V-3-5. Singular value decomposition

In case of spectral decomposition, we can decompose symmetric matrix to a product of orthogonal vectors (eigenvectors) and eigenvalue, because symmetric matrix is quadratic form and we can draw super conic curve from quadratic form. In the case of symmetric matrix, the matrix has inverse matrix. When the matrix has inverse matrix, we say the matrix is regular matrix. Regular matrix is invertible matrix and non-singular value matrix. Here, we will consider operation of diagonalization of non-regular matrix. This is a generalization of diagonalization to all real matrix including non-regular matrix. Singular value decomposition can diagonalize all real matrix. Singular value decomposition is as follow.

$$\boldsymbol{M} = \boldsymbol{U\Sigma V}^T$$

$$\boldsymbol{M}: p \times n \text{ matrix}$$

$$p \leq n$$

$$\boldsymbol{\Sigma}: \text{diagonal matrix espressing magnitude of the matrix}$$

$$\boldsymbol{U}: \text{orthogonal projection operator}$$

$$\boldsymbol{V}: \text{orthogonal projection operator}$$

$$\boldsymbol{U}^T = \boldsymbol{U}^{-1}$$

$$\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$$

$$\boldsymbol{V}^T = \boldsymbol{V}^{-1}$$

$$\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}$$

$$\boldsymbol{M} = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{p1} & m_{p2} & \cdots & m_{pn} \end{pmatrix}_{p\times n}$$

$$\boldsymbol{M}^T = \begin{pmatrix} m_{11} & m_{21} & \cdots & m_{p1} \\ m_{12} & m_{22} & \cdots & m_{p2} \\ \vdots & \vdots & \ddots & \vdots \\ m_{1n} & m_{2n} & \cdots & m_{pn} \end{pmatrix}_{n\times p}$$

We do not have any information of $\boldsymbol{\Sigma}$**,** though we hypothesize that there exist $\boldsymbol{U}$ and $\boldsymbol{V}$ which diagonalize $\boldsymbol{M}$ as follow

コメントの追加 [黒倉1]:

$$\boldsymbol{U}^T\boldsymbol{MV} = \boldsymbol{\Sigma}$$

Multiply $\boldsymbol{\Sigma^T}$ to $\boldsymbol{\Sigma}$

$$\boldsymbol{\Sigma\Sigma^T} = \boldsymbol{U}^T\boldsymbol{MV}(\boldsymbol{U}^T\boldsymbol{MV})^T == \boldsymbol{U}^T\boldsymbol{MVV}^T\boldsymbol{M}^T\boldsymbol{U} == \boldsymbol{U}^T\boldsymbol{MM}^T\boldsymbol{U} \qquad \text{i}$$

Similarly,

$$\boldsymbol{\Sigma^T\Sigma} = (\boldsymbol{U}^T\boldsymbol{MV})^T\boldsymbol{U}^T\boldsymbol{MV} == \boldsymbol{V}^T\boldsymbol{M^T}\boldsymbol{UU}^T\boldsymbol{M}\boldsymbol{U} == \boldsymbol{V}^T\boldsymbol{M}^T\boldsymbol{MV} \qquad \text{ii}$$

$$
\boldsymbol{MM^T} = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{p1} & m_{p2} & \cdots & m_{pn} \end{pmatrix} \begin{pmatrix} m_{11} & m_{21} & \cdots & m_{p1} \\ m_{12} & m_{22} & \cdots & m_{p2} \\ \vdots & \vdots & \ddots & \vdots \\ m_{1n} & m_{2n} & \cdots & m_{pn} \end{pmatrix}
$$

$$
= \begin{pmatrix} \sum_{i=1}^{n} {m_{1i}}^2 & \sum_{i=1}^{n} m_{1i} m_{2i} & \cdots & \sum_{i=1}^{n} m_{1i} m_{pi} \\ \sum_{i=1}^{n} m_{2i} m_{1i} & \sum_{i=1}^{n} {m_{2i}}^2 & \cdots & \sum_{i=1}^{n} m_{2i} m_{pi} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} m_{pi} m_{1i} & \sum_{i=1}^{n} m_{pi} m_{2i} & \cdots & \sum_{i=1}^{n} {m_{pi}}^2 \end{pmatrix}_{p \times p}
$$

$$
\boldsymbol{M^T M} = \begin{pmatrix} m_{11} & m_{21} & \cdots & m_{p1} \\ m_{12} & m_{22} & \cdots & m_{p2} \\ \vdots & \vdots & \ddots & \vdots \\ m_{1n} & m_{2n} & \cdots & m_{pn} \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{p1} & m_{p2} & \cdots & m_{pn} \end{pmatrix}
$$

$$
= \begin{pmatrix} \sum_{i=1}^{p} {m_{i1}}^2 & \sum_{i=1}^{p} m_{i1} m_{i2} & \cdots & \sum_{i=1}^{p} m_{i1} m_{in} \\ \sum_{i=1}^{p} m_{i2} m_{i1} & \sum_{i=1}^{p} {m_{i2}}^2 & \cdots & \sum_{i=1}^{p} m_{i2} m_{in} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{p} m_{in} m_{i1} & \sum_{i=1}^{p} m_{in} m_{i2} & \cdots & \sum_{i=1}^{p} {m_{in}}^2 \end{pmatrix}_{n \times n}
$$

