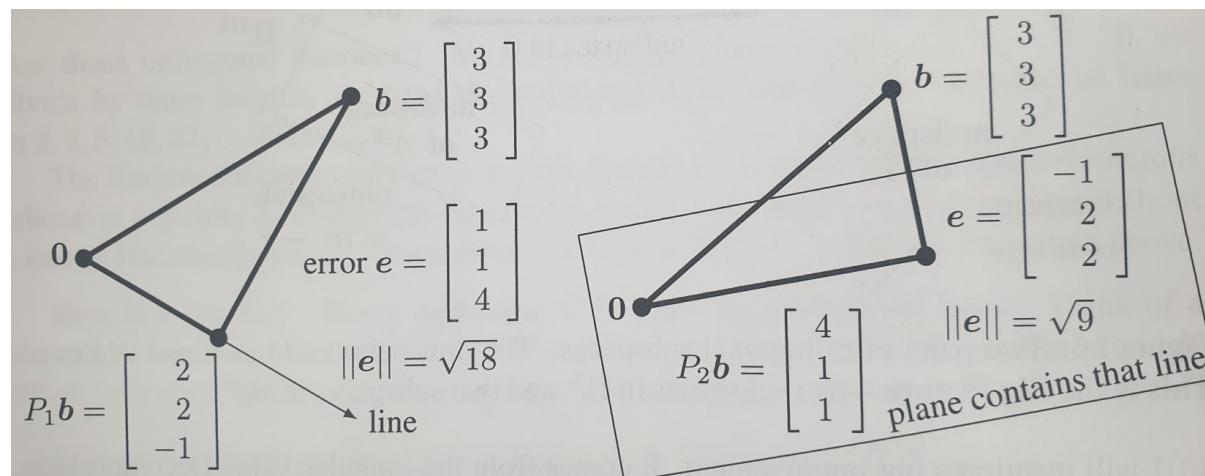
if $m > n$ then m rows cannot be orthogonal in \mathbb{R}^n : $\mathbf{QQ}^T \neq I$

$$Q_1 = \frac{1}{3} \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix}, Q_2 = \frac{1}{3} \begin{bmatrix} 2 & 2 \\ 2 & -1 \\ -1 & 2 \end{bmatrix}, Q_3 = \frac{1}{3} \begin{bmatrix} 2 & 2 & -1 \\ 2 & -1 & 2 \\ -1 & 2 & 2 \end{bmatrix} \rightarrow Q_i Q_i^T = I?$$

$P = QQ^T \rightarrow$ projection matrix: $P^2 = P = P^T \xrightarrow{\text{"least squares"}}$

$$P^2 = \frac{(Q\bar{Q}^T)(Q\bar{Q}^T)}{I} = Q\bar{Q}^T = P$$

$P\mathbf{b}$ is the orthogonal projection of \mathbf{b} onto the column space of P : $P_1\mathbf{b}$, $P_2\mathbf{b}$, $P_3\mathbf{b}$



$$\mathbf{P}_1 = \mathbf{Q}_1 \mathbf{Q}_1^T = \frac{1}{9} \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix} \begin{bmatrix} 2 & 2 & -1 \end{bmatrix} = \frac{1}{9} \begin{bmatrix} 4 & 4 & -2 \\ 4 & 4 & -2 \\ -2 & -2 & 1 \end{bmatrix} \rightarrow \mathbf{P}_1 \mathbf{b} = \frac{1}{9} \begin{bmatrix} 18 \\ 18 \\ -9 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix}$$

$$\mathbf{P}_2 = \mathbf{Q}_2 \mathbf{Q}_2^T = \frac{1}{9} \begin{bmatrix} 2 & 2 \\ 2 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 2 & & \\ & 2 & \\ & & 2 \end{bmatrix} \rightarrow \mathbf{P}_2 \mathbf{b}$$

$$\underline{\mathbf{Q}_3 \mathbf{Q}_3^T = \mathbf{I}}$$

~~$$\mathbf{Q}_1 = \frac{1}{3} \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix}, \mathbf{Q}_2 = \frac{1}{3} \begin{bmatrix} 2 & 2 \\ 2 & -1 \\ -1 & 2 \end{bmatrix}, \mathbf{Q}_3 = \frac{1}{3} \begin{bmatrix} 2 & 2 & -1 \\ 2 & -1 & 2 \\ -1 & 2 & 2 \end{bmatrix} \rightarrow \mathbf{Q}_i \mathbf{Q}_i^T = \mathbf{I}?$$~~

$\mathbf{P} = \mathbf{Q} \mathbf{Q}^T \rightarrow$ projection matrix: $\mathbf{P}^2 = \mathbf{P} = \mathbf{P}^T \xrightarrow{\text{"least squares"}}$

\mathbf{Pb} is the orthogonal projection of \mathbf{b} onto the column space of \mathbf{P} : $\mathbf{P}_1 \mathbf{b}, \mathbf{P}_2 \mathbf{b}, \mathbf{P}_3 \mathbf{b}$

$$\underline{\mathbf{P}_3 = \mathbf{Q}_3 \mathbf{Q}_3^T = \mathbf{I}} \rightarrow \underline{\mathbf{P}_3 \mathbf{b} = \mathbf{b}}$$

