

Linear Algebra

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Norms

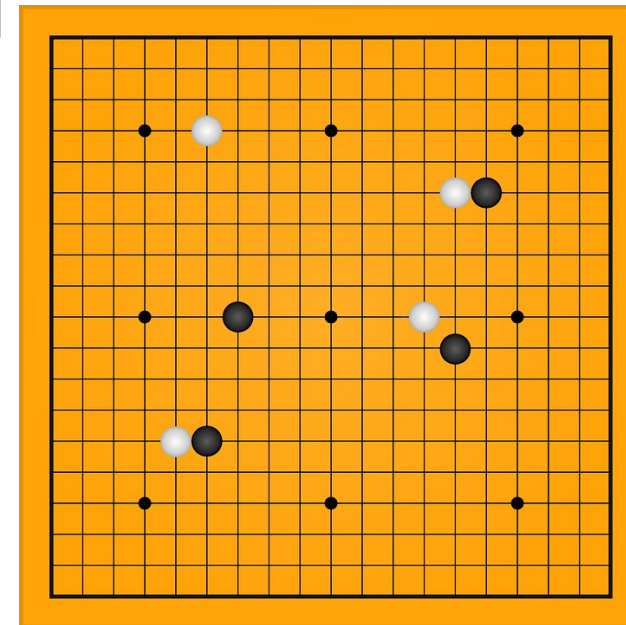
■ L^p Norms

$$\|\mathbf{x}\|_p = (\sum_i |x_i|^p)^{\frac{1}{p}} \quad \text{for } p \in \mathbf{Z}, p \geq 1$$

where $\mathbf{x} = [x_1 \quad \cdots \quad x_n]^T$

- L^1 norm : Metropolitan distance $\rightarrow \|\mathbf{x}\|_1 = |x_1| + |x_2| + |x_3|$
- L^2 norm : Euclidean distance $\rightarrow \|\mathbf{x}\|_2 = \sqrt{x_1^2 + x_2^2 + x_3^2}$
- max norm : $\rightarrow \|\mathbf{x}\|_\infty = \max_i |x_i|$
- Frobenius norm : measure the size of a matrix

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i,j} A_{i,j}^2}$$



Norms – cont.

- ❑ Functions mapping vectors to non-negative values
- ❑ Measures the distance from the origin to the point x .
- ❑ More rigorously, any function f that satisfies the following properties:
 - $f(\mathbf{x}) = 0 \rightarrow \mathbf{x} = 0$
 - $f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$: triangle inequality
 - for all $\alpha \in R$, $f(\alpha \mathbf{x}) = |\alpha|f(\mathbf{x})$

Special Kinds of Matrices and Vectors

- Diagonal matrix

$$D = \begin{bmatrix} v_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & v_n \end{bmatrix} \quad D^{-1} = \begin{bmatrix} \frac{1}{v_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{v_n} \end{bmatrix}, \quad D^{-1} \text{ exists only if } v_i \neq 0$$

- Symmetric matrix

$$A = A^T$$

- Skew-symmetric matrix

$$A = -A^T$$

- Orthogonal matrix

$$A^T A = A A^T = I \rightarrow A^{-1} = A^T$$

- Hermitian matrix

$$\bar{A}^T = A \text{ or } A^T = \bar{A}$$

- Skew-hermitian matrix

$$\bar{A}^T = -A \text{ or } A^T = -\bar{A}$$

- Unitary matrix

$$\bar{A}^T = A^{-1}$$

- Unit vector : a vector with unit norm $\|x\|_2 = 1$

Special Kinds of Matrices and Vectors – cont.

