Singular Values of a Matrix:

Let A be an $m \times n$ matrix. The product $A^t A$ is a symmetric matrix.

$$[(A^tA)^t = A^t (A^t)^t = A^t A].$$

Thus A^tA has n L.I. eigenvectors $v_1, v_2, \ldots v_n$ and real eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_n$.

We know that eigenvalues of A^tA are also all nonnegative.

Let λ be any eigenvalue of A^tA with corr. eigenvector v. Then

$$\lambda = \lambda \|v\|^2 = \lambda v^t v = v^t \lambda v = v^t A^t A v$$

$$= (Av)^t Av$$

$$= \|Av\|^2 \geq 0$$

Label the eigenvectors $v_1, v_2, \ldots, v_n$ so that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Let $\sigma_i = \sqrt{\lambda_i}$. Thus $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$

The numbers $\sigma_1, \sigma_2, \ldots \sigma_n$ are called the singular values of the matrix A.

Singular Value Decomposition:

Let A be an $m \times n$ matrix. Then there exists a factorization of A,

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

where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix, and Σ is an $m \times n$ matrix of the form

$$\Sigma = \left[\begin{array}{c|c} D & 0 \\ \hline 0 & 0 \end{array}\right], \text{ where}$$

$$D = \begin{bmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r \end{bmatrix} \quad \text{with elements } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$$

for $r \leq m, n$.

Any such factorization is called a singular value decomposition of A (SVD of A). The matrices U & V are not unique. However Σ is unique. The elements on the diagonal of D, namely $\sigma_1, \ldots, \sigma_r$ are the nonzero singular values of A. The columns of U are called left singular vectors of A and columns of V are right singular vectors of A.

Information given by SVD :-

Let $A = U\Sigma V^t$ be a singular value decomposition of an $m\times n$ matrix A.

(a) The rank of A is r, the number of nonzero singular values.

(b) $\{u_1, \ldots u_r\}$ is an orthonormal basis for col(A) - the range of A.

(c) $\{u_{r+1}, \ldots u_m\}$ is an orthonormal basis for null (A^t).

(d) $\{v_1, \ldots v_r\}$ is an orthonormal basis for row (A).

(e) $\{v_{r+1}, \ldots v_n\}$ is an orthonormal basis for null (A).

Example: Find a singular value decomposition of the following matrix A.

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

Solution: We want to find the matrices U, Σ, V such that

$$A = U \Sigma V^t.$$

Here

$$\underset{m\times n}{A} = \underset{m\times m}{U}\,\underset{m\times n}{\Sigma}\,\underset{n\times n}{V^t} \qquad \underset{2\times 3}{A} = \underset{2\times 2}{U}\,\underset{2\times 3}{\Sigma}\,\underset{3\times 3}{V^t}$$

Finding V: The columns of V will be eigenvectors of A^tA. We get

$$A^tA = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 2 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 0 & 4 \end{bmatrix}$$

In order to find eigenvectors, we need to find eigenvalues:

$$|A^tA - \lambda I| = 0 \Rightarrow \begin{vmatrix} 1-\lambda & 0 & 2 \\ 0 & 1-\lambda & 0 \\ 2 & 0 & 4-\lambda \end{vmatrix} = 0$$

$$\Rightarrow (1-\lambda)\left((1-\lambda)(4-\lambda)\right) + 2\left(0 - 2(1-\lambda)\right) = 0$$

$$\Rightarrow (1-\lambda)\left[\cancel{4} - \lambda - 4\lambda + \lambda^2 - \cancel{4}\right] = 0$$

$$(1-\lambda)(\lambda^2 - 5\lambda - 0) = 0 \Rightarrow \lambda = 1,\ \lambda = 0,\ \lambda = 5$$

In descending order of magnitude

$\lambda = 5, 1, 0.$

$AX = 5X \Rightarrow (A^tA - 5I)X = 0$

$$\begin{bmatrix} -4 & 0 & 2 \\ 0 & -4 & 0 \\ 2 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$\Rightarrow \quad -4x_1 + 2x_3 = 0 \Rightarrow x_3 = 2x_1$

