Goal: Given a matrix A compute its singular value decomposition

$$A = \underbrace{U}_{\text{orthogonal}} \cdot \underbrace{\Sigma}_{\text{diagonal}} \cdot \underbrace{V^T}_{\text{orthogonal}}$$

Note:

1) If $A = U \cdot \Sigma \cdot V^T$ then:

$$A^T A = (U\Sigma V^T)^T (U \Sigma V^T) = (V^T)^T \Sigma^T \overbrace{\cancel{U^T U}}^{U^T = U^{-1}} \Sigma V^T = V \Sigma^T \Sigma V^T$$

2) $\Sigma^T \Sigma$ is a diagonal matrix with squares of singular values on the diagonal.

E.g.:

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \end{bmatrix} \qquad \Sigma^T \Sigma = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

We obtain: $\underbrace{A^T A}_{\text{symmetric}} = \underbrace{V}_{\text{orthogonal}} \underbrace{(\Sigma^T \Sigma)}_{\text{diagonal}} V^T$ ← This is an orthogonal diagonalization of $A^T A$. We know how to compute it.

This gives matrices V and Σ:

(columns of V) = (orthonormal eigenvectors of $A^T A$)

$$\begin{pmatrix} \text{diagonal entries of } \Sigma \\ \text{i.e. singular values of } A \end{pmatrix} = \sqrt{\text{eigenvalues of } A^T A}$$

It remains to compute the matrix U:

$A = U \Sigma V^T$ gives: $AV = U\Sigma$

Note: If $U = [u_1 \dots u_m]$, $V = [v_1 \dots v_n]$,

$\sigma_1, \dots, \sigma_r$ - non-zero singular values of A

then: $AV = [Av_1 \; Av_2 \dots Av_n]$, $U\Sigma = [\sigma_1 u_1 \dots \sigma_r u_r \; 0 \dots 0]$

so: $u_1 = \frac{1}{\sigma_1} A v_1, \dots, u_r = \frac{1}{\sigma_r} A v_r$

Vectors $u_{r+1}, \dots, u_m$ can be chosen in an arbitrary way so that $\{u_1, \dots, u_m\}$ is an orthonormal basis of $\mathbb{R}^m$.

How to compute SVD of a matrix A

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

1) Compute an orthogonal diagonalization of the symmetric $n \times n$ matrix $A^T A$:

$$A^T A = Q D Q^T$$

such that eigenvalues on the diagonal of the matrix D are arranged from the largest to the smallest. We set $V = Q$.

2) If

$$D = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & \lambda_n \end{bmatrix}$$

then $\sigma_i = \sqrt{\lambda_i}$. This gives the matrix Σ.

Note: if $n > m$ then we use only $\lambda_1, \dots, \lambda_m$. The remaining eigenvalues $\lambda_{m+1}, \dots, \lambda_n$ of D will be equal to 0 in this case.

3) Let $V = \begin{bmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_n \end{bmatrix}$ and let $\sigma_1, \dots, \sigma_r$ be non-zero singular values of A. The first r columns of the matrix $U = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_m \end{bmatrix}$ are given by

$$\mathbf{u}_i = \frac{1}{\sigma_i} A \mathbf{v}_i$$

The remaining columns $\mathbf{u}_{r+1}, \dots, \mathbf{u}_m$ can be added arbitrarily so that U is an orthogonal matrix (i.e.$\{\mathbf{u}_1, \dots, \mathbf{u}_m\}$) is an orthonormal basis of $\mathbb{R}^m$.

Example. Find SVD of the following matrix:

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

3×2

$$\underset{3\times 3}{U} \cdot \underset{3\times 2}{\Sigma} \cdot \underset{2\times 2}{V^T}$$

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

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \\ 0 & 0 \end{bmatrix}$$

Solution.

1) Compute an orthogonal diagonalization of $A^T A$.

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

$$P(\lambda) = \det \begin{bmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{bmatrix} = \lambda^2 - 4\lambda + 3$$

(eigenvalues of A^TA) = (roots of $P(\lambda)$) = $(\lambda_1 = 3,\ \lambda_2 = 1)$

(basis of the eigenspace of $\lambda_1 = 3$) = $\left\{ \underset{w_1}{\begin{bmatrix} -1 \\ 1 \end{bmatrix}} \right\}$ $\quad \|w_1\| = \sqrt{2}$

(basis of the eigenspace of $\lambda_2 = 1$) = $\left\{ \underset{w_2}{\begin{bmatrix} 1 \\ 1 \end{bmatrix}} \right\}$ $\quad \|w_2\| = \sqrt{2}$

We obtain:

$$A^TA = VDV^T$$

where: $V = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$ $\qquad D = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$

σ_1^2 $\quad$ σ_2^2

2) Get matrices V and Σ.

$$V = \begin{bmatrix} \underbrace{\begin{matrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{matrix}}_{v_1} & \underbrace{\begin{matrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{matrix}}_{v_2} \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

σ_1 $\quad$ σ_2

3) Compute the matrix U.

Let $\mathcal{U} = [u_1 \ \ u_2 \ \ u_3]$

We have :

columns of the matrix V

$$u_1 = \frac{1}{\sigma_1} A v_1 \qquad\qquad u_2 = \frac{1}{\sigma_2} A v_2$$

$$\frac{1}{\sqrt{3}} \cdot \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{6} \\ -2/\sqrt{6} \\ 1/\sqrt{6} \end{bmatrix} \qquad \frac{1}{1} \cdot \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} -1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}$$

$\underline{u_3 = ?}$

- Start with some vector z_3 linearly independent of $\{u_1, u_2\}$. In our example we can take e.g. $z_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$
- $\{u_1, u_2, z_3\}$ is a basis of $\mathbb{R}^3$. Use Gram-Schmidt process to make it into an orthogonal basis. Since u_1, u_2 are already orthogonal, it suffices to modify z_3 :

$$w_3 = z_3 - \left(\frac{z_3 \cdot u_1}{u_1 \cdot u_1}\right) u_1 - \left(\frac{z_3 \cdot u_2}{u_2 \cdot u_2}\right) u_2 = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

Take $u_3 = \dfrac{w_3}{\|w_3\|} = \dfrac{1}{1/\sqrt{3}} \cdot \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$

4) Write the singular value decomposition of A.

$$A = \begin{array}{c} \begin{array}{ccc} u_1 & u_2 & u_3 \end{array} \\ \begin{bmatrix} 1/\sqrt{6} & -1/\sqrt{2} & 1/\sqrt{3} \\ 1/\sqrt{6} & 0 & 1/\sqrt{3} \\ 1/\sqrt{6} & 1/\sqrt{2} & 1/\sqrt{3} \end{bmatrix} \end{array} \cdot \begin{bmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$$\mathcal{U} \qquad \cdot \qquad \Sigma \qquad \cdot \qquad V^T$$