- Diagonal matrix

$$\mathbf{D} = \begin{bmatrix} 1.5 & 0 & 0 \\ 0 & 2.1 & 0 \\ 0 & 0 & 3.3 \end{bmatrix} \quad \mathbf{D}^{-1} = \begin{bmatrix} \frac{1}{1.5} & 0 & 0 \\ 0 & \frac{1}{2.1} & 0 \\ 0 & 0 & \frac{1}{3.3} \end{bmatrix}, \quad \mathbf{D}^{-1} \text{ exists only if } v_i \neq 0$$

- Symmetric matrix

$$\mathbf{A} = \mathbf{A}^T$$

- Skew-symmetric matrix

$$\mathbf{A} = -\mathbf{A}^T$$

- Orthogonal matrix

$$\mathbf{A}^T \mathbf{A} = \mathbf{A} \mathbf{A}^T = \mathbf{I} \rightarrow \mathbf{A}^{-1} = \mathbf{A}^T$$

$$\begin{bmatrix} -3 & 1 & 5 \\ 1 & 0 & -2 \\ 5 & -2 & 4 \end{bmatrix}, \quad \begin{bmatrix} 0 & 9 & -12 \\ -9 & 0 & 20 \\ 12 & -20 & 0 \end{bmatrix}, \quad \begin{bmatrix} \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & -\frac{2}{3} \end{bmatrix}$$

Special Kinds of Matrices and Vectors – cont.

- Hermitian matrix $\bar{A}^T = A \text{ or } A^T = \bar{A}$
- Skew-hermitian matrix $\bar{A}^T = -A \text{ or } A^T = -\bar{A}$
- Unitary matrix $\bar{A}^T = A^{-1}$
- Unit vector : a vector with unit norm $\|x\|_2 = 1$

$$A = \begin{bmatrix} 4 & 1 - 3i \\ 1 + 3i & 7 \end{bmatrix} \quad B = \begin{bmatrix} 3i & 2 + i \\ -2 + i & -i \end{bmatrix} \quad C = \begin{bmatrix} \frac{1}{2}i & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2}i \end{bmatrix}$$

$$\text{Unit vector : } v = \left[\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2} \right]$$

Eigendecomposition

- Decompose a matrix into a set of eigenvectors and eigenvalues.

$$A\mathbf{v} = \lambda\mathbf{v} \quad \lambda: \text{eigen value} \quad \mathbf{v}: \text{eigen vector}$$

$$\mathbf{v}^T A = \lambda\mathbf{v}^T \quad \text{left eigen vector}$$

- Suppose A has linearly independent eigenvectors $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$ with corresponding eigenvalues $\{\lambda_1, \dots, \lambda_n\}$

Eigen decomposition : $A = V \text{diag}(\lambda) V^{-1}$, 여기서 $V = [\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}]$
($\because AV = V \text{diag}(\lambda)$)

- Every real symmetric matrix can be decomposed into a real-valued eigenvectors and eigenvalues.

$$A = Q \text{diag}(\lambda) Q^T$$

Eigendecomposition – cont.

- $A = \begin{bmatrix} 6 & -3 \\ 4 & -1 \end{bmatrix}$ 일때 eigen value, eigenvector 계산

- Step 1 :

$$\det(\lambda I - A) = \begin{vmatrix} \lambda - 6 & 3 \\ -4 & \lambda + 1 \end{vmatrix} = \lambda^2 - 5\lambda + 6 = 0 \rightarrow \lambda = 3, 2$$

- Step 2 :

- i) $\lambda_1 = 3$:

$$\lambda_1 I - A = \begin{bmatrix} -3 & 3 \\ -4 & 4 \end{bmatrix} \rightarrow \begin{bmatrix} -3 & 3 \\ -4 & 4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0 \rightarrow x - y = 0$$
$$\therefore v^{(1)} = [1, 1]^T$$

- ii) $\lambda_2 = 2$: $v^{(2)} = [3, 4]^T$

Eigendecomposition – cont.

■ Step 2 :

□ ii) $\lambda_2 = 2$:

$$\lambda_2 I - A = \begin{bmatrix} -4 & 3 \\ -4 & 3 \end{bmatrix} \rightarrow \begin{bmatrix} -4 & 3 \\ -4 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0 \rightarrow -4x + 3y = 0$$

$$\therefore v^{(2)} = [3, 4]^T$$

Eigendecomposition – cont.