- 5. Orthogonal matrices are square with orthonormal columns: $Q^T = Q^{-1}$

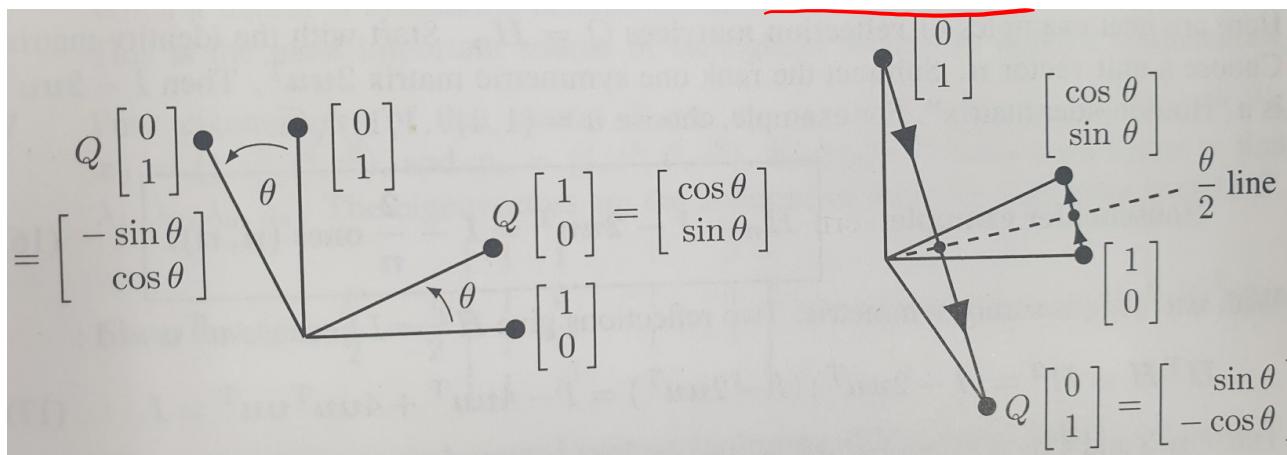
$$Q \text{ is square} \rightarrow \begin{cases} Q^T Q = I \\ Q Q^T = I \end{cases} \rightarrow Q^{-1} = Q^T$$

$$Q_{\text{rotate}} = \underbrace{\begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}}_{\text{rotation through an angle } \theta}, \quad Q_{\text{reflect}} = \underbrace{\begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix}}_{\text{reflection across the } \frac{\theta}{2} \text{ line}}$$

$$Q_1, Q_2 : \text{orthogonal} \rightarrow Q_1 Q_2 : \text{orthogonal}$$

$$(Q_1 Q_2)^T (Q_1 Q_2)$$

$$\begin{aligned} &= Q_2^T Q_1^T Q_1 Q_2 \\ &\stackrel{T}{=} I \end{aligned}$$



Orthogonal basis = orthogonal axes in \mathbb{R}^n
 orthogonal $\mathbf{Q}(n \times n)$: $\mathbf{v} = c_1\mathbf{q}_1 + \dots + c_n\mathbf{q}_n \rightarrow c_i = \mathbf{q}_i^T \mathbf{v}$
 $\mathbf{v} = \mathbf{Q}\mathbf{c} \rightarrow \mathbf{Q}^T \mathbf{v} = \mathbf{Q}^T \mathbf{Q}\mathbf{c} = \mathbf{c}$

Householder reflections: $\mathbf{Q} = \mathbf{H}_n = \mathbf{I} - 2\mathbf{u}\mathbf{u}^T$
 $\mathbf{u} = (1, 1, \dots, 1)/\sqrt{n} \rightarrow \mathbf{Q} = \mathbf{H}_n = \mathbf{I} - \frac{2}{n} \mathbf{ones}(n, n) \xrightarrow{\mathbf{u} \perp \mathbf{w}}$

$\mathbf{H}^T \mathbf{H} = \mathbf{H}^2 = \mathbf{I}$ $(\mathbf{I} - 2\mathbf{u}\mathbf{u}^T)(\mathbf{I} - 2\mathbf{u}\mathbf{u}^T) = \mathbf{I} - 4\mathbf{u}\mathbf{u}^T + 4\mathbf{u}\mathbf{u}^T\mathbf{u}\mathbf{u}^T$

$\mathbf{H}_3 = \mathbf{I} - \frac{2}{3} \mathbf{ones} = \frac{1}{3} \begin{bmatrix} 1 & -2 & -2 \\ -2 & 1 & -2 \\ -2 & -2 & 1 \end{bmatrix}$, $\mathbf{H}_4 = \mathbf{I} - \frac{2}{4} \mathbf{ones} = \frac{1}{2} \begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{bmatrix}$

eigenvalues of \mathbf{H}_n are -1 (once) and $+1$ ($n-1$ times)
 All reflection matrices have eigenvalues -1 and 1

$$H = I - 2 \frac{vv^T}{\|v\|^2} = I - 2uu^T$$

$u = \frac{v}{\|v\|}$

key point: if $v = a - r$ and $\|a\| = \|r\|$, then $Ha = r$

$$\underbrace{H_{n-1} \cdots H_2 H_1 A}_{\text{matrix}} = \begin{bmatrix} r_1 & r_2 & \cdots & r_n \end{bmatrix} \rightarrow Q^T A = R$$

$$A = \begin{bmatrix} 4 & x \\ 3 & x \end{bmatrix} \rightarrow a = \begin{bmatrix} 4 \\ 3 \end{bmatrix}, r = \begin{bmatrix} 5 \\ 0 \end{bmatrix} \rightarrow v = a - r = \begin{bmatrix} -1 \\ 3 \end{bmatrix} \rightarrow u = \frac{1}{\sqrt{10}} \begin{bmatrix} -1 \\ 3 \end{bmatrix}$$