$x_2 = 0$

$$E_5 = \left\{ \begin{pmatrix} x_1 \\ 0 \\ 2x_1 \end{pmatrix} : x_1 \in \mathbb{R} \right\} = \text{span} \left\{ \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} \right\}$$

$X_1 = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix}$ corresponding to $\lambda = 5.$

$X_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ " " $\lambda = 1$

$X_3 = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix}$ " " $\lambda = 0$

$$V_1 = \begin{pmatrix} 1/\sqrt{5} \\ 0 \\ 2/\sqrt{5} \end{pmatrix}, \quad V_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad V_3 = \begin{pmatrix} -2/\sqrt{5} \\ 0 \\ 1/\sqrt{5} \end{pmatrix}$$

$(\lambda = 5) \qquad \lambda = 1, \qquad \lambda = 0.$

Observe that these vectors are orthogonal.
Let these vectors be the columns of the matrix V. V is an orthonormal matrix.

$$V = \begin{bmatrix} 1/\sqrt{5} & 0 & -\frac{2}{\sqrt{5}} \\ 0 & 1 & 0 \\ 2/\sqrt{5} & 0 & \frac{1}{\sqrt{5}} \end{bmatrix}.$$

Finding the Singular Values:-
The singular values of A are the positive square roots of the eigenvalues A^tA. The singular values are

$$\sigma_1 = \sqrt{5}, \quad \sigma_2 = 1, \quad \sigma_3 = 0.$$

Finding Σ: Σ is to be a 2×3 matrix, with upper left block being a diagonal matrix D with diagonal elements $\sigma_1 = \sqrt{5}$, $\sigma_2 = 1$.

$$D = \begin{bmatrix} \sqrt{5} & 0 \\ 0 & 1 \end{bmatrix}. \quad \Sigma = \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

Finding U :- U is a 2×2 matrix. The columns of U are selected to be the vectors, $u_1 = \frac{1}{\sigma_1} A v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$,

$$u_2 = \frac{1}{\sigma_2} A v_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\frac{1}{\sqrt{5}}\begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} 1/\sqrt{5} \\ 0 \\ 2/\sqrt{5} \end{bmatrix} = \frac{1}{5}\begin{bmatrix} 5 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = u_1$$

$$u_2 = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

These vectors are orthonormal. U is the orthogonal matrix,

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

We get the following SVD for the matrix A.

$$A = U \Sigma V^t = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} 1/\sqrt{5} & 0 & 2/\sqrt{5} \\ 0 & 1 & 0 \\ -2/\sqrt{5} & 0 & 1/\sqrt{5} \end{bmatrix}.$$

Remark: In previous example, there were enough nonzero singular values for A to provide orthonormal columns for U. This is not always the case, as in the following example:

Ex: Find a singular value decomposition of the following matrix A,

$$A = \begin{bmatrix} 3 & 0 & -3 \\ 2 & 0 & -2 \\ 6 & 0 & -6 \end{bmatrix}.$$

Soln:

$$\underset{m\times n}{A} = \underset{m\times m}{U} \; \underset{m\times n}{\Sigma} \; \underset{n\times n}{V^t}$$

$$\Rightarrow A_{3\times 3} = U_{3\times 3} \; \Sigma_{3\times 3} \; V^t_{3\times 3}$$

Finding V: The columns of V will be eigenvectors of A^tA. We get

$$A^t A = \begin{bmatrix} 49 & 0 & -49 \\ 0 & 0 & 0 \\ -49 & 0 & 49 \end{bmatrix}$$

eigenvalues of $A^t A$ are found to be

$$\lambda = 98,\ 0,\ 0.$$

eigenvectors of $A^t A$

$$X_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},\ X_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix},\ X_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$(\lambda = 98)$ $(\lambda = 0)$ $(\lambda = 0)$

Normalized eigenvectors

$$v_1 = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{pmatrix},\ v_2 = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix},\ v_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$(\lambda = 98)$ $(\lambda = 0)$ $\lambda = 3-$

These vectors are orthogonal.