- $\{v^{(1)}, v^{(2)}\}$: linearly independent eigenvectors with corresponding eigenvalues $\{3, 2\}$

□ Eigen decomposition : $A = V \text{diag}(\lambda) V^{-1}$

$$\begin{bmatrix} 6 & -3 \\ 4 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix}^{-1} \quad \text{그런데, } \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix}^{-1} = \begin{bmatrix} 4 & -3 \\ -1 & 1 \end{bmatrix} \text{이므로}$$

$$\begin{bmatrix} 6 & -3 \\ 4 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 4 & -3 \\ -1 & 1 \end{bmatrix} \text{로 나타낼 수 있다.}$$

□ Diagonalization: $\text{diag}(\lambda) = V^{-1} A V$

$$\begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} = \begin{bmatrix} 4 & -3 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 6 & -3 \\ 4 & -1 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix}$$

Eigendecomposition – cont.

- $A = \begin{bmatrix} 5 & 2 \\ 2 & 2 \end{bmatrix}$ 일때 eigen values, eigenvectors 계산

- Step 1 :

$$\det(\lambda I - A) = \begin{vmatrix} \lambda - 5 & -2 \\ -2 & \lambda - 2 \end{vmatrix} = \lambda^2 - 7\lambda + 6 = 0 \rightarrow \lambda = 1, 6$$

- Step 2 :

- i) $\lambda_1 = 1$:

$$\lambda_1 I - A = \begin{bmatrix} -4 & -2 \\ -2 & -1 \end{bmatrix} \rightarrow \begin{bmatrix} -4 & -2 \\ -2 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0 \rightarrow 2x + y = 0$$

$$\therefore v^{(1)} = [1, -2]^T$$

- ii) $\lambda_2 = 6$:

Eigendecomposition – cont.

■ Step 2 :

□ ii) $\lambda_2 = 6$:

$$\lambda_2 I - A = \begin{bmatrix} 1 & -2 \\ -2 & 4 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & -2 \\ -2 & 4 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0 \rightarrow x - 2y = 0$$

$$\therefore v^{(2)} = [2, \ 1]^T$$

■ Step 3 :

$$A = V \operatorname{diag}(\lambda) V^{-1} = \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}^{-1}$$

$$\begin{aligned} \left(\begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}^{-1} = \frac{1}{5} \begin{bmatrix} 1 & -2 \\ 2 & 1 \end{bmatrix} \right) &= \frac{1}{5} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix} \begin{bmatrix} 1 & -2 \\ 2 & 1 \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 6 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix} = \mathbf{Q} \operatorname{diag}(\lambda) \mathbf{Q}^T \end{aligned}$$

Eigendecomposition – cont.

- Every real symmetric matrix can be decomposed into a real-valued eigenvectors and eigenvalues.

$$\bar{x}^T A x = \lambda \bar{x}^T x \rightarrow \lambda = \frac{\bar{x}^T A x}{\bar{x}^T x} \quad (\because \bar{x}^T A x = x^T A^T \bar{x} = \overline{\bar{x}^T A x}, (AB)^T = B^T A^T)$$

- A : symmetric $\Leftrightarrow \langle Av, w \rangle = \langle v, Aw \rangle$

$$\Leftrightarrow \langle Av, w \rangle = (Av)^T w = v^T A^T w = \langle v, A^T w \rangle = \langle v, Aw \rangle$$

- A : symmetric and v, w : eigenvectors with different eigenvalue

$$\Leftrightarrow \langle v, w \rangle = 0$$

$$(\text{proof}): \text{suppose } Av = \lambda_1 v \text{ and } Aw = \lambda_2 w$$

$$\Leftrightarrow \lambda_1 \langle v, w \rangle = \langle \lambda_1 v, w \rangle = \langle Av, w \rangle = \langle v, Aw \rangle = \langle v, \lambda_2 w \rangle = \lambda_2 \langle v, w \rangle$$

$$\Leftrightarrow \text{eigenvectors are orthogonal} \Leftrightarrow \mathbf{Q}^T = \mathbf{Q}^{-1}$$