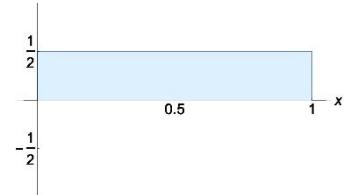
$$H = I - 2uu^T = \frac{1}{5} \begin{bmatrix} 4 & 3 \\ 3 & -4 \end{bmatrix} = Q^T \rightarrow HA = \begin{bmatrix} 5 & x \\ 0 & x \end{bmatrix} = R$$

$$\underline{R\hat{x} = Q^T b}$$

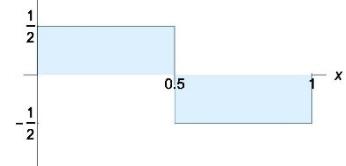
Examples

- Rotations
- Reflections
- Hadamard matrices
- Haar wavelets
- Discrete Fourier Transform (DFT)
- Complex inner product

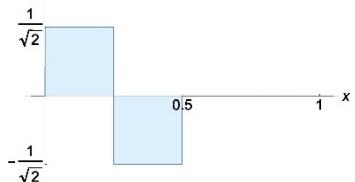
$$\mathbf{W} = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & -1 & 0 \\ 1 & -1 & 0 & 1 \\ 1 & -1 & 0 & -1 \end{bmatrix}$$



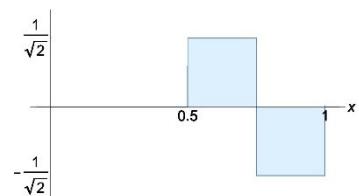
(a) Haar function of $h_0(x)$



(b) Haar function of $h_1(x)$



(c) Haar function of $h_2(x)$



(d) Haar function of $h_3(x)$

6. Eigenvalues and Eigenvectors

eigenvectors of \mathbf{A} don't change direction when you multiply them by \mathbf{A}

$$\left. \begin{array}{l} \mathbf{x} : \text{eigenvector of } \mathbf{A} \\ \lambda : \text{eigenvector of } \mathbf{A} \end{array} \right\} \rightarrow \boxed{\mathbf{Ax} = \lambda \mathbf{x}} \rightarrow \mathbf{A}(\mathbf{Ax}) = \mathbf{A}(\lambda \mathbf{x}) = \lambda(\mathbf{Ax}) = \lambda^2 \mathbf{x} \rightarrow \boxed{\mathbf{A}^k \mathbf{x} = \lambda^k \mathbf{x}}$$

$n \times n$ matrices \rightarrow n independent eigenvectors \mathbf{x}_1 to \mathbf{x}_n with n different eigenvalues λ_1 to λ_n

$$\mathbf{v} = c_1 \mathbf{x}_1 + \dots + c_n \mathbf{x}_n \rightarrow \mathbf{Av} = c_1 \lambda_1 \mathbf{x}_1 + \dots + c_n \lambda_n \mathbf{x}_n \rightarrow \boxed{\mathbf{A}^k \mathbf{v} = c_1 \lambda_1^k \mathbf{x}_1 + \dots + c_n \lambda_n^k \mathbf{x}_n}$$

How useful? $\begin{cases} \text{solution of differential equations} \\ \text{similar matrices} \rightarrow \text{same eigenvalues} \\ \text{diagonalize a matrix} \end{cases}$

Four properties: matrix \mathbf{A} (real), \mathbf{S} (symmetric), \mathbf{Q} (orthogonal)

$\underbrace{\mathbf{S} \text{ (symmetric)}}_{\text{like real numbers: } \lambda}, \quad \underbrace{\mathbf{Q} \text{ (orthogonal)}}_{\text{like complex numbers: } e^{i\theta}}$

(Trace of \mathbf{S}) $\sum_{i=1}^n \lambda_i$ = trace of matrix

(Determinant) $\prod \lambda_i$ = determinant of matrix

(Real eigenvalues of \mathbf{S}) \mathbf{S} : real eigenvalues, orthogonal eigenvectors

(Orthogonal eigenvectors) if $\lambda_1 \neq \lambda_2$, then $\mathbf{x}_1 \cdot \mathbf{x}_2 = 0$, eigenvectors of \mathbf{A} are orthogonal iff $\mathbf{A}^T \mathbf{A} = \mathbf{A} \mathbf{A}^T$

$$\mathbf{S} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \rightarrow \left\{ \mathbf{S} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ and } \mathbf{S} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = 1 \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right\}, \quad \mathbf{Q} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \rightarrow \left\{ \mathbf{Q} \begin{bmatrix} 1 \\ -i \end{bmatrix} = i \begin{bmatrix} 1 \\ -i \end{bmatrix} \text{ and } \mathbf{Q} \begin{bmatrix} 1 \\ i \end{bmatrix} = -i \begin{bmatrix} 1 \\ i \end{bmatrix} \right\}$$