V is orthonormal matrix where

$$V = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix}.$$

Finding Σ: The singular values of A are

$$\sigma_1 = \sqrt{98} = 7\sqrt{2}, \quad \sigma_2 = 0, \sigma_3 = 0$$

Σ is to be a 3×3 matrix. Then

$$\Sigma = \begin{bmatrix} 7\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Finding U: U is a 3×3 matrix. We find suitable orthonormal column vectors u_1, u_2 and u_3 for U.

Let $$u_1 = \frac{1}{\sigma_1} A v_1 = \frac{1}{7\sqrt{2}} \begin{bmatrix} 3 & 6 & -3 \\ 2 & 0 & -2 \\ 6 & 0 & -6 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 3/7 \\ 2/7 \\ 6/7 \end{bmatrix}$$

Since σ_2 and σ_3 are zero. We cannot use the formula $u_i = \frac{1}{\sigma_i} A v_i$ as in the previous example.

Let us determine the subspace W orthogonal to u_1, then find two orthogonal vectors in W. Normalize ~~these~~ these to get u_2 and u_3.

Let $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$ be any vector in W then

$$u_1 \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \Rightarrow \begin{pmatrix} 3/7 \\ 2/7 \\ 6/7 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$$

$$\Rightarrow 3a + 2b + 6c = 0$$

i.e. $a = -\frac{2}{3}b - 2c$.

$$W = \left\{ \begin{pmatrix} a \\ b \\ c \end{pmatrix} \middle| \ a = -\frac{2}{3}b - 2c \right\}$$

$$= \left\{ \begin{pmatrix} -\frac{2}{3}b - 2c \\ b \\ c \end{pmatrix} \middle| \ a, b, c \in \mathbb{R} \right\}.$$

Find one of these vectors by putting $b = 0$, $c = 1$

$$Y_2 = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix}, \quad u_2 = \begin{pmatrix} -2/\sqrt{5} \\ 0 \\ 1/\sqrt{5} \end{pmatrix}.$$

We still need to find one more vector, in W, orthogonal to $\begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix}$.

i.e. $\begin{pmatrix} -\frac{2}{3}b - 2c \\ b \\ c \end{pmatrix} \cdot \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} = 0$

$\Rightarrow +\frac{4b}{3} + 4c + c = 0$

$\Rightarrow 4b + 15c = 0$

$\Rightarrow b = \frac{-15}{4} c.$

a third vector is of the form:

$\begin{pmatrix} -\frac{2}{3} \times \left(\frac{-15}{4}\right) c - 2c \\ \frac{-15}{4} c \\ c \end{pmatrix}$

let $c = 1$ $\quad X_3 = \begin{pmatrix} 1/2 \\ -15/4 \\ 1 \end{pmatrix}$ so $y_3 = \begin{pmatrix} 2/7\sqrt{5} \\ -15/7\sqrt{5} \\ 4/7\sqrt{5} \end{pmatrix}$

so $U = \begin{bmatrix} 3/7 & -2/\sqrt{5} & 2/7\sqrt{5} \\ 2/7 & 0 & -15/7\sqrt{5} \\ 6/7 & 1/\sqrt{5} & 4/7\sqrt{5} \end{bmatrix}$

We get the following SVD of A,

$$A = U \cdot \Sigma \cdot V^t$$

$$= \underbrace{\begin{bmatrix} 3/7 & -2/\sqrt{5} & 2/7\sqrt{5} \\ 2/7 & 0 & -15/7\sqrt{5} \\ 6/7 & 1/\sqrt{5} & 4/7\sqrt{5} \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 7\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \end{bmatrix}}_{V^t}$$

Remark: In general, the matrices U and V are not unique in singular value decomposition but Σ is unique.