Quadratic Forms

$$\begin{aligned} Q = \mathbf{x}^T \mathbf{A} \mathbf{x} &= \sum_{j=1}^n \sum_{k=1}^n a_{jk} x_j x_k \\ &= a_{11} x_1^2 + a_{12} x_1 x_2 + \cdots + a_{1n} x_1 x_n \\ &\quad + a_{21} x_2 x_1 + a_{22} x_2^2 + \cdots + a_{2n} x_2 x_n \\ &\quad + \cdots \cdots \cdots \\ &\quad + a_{n1} x_n x_1 + a_{n2} x_n x_2 + \cdots + a_{nn} x_n^2. \end{aligned}$$

Quadratic Form. Symmetric Coefficient Matrix

Let

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & 4 \\ 6 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 3x_1^2 + 4x_1x_2 + 6x_2x_1 + 2x_2^2 = 3x_1^2 + 10x_1x_2 + 2x_2^2.$$

Here $4 + 6 = 10 = 5 + 5$. From the corresponding *symmetric* matrix $\mathbf{C} = [c_{jk}]$, where $c_{jk} = \frac{1}{2}(a_{jk} + a_{kj})$, thus $c_{11} = 3, c_{12} = c_{21} = 5, c_{22} = 2$, we get the same result; indeed,

$$\mathbf{x}^T \mathbf{C} \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & 5 \\ 5 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 3x_1^2 + 5x_1x_2 + 5x_2x_1 + 2x_2^2 = 3x_1^2 + 10x_1x_2 + 2x_2^2. \quad \blacksquare$$

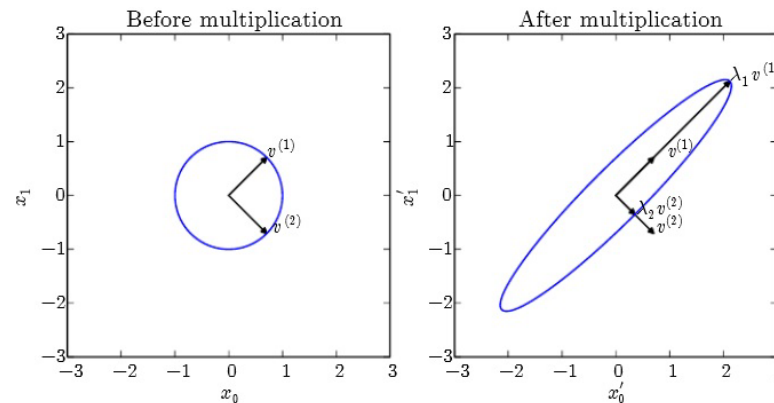
Quadratic Forms – cont.

■ $f(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$ ($\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T$) 이용하면

$$\begin{aligned} &= \mathbf{x}^T \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T \mathbf{x} = \mathbf{x}^T \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T \mathbf{x} = (\mathbf{Q}^T \mathbf{x})^T \mathbf{\Lambda} (\mathbf{Q}^T \mathbf{x}) = \mathbf{y}^T \mathbf{\Lambda} \mathbf{y}, \quad (\mathbf{y} = \mathbf{Q}^T \mathbf{x}) \text{ 이용} \\ &= [y_1 \quad y_2] \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \\ &= \lambda_1 y_1^2 + \lambda_2 y_2^2 \end{aligned}$$

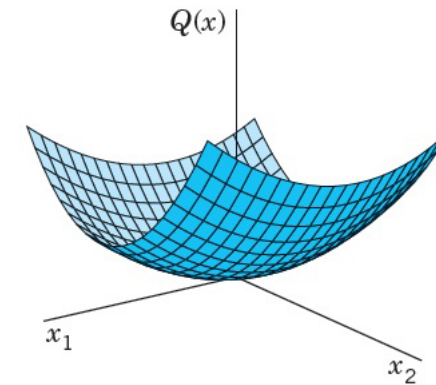
□ Optimization of quadratic form $f(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$ subject to $\|\mathbf{x}\|_2 = 1$

$$\|\mathbf{x}\|_2 = 1 \equiv \sqrt{x_1^2 + x_2^2} = 1 \rightarrow \mathbf{x}^T \mathbf{x} = \mathbf{1}$$

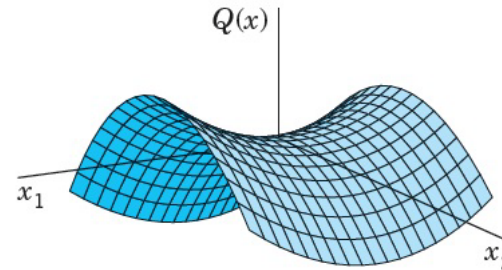


Quadratic Forms – cont.