$\text{eig}(\mathbf{A} + \mathbf{B}) \neq \text{eig}(\mathbf{A}) + \text{eig}(\mathbf{B})$
 $\text{eig}(\mathbf{AB}) \neq \text{eig}(\mathbf{A}) \text{eig}(\mathbf{B})$
 $\lambda_1 = \lambda_2$ might or might not have
two independent eigenvectors

$$\overline{\mathbf{x}_1} \cdot \mathbf{x}_2 = 0$$

(1) \mathbf{A} controls a system of linear differential equations: $\frac{d\mathbf{u}}{dt} = \boxed{\mathbf{A}\mathbf{u}}$ with $\mathbf{u}(0) = \mathbf{u}_0 = \boxed{e^{\lambda t}}$

$$\mathbf{u}(0) = c_1 \mathbf{x}_1 + \cdots + c_n \mathbf{x}_n$$

$$\mathbf{u}(t) = c_1 e^{\lambda_1 t} \mathbf{x}_1 + \cdots + c_n e^{\lambda_n t} \mathbf{x}_n \xrightarrow{\lambda = a + ib} \begin{cases} e^{at} & \begin{cases} \text{Re } \lambda > 0 : \text{ grow} \\ \text{Re } \lambda < 0 : \text{ decay} \end{cases} \\ e^{ibt} & \text{oscillate} \end{cases}$$

shift in $\mathbf{A} \rightarrow$ shift in λ : $\underbrace{(\mathbf{A} + s\mathbf{I})\mathbf{x}}_{\mathbf{x}} = \lambda \mathbf{x} + s\mathbf{x} = (\lambda + s)\mathbf{x}$

(2) \mathbf{B} similar to $\mathbf{A} \rightarrow \mathbf{B} = \underset{\text{invertible}}{\mathbf{M}} \mathbf{A} \mathbf{M}^{-1} \rightarrow \text{eig}(\mathbf{B}) = \text{eig}(\mathbf{A})$: compute eigenvalues of large matrices

Make \mathbf{B} gradually into a triangular matrix \rightarrow Gradually show up on the main diagonal

$$\mathbf{B}\mathbf{y} = \lambda\mathbf{y} \rightarrow \mathbf{M}\mathbf{A}\mathbf{M}^{-1}\mathbf{y} = \lambda\mathbf{y} \rightarrow \mathbf{A}(\mathbf{M}^{-1}\mathbf{y}) = \lambda(\mathbf{M}^{-1}\mathbf{y})$$

$$\underbrace{\mathbf{M}^{-1}\mathbf{M}\mathbf{A}(\mathbf{M}^{-1}\mathbf{y})}_{\mathbf{A}\mathbf{x}} = \lambda(\mathbf{M}^{-1}\mathbf{y}) \rightarrow \mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

$$A = X \Lambda X^{-1} = \begin{bmatrix} 3 & 1 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} 10 & 5 \\ 5 & 5 \end{bmatrix} \begin{bmatrix} -1 & -1 \\ -2 & 3 \end{bmatrix}^{-1}$$

(3) diagonalize a matrix

$$A \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} A\mathbf{x}_1 & \cdots & A\mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \lambda_1 \mathbf{x}_1 & \cdots & \lambda_n \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

$$X^{-1}AX = \Lambda$$

$$\begin{cases} AX = X\Lambda \\ A = X\Lambda X^{-1} \\ A^2 = X\Lambda^2 X^{-1} \end{cases}$$

$$A^k \mathbf{v} = X \Lambda^k X^{-1} \mathbf{v} : \mathbf{v} = X\mathbf{c} \rightarrow \underbrace{\mathbf{c}}_{c_i} = \underbrace{X^{-1}\mathbf{v}}_{c_i \lambda_i^k} \rightarrow \underbrace{\Lambda^k X^{-1}\mathbf{v}}_{c_i \lambda_i^k x_i} \rightarrow \underbrace{X\Lambda X^{-1}\mathbf{v}}$$

$$(X\Lambda X^{-1})(X\Lambda X^{-1})$$

Example: ~~$A = \begin{bmatrix} 8 & 3 \\ 2 & 7 \end{bmatrix}$~~ divide by 10 $\rightarrow A = \underbrace{\begin{bmatrix} 0.8 & 0.3 \\ 0.2 & 0.7 \end{bmatrix}}_{\text{Markov matrix with positive columns adding to 1}} \rightarrow \begin{cases} A^k \mathbf{v} = c_1 (1)^k \mathbf{x}_1 + c_2 \left(\frac{1}{2}\right)^k \mathbf{x}_2 \\ \text{as } k \text{ increases } A^k \mathbf{v} \text{ approaches to } c_1 \mathbf{x}_1 \end{cases}$

the action of the whole matrix A is broken into simple actions (just multiply by λ)

[nondiagonalizable matrices: when GM < AM, A is not diagonalizable]

