Singular Value Decomposition

Spectral theorem (Real symmetric case)

A is a $n \times n$ real symmetric matrix. Then,

(i) All eigenvalues of A are real

(ii) A is orthogonally diagonalizable, i.e., $\exists$ a orthogonal matrix Q ($\Leftrightarrow Q^T Q = I$)

s.t. $A = Q \Lambda Q^T$

$$= \underbrace{\begin{bmatrix} | & & | \\ x_1 & \cdots & x_n \\ | & & | \end{bmatrix}}_{\text{eigenvectors of } A} \underbrace{\begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}}_{\text{eigenvalues of } A} \begin{bmatrix} - & x_1^T & - \\ - & x_2^T & - \\ & \vdots & \\ - & x_n^T & - \end{bmatrix}$$

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

Eigenvalues: $\lambda_1 = -3$, $\lambda_2 = 2$ Eigenvectors: $x_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ $x_2 = \begin{bmatrix} -2 \\ 1 \end{bmatrix}$

Normalized eigenvectors: $q_1 = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}$ $q_2 = \begin{bmatrix} -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}$

$Q = \begin{bmatrix} | & | \\ q_1 & q_2 \\ | & | \end{bmatrix}$ $\longrightarrow$ Check $Q^T Q = I$

$Q \Lambda Q^T = \begin{bmatrix} 1/\sqrt{5} & -2/\sqrt{5} \\ 2/\sqrt{5} & 1/\sqrt{5} \end{bmatrix} \begin{bmatrix} -3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1/\sqrt{5} & 2/\sqrt{5} \\ -2/\sqrt{5} & 1/\sqrt{5} \end{bmatrix} \overset{\text{Check this}}{=} A$

Singular value decomposition

Every matrix cannot be diagonalized

But, any "real" $m \times n$ matrix A can be decomposed in the "SVD" form, i.e., A can be written as $A = Q_1 \Sigma Q_2^T$ —— (*)

A: $m \times n$; Q_1: $m \times m$ matrix; Q_2: $n \times n$ matrix

Q_1, Q_2 are orthogonal i.e., $Q_1^T Q_1 = \underbrace{I}_{m \times m}$, $Q_2^T Q_2 = \underbrace{I}_{n \times n}$

$$\Sigma = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix}, \text{ where } D = \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r \end{bmatrix}, \sigma_i > 0$$

Why does the decomposition (*) hold for any $m \times n$ real matrix A?

Pf> A is $m \times n$, $A^T A$ is $n \times n$, $A^T A$ is symmetric & real

$\Rightarrow$ There exist a basis of orthonormal eigenvectors $\{x_1, \dots, x_n\}$ corresponding to the eigenvalues $\{\lambda_1, \dots, \lambda_n\}$

We have $A^T A x_i = \lambda_i x_i$, for $i = 1, \dots, n$

$\forall i$, $\|x_i\| = 1$, $x_i \cdot x_j = 0$ $\forall i \neq j$

So, $(A^T A x_i) \cdot x_i = (\lambda_i x_i) \cdot x_i = \underline{\lambda_i}$ (since $\|x_i\|^2 = 1$) — ①

$(A^T A x_i) \cdot x_i = (A^T A x_i)^T x_i = x_i^T A^T A x_i = (Ax_i)^T A x_i = \underline{\|Ax_i\|^2} \geq 0$ — ②

① & ② $\Rightarrow$ $\lambda_i \geq 0$

Order the eigenvalues of $A^T A$: $\lambda_1, \lambda_2, \ldots, \lambda_r, \lambda_{r+1}, \ldots \lambda_n$

$\lambda_1 > 0 \ldots \lambda_r > 0, \quad \lambda_{r+1} = \ldots = \lambda_n = 0$

σ_i's are called singular values & for each $i = 1 \ldots r$, $\sigma_i = \sqrt{\lambda_i}$ (So, the matrix Σ is now clear)

Let $y_i = \frac{1}{\sigma_i} A x_i$, for $i = 1, \ldots r$, $y_i \in \mathbb{R}^m$

$\|y_i\| = \frac{1}{\sigma_i} \|Ax_i\| = \frac{\sqrt{\lambda_i}}{\sigma_i} = 1.$

from ① & ②, $\|Ax_i\|^2 = \lambda_i$

$A^T A x_j = \lambda_j x_j$

$i \neq j$, $\quad y_i \cdot y_j = \dfrac{1}{\sigma_i \sigma_j} (A x_i) \cdot (A x_j) = \dfrac{1}{\sigma_i \sigma_j} x_i^T A^T A x_j = \dfrac{1}{\sigma_i \sigma_j} x_i^T \lambda_j x_j$

$= \dfrac{\lambda_j}{\sigma_i \sigma_j} x_i^T x_j = 0$ since $\{x_1, \dots x_n\}$ is an orthonormal basis (so) $x_i^T x_j = 0 \;\forall\, i \neq j$

So, we have a set $\{y_1, \dots, y_r\}$ of orthonormal vectors

Since $r \leq m$, the set $\{y_1, \dots y_r\}$ is not a basis.

However, we could extend $\{y_1, \dots y_r\}$ to form a orthonormal basis of $\mathbb{R}^m$.

Let $\{y_1, \dots\dots y_m\}$ be the orthonormal basis obtained by extending $\{y_1, \dots y_r\}$

$$Q_1 = \begin{bmatrix} | & & | \\ y_1 & \cdots & y_m \\ | & & | \end{bmatrix} \qquad Q_2 = \begin{bmatrix} | & & | \\ x_1 & \cdots & x_n \\ | & & | \end{bmatrix}$$

So, all components of SVD are defined.
Need to check if
$A = Q_1 \Sigma Q_2^T$

$$\Sigma = Q_1^T \; A \; Q_2$$

$$= \begin{bmatrix} - & y_1^T & - \\ & \vdots & \\ - & y_m^T & - \end{bmatrix} \begin{bmatrix} | & & | \\ Ax_1 & \cdots & Ax_n \\ | & & | \end{bmatrix}$$

$$(\Sigma)_{ij} = y_i^T (A x_j)$$

For $j \leq r$, $y_j = \frac{1}{\sigma_j} A x_j$

$$y_i^T (A x_j) = y_i^T \sigma_j y_j = \sigma_j y_i^T y_j$$

$$= \begin{cases} \sigma_j & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

For $j > r$, $\|A x_j\|^2 = \lambda_j = 0$

$\Rightarrow A x_j = 0$

$\Rightarrow y_i^T A x_j = 0$

$$\Sigma = \left[\begin{array}{ccc|c} \sigma_1 & & 0 & \\ & \ddots & & 0 \\ 0 & & \sigma_r & \\ \hline & 0 & & 0 \end{array}\right] = \begin{bmatrix} \underset{\text{r×r diagonal matrix}}{D} & 0 \\ 0 & 0 \end{bmatrix}$$

$$Q_1^T A Q_2 = \Sigma \iff \underbrace{Q_1 \Sigma Q_2^T}_{\text{SVD of } A} = A$$

Remarks: ① $A = Q_1 \Sigma Q_2^T$

$$\boxed{AA^T = Q_1 \Sigma \Sigma^T Q_1^T}$$ eigendecomposition of AA^T (real symmetric matrix)

So, the eigenvectors of AA^T go into Q_1

9. $A^T A = Q_2 \Sigma^T \Sigma Q_2^T$

$\Rightarrow$ the eigenvectors of $A^T A$ go into Q_2