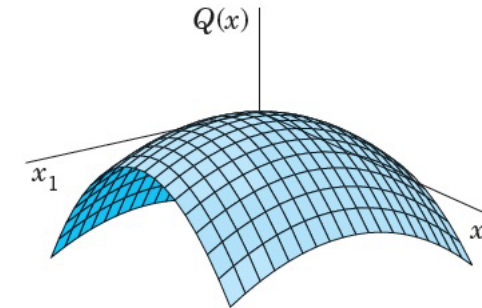
- Effect of eigenvectors and eigenvalues
 - ❑ Matrix is singular iff any of the eigenvalues are 0. (error)
 - ❑ Matrix whose eigenvalues are all positive \Rightarrow positive definite
 - ❑ cf: positive semidefinite, negative (semi)definite.
 - ❑ Positive definite matrix satisfying $\mathbf{x}^T \mathbf{A} \mathbf{x} = 0 \Rightarrow \mathbf{x} = 0$



(a) Positive definite form



(c) Indefinite form



(b) Negative definite form

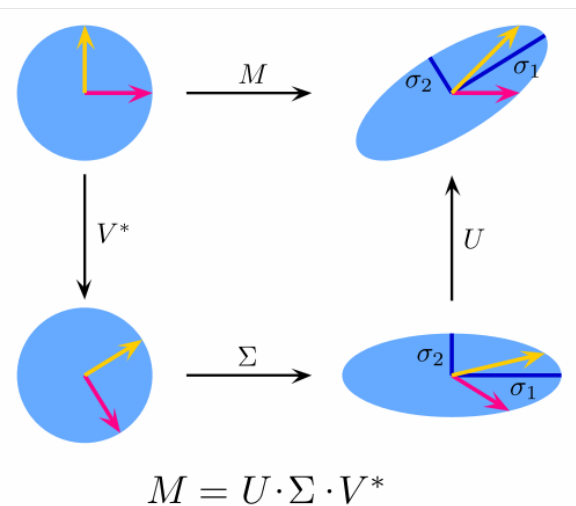
Singular value decomposition

- *More general than eigenvalue decomposition*
- $A = UDV^T$ where $A_{m \times n}$, $U_{m \times m}$, $D_{m \times n}$, $V_{n \times n}$
 U, V : orthogonal matrix

columns of U : left-singular vectors, eigenvectors of AA^T

columns of V : right-singular vectors, eigenvectors of $A^T A$

nonzero singular values of A : square roots of eigenvalues of AA^T
or $A^T A$



Singular value decomposition – cont'd

■ *SVD Example*

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$$

$$AA^T = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix} \quad A^T A = \begin{bmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{bmatrix}$$

$$\det(AA^T - \lambda I) = \lambda^2 - 34\lambda + 225 = (\lambda - 25)(\lambda - 9) = 0$$

Singular values: $\sigma_1 = 5, \sigma_2 = 3$

- $A^T A$ is symmetric \rightarrow orthogonal eigenvectors
- For $\lambda = 25$,

$$A^T A - 25I = \begin{bmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{bmatrix} \xrightarrow{\text{row reduced}} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

Singular value decomposition – cont'd

■ *SVD Example*

- $A^T A$ is symmetric \rightarrow orthogonal eigenvectors
- For $\lambda = 25$,

$$A^T A - 25I = \begin{bmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{bmatrix} \xrightarrow{\text{row reduced}} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$(A^T A - 25I)v = 0 \rightarrow \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 0 \rightarrow \begin{matrix} x_1 - x_2 = 0 \\ x_3 = 0 \end{matrix}, \quad x_1 = 1, x_2 = 1, x_3 = 0$$

$$v^T = [1 \quad 1 \quad 0] \equiv \text{normalize} \quad v_1^T = \left[\frac{1}{\sqrt{2}} \quad \frac{1}{\sqrt{2}} \quad 0 \right]$$