- {} (Geometric Multiplicity = GM): count the independent eigenvectors, $\dim N(A - \lambda I)$
- {} (Algebraic Multiplicity = AM): count the repetitions of eigenvalues, $\det(A - \lambda I) = 0$

$$A = \begin{bmatrix} 5 & 1 \\ 0 & 5 \end{bmatrix}, \begin{bmatrix} 6 & -1 \\ 1 & 4 \end{bmatrix}, \begin{bmatrix} 7 & 2 \\ -2 & 3 \end{bmatrix} \rightarrow \begin{cases} \det(A - \lambda I) = (\lambda - 5)^2 = 0 \rightarrow AM = 2 \\ \text{rank}(A - 5I) = 1 \rightarrow GM = 1 \end{cases}$$

8. Singular Value Decomposition (SVD)

best matrices (real symmetric matrices \mathbf{S}): real eigenvalues and orthogonal eigenvectors

other matrices (\mathbf{A} is not square, $m \times n$): complex eigenvalues and not orthogonal eigenvectors

key point: two sets of singular vectors $\begin{cases} n \text{ right singular vectors } (\mathbf{v}_1, \dots, \mathbf{v}_n) \text{ orthogonal in } \mathbf{R}^n \\ m \text{ left singular vectors } (\mathbf{u}_1, \dots, \mathbf{u}_m) \text{ orthogonal in } \mathbf{R}^m \end{cases}$

connection between n v's and m u's

$$\underbrace{\mathbf{Av}_1 = \sigma_1 \mathbf{u}_1, \dots, \mathbf{Av}_r = \sigma_r \mathbf{u}_r}_{\begin{array}{l} r = \text{rank}(\mathbf{A}) \\ \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0 \end{array}}, \underbrace{\mathbf{Av}_{r+1} = \mathbf{0}, \dots, \mathbf{Av}_n = \mathbf{0}}_{\begin{array}{l} (n-r) \text{ v's in } N(\mathbf{A}) \\ (m-r) \text{ u's in } N(\mathbf{A}^T) \end{array}}$$

$$\mathbf{A} \begin{bmatrix} & & & & \\ \mathbf{v}_1 & \cdots & \mathbf{v}_r & \cdots & \mathbf{v}_n \\ & & & & \end{bmatrix} = \begin{bmatrix} & & & & \\ \mathbf{u}_1 & \cdots & \mathbf{u}_r & \cdots & \mathbf{u}_m \\ & & & & \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \rightarrow \begin{cases} \mathbf{AV} = \mathbf{U}\Sigma \Leftrightarrow \mathbf{AX} = \mathbf{X}\Lambda \\ \mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T \\ = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \dots + \sigma_r \mathbf{u}_r \mathbf{v}_r^T \\ (\mathbf{A} \rightarrow r \text{ pieces of rank 1}) \end{cases}$$

Proof of SVD

$$\mathbf{AX} = \mathbf{X}\Lambda \Leftrightarrow \mathbf{AV} = \mathbf{U}\Sigma$$

$$\begin{bmatrix} 3 & 0 \\ 4 & 5 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 & -3 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 3\sqrt{5} \\ \sqrt{5} \end{bmatrix}$$

not symmetric
 $\mathbf{V} \neq \mathbf{U}$

$\mathbf{V}^T = \mathbf{V}^{-1}$
 $\mathbf{U}^T = \mathbf{U}^{-1}$

$\text{rank}(\mathbf{A}) = 2 \rightarrow \sigma_1, \sigma_2$
 $\sigma_1 \sigma_2 = \det(\mathbf{A})$

$$\sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^T = \frac{3\sqrt{5}}{\sqrt{10}\sqrt{2}} \begin{bmatrix} 1 \\ 3 \end{bmatrix} [1 \ 1] + \frac{\sqrt{5}}{\sqrt{10}\sqrt{2}} \begin{bmatrix} -3 \\ 1 \end{bmatrix} [-1 \ 1] = \frac{3}{2} \begin{bmatrix} 1 & 1 \\ 3 & 3 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 3 & -3 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 4 & 5 \end{bmatrix} = \mathbf{A}$$

$\left\{ \begin{array}{l} \mathbf{V} \text{ contains orthonormal eigenvectors of } \mathbf{A}^T \mathbf{A} \\ \mathbf{U} \text{ contains orthonormal eigenvectors of } \mathbf{A} \mathbf{A}^T \\ \sigma_1^2 \text{ to } \sigma_r^2 \text{ are the nonzero eigenvalues of both } \mathbf{A}^T \mathbf{A} \text{ and } \mathbf{A} \mathbf{A}^T \end{array} \right.$

SVD requires that $\mathbf{Av}_k = \sigma_k \mathbf{u}_k$: $\mathbf{v}_k (\mathbf{A}^T \mathbf{A} \mathbf{v}_k = \sigma_k^2 \mathbf{v}_k) \rightarrow \mathbf{u}_k$'s

$$\left(\mathbf{u}_k = \frac{\mathbf{Av}_k}{\sigma_k} \text{ for } k = 1, \dots, r \right)$$

sign, multiple eigenvalues

(check 1) \mathbf{u} 's are eigenvectors of $\mathbf{A} \mathbf{A}^T \rightarrow \mathbf{A} \mathbf{A}^T \mathbf{u}_k = \sigma_k^2 \mathbf{u}_k$

(check 2) \mathbf{u} 's are also orthonormal $\rightarrow \mathbf{u}_j^T \mathbf{u}_k = \frac{\sigma_k}{\sigma_j} \mathbf{v}_j^T \mathbf{v}_k = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases}$

choose $(n-r)$ \mathbf{v} 's in $N(\mathbf{A})$ and $(m-r)$ \mathbf{u} 's in $N(\mathbf{A}^T)$

$$\begin{aligned} \mathbf{A} \mathbf{A}^T \frac{\mathbf{Av}_k}{\sigma_k} &= \frac{\mathbf{A} \sigma_k^2 \mathbf{v}_k}{\sigma_k} \\ &= \sigma_k \mathbf{Av}_k \\ &\stackrel{?}{=} \sigma_k \mathbf{u}_k \end{aligned}$$

$$\left(\frac{\mathbf{Av}_j}{\sigma_j} \right)^T \left(\frac{\mathbf{Av}_k}{\sigma_k} \right) = \frac{\mathbf{v}_j^T (\mathbf{A} \mathbf{A}^T \mathbf{v}_k)}{\sigma_j \sigma_k}$$

8. Singular Value Decomposition (SVD)

- Columns of V are orthogonal eigenvectors of $A^T A$
- $Av = \sigma u$ gives orthonormal eigenvectors u of $A A^T$
- $\sigma^2 = \text{eigenvalue of } A^T A = \text{eigenvalue of } A A^T \neq 0$
- Why is the SVD so important?
 - It separates the matrix into rank one pieces like the other factorizations $A=LU$, $A=QR$, $S=Q\Lambda Q^T$
 - Those pieces come in order of importance
 - First piece $\sigma_1 u_1 v_1^T$ is the closest rank one matrix to A
 - Sum of the first k pieces is best possible for rank k

$\mathbf{A}_k = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \dots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T$ is the best rank k approximation to \mathbf{A} :

If \mathbf{B} has rank k then $\|\mathbf{A} - \mathbf{A}_k\| \leq \|\mathbf{A} - \mathbf{B}\|$

Example

Find the matrices $\mathbf{U}, \Sigma, \mathbf{V}$ for $\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 4 & 5 \end{bmatrix} \rightarrow \mathbf{A}^T \mathbf{A} = \begin{bmatrix} 25 & 20 \\ 20 & 25 \end{bmatrix}, \mathbf{A} \mathbf{A}^T = \begin{bmatrix} 9 & 12 \\ 12 & 41 \end{bmatrix}$

$$\mathbf{U} = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 & -3 \\ 3 & 1 \end{bmatrix}, \Sigma = \begin{bmatrix} \sqrt{45} & 0 \\ 0 & \sqrt{5} \end{bmatrix}, \mathbf{V} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$\sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^T = \mathbf{A}$$

- If $S = Q \Lambda Q^T$ is symmetric positive definite, what is its SVD? $S = \mathbf{U} \Sigma \mathbf{V}^T$
- If $S = Q \Lambda Q^T$ has a negative eigenvalue ($Sx = -\alpha x$), what is the singular value and what are the vectors v and u ? $S(v) = 0 \cdot v$ $Q^T Q = I$ $A = Q = V \Sigma V^T$
- If $A = Q$ is an orthogonal matrix, why does every singular value equal 1?
- Why are all eigenvalues of a square matrix A less than or equal to σ_1 ?
- If $A = xy^T$ has rank 1, what are u_1, v_1, σ_1 ? Check that $|\lambda_1| \leq \sigma_1$
- What is the Karhunen-Loève transform and its connection to SVD?

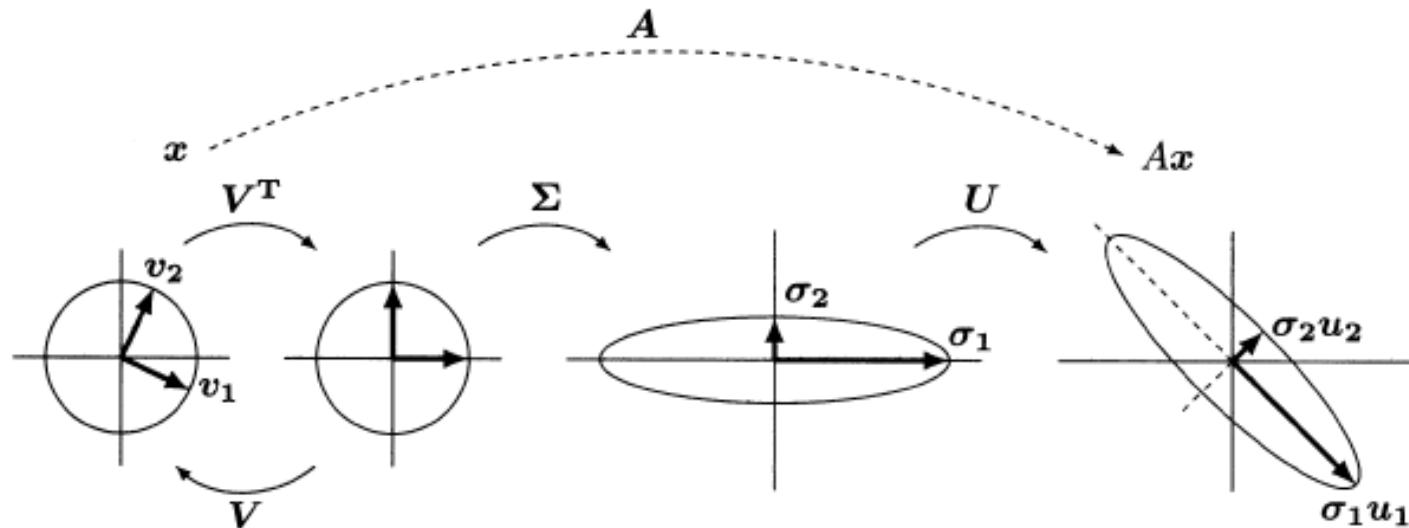
$$\|Ax\| = \|\mathbf{U} \Sigma \mathbf{V}^T x\| = \|\Sigma \mathbf{V}^T x\| \leq \sigma_1 \|x\| = \sigma_1 \|x\| \quad \frac{x}{\|x\|} \rightarrow \frac{\mathbf{V}^T x}{\|\mathbf{V}^T x\|}$$