Singular value decomposition – cont'd

■ SVD Example

□ $A^T A$ is symmetric \rightarrow orthogonal eigenvectors

□ For $\lambda = 9$,

$$A^T A - 9I = \begin{bmatrix} 4 & 12 & 2 \\ 12 & 4 & -2 \\ 2 & -2 & -1 \end{bmatrix} \xrightarrow{\text{row reduced}} \begin{bmatrix} 1 & 0 & -\frac{1}{4} \\ 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 \end{bmatrix}$$

$$(A^T A - 9I)v_2 = 0 \rightarrow \begin{bmatrix} 1 & 0 & -\frac{1}{4} \\ 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 0 \rightarrow \begin{aligned} x_1 - \frac{1}{4}x_3 &= 0 \\ x_2 + \frac{1}{4}x_3 &= 0 \end{aligned} \quad x_1 = 1, x_2 = -1, x_3 = 4$$

$$v^T = [1 \quad -1 \quad 4] \xrightarrow{\text{normalize}} v_2^T = \left[\frac{1}{\sqrt{18}} \quad -\frac{1}{\sqrt{18}} \quad \frac{4}{\sqrt{18}} \right]$$

Singular value decomposition – cont'd

■ *SVD Example*

- for the last eigenvector $v_3^T = [a \ b \ c]$,

$$v_1^T v_3 = 0, v_2^T v_3 = 0 \rightarrow a + b = 0, \frac{2}{\sqrt{18}}a + \frac{4}{\sqrt{18}}c = 0$$

$$\rightarrow v_3^T = \begin{bmatrix} a & -a & -\frac{1}{2}a \end{bmatrix} \rightarrow v_3^T = \begin{bmatrix} \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}$$

$$\square \mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T = \mathbf{U} \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}$$

$$\square \text{ Finally, } \mathbf{A}v_i = \sigma_i u_i \text{ and } \mathbf{A}^T u_i = \sigma_i v_i \rightarrow u_i = \frac{1}{\sigma_i} \mathbf{A}v_i \rightarrow \mathbf{U} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

Quiz

- 다음 행렬을 eigendecomposition 하시오.

(문제를 풀고 사진을 찍어서 3월 20일 오후 12시까지 이클래스에 제출하세요.)

$$A = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

강의 정리

- 머신러닝을 이해하는데 필요한 최소한의 Linear algebra 리뷰
 - Symmetric, Hermitian, orthogonal, unitary matrix 등의 구조 및 특성 설명
 - Eigendecomposition 내용 및 계산하는 방법 설명
 - Quadratic Form 설명
 - Singular value decomposition 예제를 통한 계산법 설명

Moore-Penrose pseudoinverse

- Matrix inverse is not defined for matrices that are not square.
- given $\mathbf{Ax} = \mathbf{y}$, get a left-inverse of \mathbf{A} s.t. $\mathbf{x} = \mathbf{B}\mathbf{y}$ and $\mathbf{A}_{m \times n}$
 - If $m > n$, possibly no solution
 - If $m < n$, multiple possible solutions

- Pseudoinverse is defined as

$$\mathbf{A}^+ = \lim_{\alpha \rightarrow 0} (\mathbf{A}^T \mathbf{A} + \alpha \mathbf{I})^{-1} \mathbf{A}^T$$

- Practically,

$$\mathbf{A}^+ = \mathbf{V} \mathbf{D}^+ \mathbf{U}^T$$

- If $m < n$, solution $\mathbf{x} = \mathbf{A}^+ \mathbf{y}$ has minimal Euclidean norm $\|\mathbf{x}\|_2$
- If $m > n$, possibly no solution, or \mathbf{x} s.t. \mathbf{Ax} is as close as possible to \mathbf{y} in terms of Euclidean norm $\|\mathbf{Ax} - \mathbf{y}\|_2$
- \mathbf{D}^+ is obtained by taking the reciprocal of its nonzero elements and taking the transpose of the resulting matrix.