$$= \|\mathbf{V}^T x\|$$

Geometry of SVD



- $A = (\text{rotation})(\text{stretching})(\text{rotation}) U\Sigma V^T$ for every A
- If A is m by n and B is n by m , then AB and BA have the same nonzero eigenvalues



$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} \sigma_1 & \\ & \sigma_2 \end{bmatrix} \begin{bmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{bmatrix}$$

4 parameters: two angles, two numbers

First singular vector \mathbf{v}_1

$$\max \lambda = \frac{\|\mathbf{Ax}\|}{\|\mathbf{x}\|}$$

Maximize the ratio $\frac{\|\mathbf{Ax}\|}{\|\mathbf{x}\|} \rightarrow$ The maximum is σ_1 at the vector $\mathbf{x} = \underline{\mathbf{v}_1}$

maximizing \mathbf{x} is \mathbf{v}_1 : $\mathbf{Av}_1 = \sigma_1 \mathbf{u}_1$ (the longest axis of the ellipse), $\|\mathbf{v}_1\| = 1 \rightarrow \|\mathbf{Av}_1\| = \sigma_1$

\Rightarrow Find the maximum value λ of $\frac{\|\mathbf{Ax}\|^2}{\|\mathbf{x}\|^2} = \frac{(\mathbf{Ax})^T \mathbf{Ax}}{\mathbf{x}^T \mathbf{x}} = \frac{\mathbf{x}^T \mathbf{Sx}}{\mathbf{x}^T \mathbf{x}}$

$\frac{\partial}{\partial x_i} \left(\frac{\mathbf{x}^T \mathbf{Sx}}{\mathbf{x}^T \mathbf{x}} \right) = (\mathbf{x}^T \mathbf{x}) 2(\mathbf{Sx})_i - (\mathbf{x}^T \mathbf{Sx}) 2(\mathbf{x})_i = 0$ for $i = 1, \dots, n$

$\rightarrow (\mathbf{Sx})_i = \left(\frac{\mathbf{x}^T \mathbf{Sx}}{\mathbf{x}^T \mathbf{x}} \right) (\mathbf{x})_i \rightarrow \mathbf{Sx} = \lambda \mathbf{x}$

Maximize $\frac{\|\mathbf{Ax}\|}{\|\mathbf{x}\|}$ under the condition $\mathbf{v}_1^T \mathbf{x} = 0 \rightarrow$ The maximum is σ_2 at $\mathbf{x} = \mathbf{v}_2$

Polar decomposition

$$x + iy \underset{\text{complex number}}{=} re^{i\theta} \underset{\text{polar form}}{=} \begin{cases} e^{i\theta} : \text{orthogonal matrix } \mathbf{Q} \\ r \geq 0 : \text{positive semidefinite matrix } \mathbf{S} \end{cases}$$

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T = (\mathbf{U}\mathbf{V}^T)(\mathbf{V}\Sigma\mathbf{V}^T) = \underline{\mathbf{QS}} \quad S = Q \Lambda Q^T$$

if \mathbf{A} is invertible, then Σ and \mathbf{S} are also invertible

$$\boxed{\mathbf{S}^2 = \mathbf{V}\Sigma^2\mathbf{V}^T = \mathbf{A}^T\mathbf{A}} \rightarrow \begin{cases} \text{eigenvalues of } \mathbf{S} = \text{singular values of } \mathbf{A} \\ \text{eigenvectors of } \mathbf{S} = \text{singular vectors } \mathbf{v} \text{ of } \mathbf{A} \end{cases}$$

$$\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 4 & 5 \end{bmatrix} \rightarrow \mathbf{U} = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 & -3 \\ 3 & 1 \end{bmatrix}, \Sigma = \begin{bmatrix} \sqrt{45} & \\ & \sqrt{5} \end{bmatrix}, \mathbf{V} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$\mathbf{Q} = \mathbf{U}\mathbf{V}^T = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 & -3 \\ 3 & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & -1 \\ 1 & 2 \end{bmatrix}$$

$$\mathbf{S} = \mathbf{V}\Sigma\mathbf{V}^T = \frac{\sqrt{5}}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & \\ & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \sqrt{5} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$\boxed{\mathbf{A} = \begin{matrix} \mathbf{Q} & \mathbf{S} \\ \downarrow & \downarrow \\ \text{rotation} & \text{stretch} \end{matrix}}$$