Moore-Penrose pseudoinverse – cont'd

- When A has more columns than rows, it provides one of the many possible solutions.
- Solution $x = A^+ y$ has minimal Euclidean norm among all possible solutions.

Trace operator

- Definition

$$\text{Tr}(\mathbf{A}) = \sum_i A_{i,i}$$

- Example

$$\|\mathbf{A}\|_F = \sqrt{\text{Tr}(\mathbf{A}\mathbf{A}^T)}$$

$$\text{Tr}(\mathbf{A}) = \text{Tr}(\mathbf{A}^T)$$

$$\text{Tr}(\mathbf{A}\mathbf{B}\mathbf{C}) = \text{Tr}(\mathbf{C}\mathbf{A}\mathbf{B}) = \text{Tr}(\mathbf{B}\mathbf{C}\mathbf{A})$$

$$\text{Tr}(\mathbf{A}\mathbf{B}) = \text{Tr}(\mathbf{B}\mathbf{A})$$

$$(\text{if } \mathbf{A}_{m \times n}, \mathbf{B}_{n \times m} \text{ then } \mathbf{A}\mathbf{B}_{m \times m}, \mathbf{B}\mathbf{A}_{n \times n})$$

Principal component analysis

- Suppose a collection of m points $\{x^{(1)} \dots x^{(m)}\}$ in \mathbf{R}^n
 - lossy compression assumed.
 - for each point $x^{(k)}$, corresponding code vector $c^{(k)} \in \mathbf{R}^l, l \leq n$
 - Find some encoding function $f(x) = c$ and decoding function $x \approx g(f(x))$
 - Let $g(c) = Dc$ where $D \in \mathbf{R}^{n \times l}$
constraints: columns of D are orthonormal to each other.
 - For optimal code \Rightarrow minimize the distance between x and $g(c)$
 - i.e.

$$\begin{aligned} c^* &= \operatorname{argmin}_c \|x - g(c)\|_2 \\ &= \operatorname{argmin}_c (x - g(c))^T (x - g(c)) \\ &= \operatorname{argmin}_c (x^T x - x^T g(c) - g(c)^T x + g(c)^T g(c)) \\ &= \operatorname{argmin}_c (-2x^T g(c) + g(c)^T g(c)) \end{aligned}$$

Principal component analysis

$$\begin{aligned}\mathbf{c}^* &= \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{x} - g(\mathbf{c})\|_2 \\ &= \underset{\mathbf{c}}{\operatorname{argmin}} (\mathbf{x} - g(\mathbf{c}))^T (\mathbf{x} - g(\mathbf{c})) \\ &= \underset{\mathbf{c}}{\operatorname{argmin}} (\mathbf{x}^T \mathbf{x} - \mathbf{x}^T g(\mathbf{c}) - g(\mathbf{c})^T \mathbf{x} + g(\mathbf{c})^T g(\mathbf{c})) \\ &= \underset{\mathbf{c}}{\operatorname{argmin}} (-2\mathbf{x}^T g(\mathbf{c}) + g(\mathbf{c})^T g(\mathbf{c})) \\ &= \underset{\mathbf{c}}{\operatorname{argmin}} (-2\mathbf{x}^T \mathbf{D}\mathbf{c} + \mathbf{c}^T \mathbf{D}^T \mathbf{D}\mathbf{c}) \\ &= \underset{\mathbf{c}}{\operatorname{argmin}} (-2\mathbf{x}^T \mathbf{D}\mathbf{c} + \mathbf{c}^T \mathbf{c}) \quad (\mathbf{D}^T \mathbf{D} = \mathbf{I}) \\ \therefore \mathbf{c} &= \mathbf{D}^T \mathbf{x} \quad \Leftrightarrow \quad f(\mathbf{x}) = \mathbf{D}^T \mathbf{x} \text{ and} \\ &\quad r(\mathbf{x}) = g(f(\mathbf{x})) = \mathbf{D}\mathbf{D}^T \mathbf{x}\end{aligned}$$

Principal component analysis

- How to choose the encoding matrix $\mathbf{D} \in \mathbb{R}^{n \times l}$

$$\mathbf{D}^* = \underset{\mathbf{D}}{\operatorname{argmin}} \sqrt{\sum_{i,j} \left(x_j^{(i)} - r(\mathbf{x}^{(i)})_j \right)^2} \quad \text{subject to } \mathbf{D}^T \mathbf{D} = \mathbf{I}$$

Consider the case of $l = 1$.

$$\begin{aligned} \mathbf{d}^* &= \underset{\mathbf{d}}{\operatorname{argmin}} \sum_i \left\| \mathbf{x}^{(i)} - \mathbf{d} \mathbf{d}^T \mathbf{x}^{(i)} \right\|_2^2 \quad \text{subject to } \|\mathbf{d}\|_2 = 1 \\ &= \underset{\mathbf{d}}{\operatorname{argmin}} \sum_i \left\| \mathbf{x}^{(i)} - \mathbf{d}^T \mathbf{x}^{(i)} \mathbf{d} \right\|_2^2 \quad \text{subject to } \|\mathbf{d}\|_2 = 1 \\ &= \underset{\mathbf{d}}{\operatorname{argmin}} \sum_i \left\| \mathbf{x}^{(i)} - \mathbf{x}^{(i)T} \mathbf{d} \mathbf{d} \right\|_2^2 \quad \text{subject to } \|\mathbf{d}\|_2 = 1 \\ &= \underset{\mathbf{d}}{\operatorname{argmin}} \|\mathbf{X} - \mathbf{X} \mathbf{d} \mathbf{d}^T\|_F^2 \quad \text{subject to } \mathbf{d}^T \mathbf{d} = 1 \\ &= \underset{\mathbf{d}}{\operatorname{argmin}} \operatorname{Tr}((\mathbf{X} - \mathbf{X} \mathbf{d} \mathbf{d}^T)^T (\mathbf{X} - \mathbf{X} \mathbf{d} \mathbf{d}^T)) \quad \text{subject to } \|\mathbf{d}\|_2 = 1 \\ &= \underset{\mathbf{d}}{\operatorname{argmin}} (\operatorname{Tr}(\mathbf{X}^T \mathbf{X} - \mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T - \mathbf{d} \mathbf{d}^T \mathbf{X}^T \mathbf{X} + \mathbf{d} \mathbf{d}^T \mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T)) \end{aligned}$$

Principal component analysis

- How to choose the encoding matrix $\mathbf{D} \in \mathbf{R}^{n \times l}$

$$\mathbf{d}^* = \underset{\mathbf{d}}{\operatorname{argmin}} \sum_i \|\mathbf{x}^{(i)} - \mathbf{d}\mathbf{d}^T \mathbf{x}^{(i)}\|_2^2 \quad \text{subject to } \|\mathbf{d}\|_2 = 1 \quad (= \mathbf{d}^T \mathbf{d} = 1)$$

$$= \underset{\mathbf{d}}{\operatorname{argmin}} (-2\operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T) + \operatorname{Tr}(\mathbf{d} \mathbf{d}^T \mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T))$$

$$= \underset{\mathbf{d}}{\operatorname{argmin}} (-2\operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T) + \operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T \mathbf{d} \mathbf{d}^T)) \quad \text{subject to } \mathbf{d}^T \mathbf{d} = 1$$

$$= \underset{\mathbf{d}}{\operatorname{argmin}} (-2\operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T) + \operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T)) \quad \text{subject to } \mathbf{d}^T \mathbf{d} = 1$$

$$= \underset{\mathbf{d}}{\operatorname{argmax}} (\operatorname{Tr}(\mathbf{X}^T \mathbf{X} \mathbf{d} \mathbf{d}^T)) \quad \text{subject to } \mathbf{d}^T \mathbf{d} = 1$$

$$= \underset{\mathbf{d}}{\operatorname{argmax}} (\operatorname{Tr}(\mathbf{d}^T \mathbf{X}^T \mathbf{X} \mathbf{d})) \quad \text{subject to } \mathbf{d}^T \mathbf{d} = 1$$

\Leftrightarrow optimal $\mathbf{d} = \mathbf{d}^*$ = eigenvector of $\mathbf{X}^T \mathbf{X}$ corresponding to the largest eigenvalue