9. Principal Components and the Best Low Rank Matrix

- major tool in understanding a matrix of data
 - Schmidt(1907) → Eckart and Young(1936, $\|\mathbf{A}\|_F$) → Mirsky(1955)
- Eckart-Young low rank approximation theorem
 - The norm of $\mathbf{A} - \mathbf{A}_k$ is below the norm of all other $\mathbf{A} - \mathbf{B}_k$
 - $\mathbf{A}_k = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \dots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T$

Eckart-Young: If \mathbf{B} has rank k , then $\|\mathbf{A} - \mathbf{B}\| \geq \|\mathbf{A} - \mathbf{A}_k\|$

$\mathbf{A}_k = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \dots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T$: the closest rank k matrix to \mathbf{A}

$$\left\{ \begin{array}{l} \text{Spectral norm: } \|\mathbf{A}\|_2 = \max_{\mathbf{x} \neq 0} \frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|} = \sigma_1 (\ell^2 \text{ norm}) \\ \text{Frobenius norm: } \|\mathbf{A}\|_F = \sqrt{\sigma_1^2 + \dots + \sigma_r^2} \\ \text{Nuclear norm: } \|\mathbf{A}\|_N = \sigma_1 + \dots + \sigma_r (\text{the trace norm}) \\ \|\mathbf{I}\|_2 = 1 = \|\mathbf{Q}\|_2, \quad \|\mathbf{I}\|_F = \sqrt{n} = \|\mathbf{Q}\|_F, \quad \|\mathbf{I}\|_N = n = \|\mathbf{Q}\|_N \end{array} \right.$$

Eckart-Young Theorem

- Best approximation by A_k

Eckart-Young in L^2 :

$$\text{If } \text{rank}(\mathbf{B}) \leq k, \text{ then } \|\mathbf{A} - \mathbf{B}\| = \max_{\mathbf{x} \neq 0} \frac{\|(\mathbf{A} - \mathbf{B})\mathbf{x}\|}{\|\mathbf{x}\|} \geq \sigma_{k+1}$$

Eckart-Young in the Frobenius norm:

If \mathbf{B} is closest to \mathbf{A} , then $\mathbf{U}^T \mathbf{B} \mathbf{V}$ is closest to $\mathbf{U}^T \mathbf{A} \mathbf{V}$

$$\mathbf{B} = \mathbf{U} \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}_{k \times k} \mathbf{V}^T, \mathbf{A} = \begin{bmatrix} \mathbf{L} + \mathbf{E} + \mathbf{R} & \mathbf{F} \\ \mathbf{G} & \mathbf{H} \end{bmatrix}$$

The matrix \mathbf{D} must be the same as $\mathbf{E} = \text{diag}(\sigma_1, \dots, \sigma_k)$

The singular values of \mathbf{H} must be the smallest $(n - k)$ singular values of \mathbf{A}

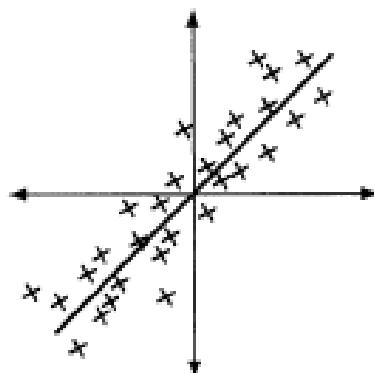
The smallest error $\|\mathbf{A} - \mathbf{B}\|_F$ must be $\|\mathbf{H}\|_F = \sqrt{\sigma_{k+1}^2 + \dots + \sigma_r^2}$

$$\mathbf{A} = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \xrightarrow{\text{rank 2 matrix closest to A}}$$

$$\mathbf{A}_2 = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \mathbf{B}_2 = \begin{bmatrix} 3.5 & 3.5 & 0 & 0 \\ 3.5 & 3.5 & 0 & 0 \\ 0 & 0 & 1.5 & 1.5 \\ 0 & 0 & 1.5 & 1.5 \end{bmatrix}$$

Principal Component Analysis

- Understand n sample points in m -dimensional space
- Data matrix A_0 : n samples, m variables
 - Find the average (the sample mean) along each row of A_0
 - Subtract that mean from m entries in the row
 - Centered matrix $A = A_0 - (\text{mean})$
 - How will linear algebra find that closest line through $(0,0)$? It is in the direction of the first singular vector u_1 of A ?



A is $2 \times n$ (large nullspace)

AA^T is 2×2 (small matrix)

$A^T A$ is $n \times n$ (large matrix)

Two singular values $\sigma_1 > \sigma_2 > 0$

- **Statistics** behind PCA
 - Variances: diagonal entries of the matrix AA^T
 - Covariances: off-diagonal entries of the matrix AA^T
 - Sample covariance matrix: $S = AA^T/(n-1)$
- **Geometry** behind PCA
 - Sum of squared distances from the data points to the line is a minimum
- **Linear algebra** behind PCA
 - Singular values σ_i and singular vectors u_i of A
 - Total variance:

$$T = \frac{\|A\|_F^2}{n-1} = \frac{\sigma_1^2 + \dots + \sigma_r^2}{n-1}$$