Both $\boldsymbol{MM}^T$ and $\boldsymbol{M}^T\boldsymbol{M}$ are symmetric. The right side of the equations i and ii are Diagonalization of symmetric matrix. This calculation demonstrates that projection operators of $\boldsymbol{MM}^T$ and $\boldsymbol{M}^T\boldsymbol{M}$ can be candidate of left and right single operator. When we accept the hypothesis.

$$
\boldsymbol{\Sigma\Sigma^T} = \boldsymbol{U}^T\boldsymbol{MM}^T\boldsymbol{U} = \boldsymbol{\lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_p} \end{pmatrix} \begin{pmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_p} \end{pmatrix}^T
$$

$$
\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p \geq
$$

$$
\boldsymbol{\Sigma\Sigma^T} = \boldsymbol{\lambda}
$$

Mathematically, this is correct, though it has problem in form of notation. When we select $\boldsymbol{U}$ in following equation as left singular operator, $\boldsymbol{U}^T$ is $p \times p$ matrix, $\boldsymbol{V}$ is $n \times n$ matrix, and $\boldsymbol{M}$ **is** $p \times n$ matrix.

$$\boldsymbol{U}^T\boldsymbol{M}\boldsymbol{V} = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1p} \\ u_{21} & u_{22} & \cdots & u_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ u_{p1} & u_{p2} & \cdots & u_{pp} \end{pmatrix}^{\boldsymbol{T}} \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{p1} & m_{p2} & \cdots & m_{pn} \end{pmatrix} \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{pmatrix}$$

$$= \begin{pmatrix} u_{11} & u_{21} & \cdots & u_{p1} \\ u_{12} & u_{22} & \cdots & u_{p2} \\ \vdots & \vdots & \ddots & \vdots \\ u_{1p} & u_{2p} & \cdots & u_{pp} \end{pmatrix}_{p\times p} \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1n} \\ m_{21} & m_{22} & \cdots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{p1} & m_{p2} & \cdots & m_{pn} \end{pmatrix}_{p\times n} \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{pmatrix}_{n\times n}$$

$$= \begin{pmatrix} \sum_{i=1}^{p} u_{i1}\, m_{i1} & \sum_{i=1}^{p} u_{i1}\, m_{i2} & \cdots & \sum_{i=1}^{p} u_{i1}\, m_{in} \\ \sum_{i=1}^{p} u_{i2}\, m_{i1} & \sum_{i=1}^{p} u_{i2}\, m_{i2} & \cdots & \sum_{i=1}^{p} u_{i2}\, m_{in} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{p} u_{ip}\, m_{i1} & \sum_{i=1}^{p} u_{ip}\, m_{i2} & \cdots & \sum_{i=1}^{p} u_{ip}\, m_{in} \end{pmatrix} \begin{pmatrix} v_{11} & v_{12} & \cdots & v_{1n} \\ v_{21} & v_{22} & \cdots & v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \cdots & v_{nn} \end{pmatrix}$$

$$= \begin{pmatrix} \sum_{j=}^{n} v_{j1} \sum_{i=1}^{p} u_{i1}\, m_{ij} & \sum_{j=}^{n} v_{j2} \sum_{i=1}^{p} u_{i1}\, m_{ij} & \cdots & \sum_{j=}^{n} v_{jn} \sum_{i=1}^{p} u_{i1}\, m_{ij} \\ \sum_{j=}^{n} v_{j1} \sum_{i=1}^{p} u_{i2}\, m_{ij} & \sum_{j=}^{n} v_{j2} \sum_{i=1}^{p} u_{i2}\, m_{ij} & \cdots & \sum_{j=}^{n} v_{jn} \sum_{i=1}^{p} u_{i2}\, m_{ij} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{j=}^{n} v_{j1} \sum_{i=1}^{p} u_{ip}\, m_{ij} & \sum_{j=}^{n} v_{j2} \sum_{i=1}^{p} u_{ip}\, m_{ij} & \cdots & \sum_{j=}^{n} v_{jn} \sum_{i=1}^{p} u_{ip}\, m_{ij} \end{pmatrix}_{p\times n}$$

$$= \begin{pmatrix} \sum_{j=}^{n} \sum_{i=1}^{p} v_{j1} u_{i1}\, m_{ij} & \sum_{j=}^{n} \sum_{i=1}^{p} v_{j2} u_{i1}\, m_{ij} & \cdots & \sum_{j=}^{n} \sum_{i=1}^{p} v_{jn} u_{i1}\, m_{ij} \\ \sum_{j=}^{n} \sum_{i=1}^{p} v_{j1} u_{i2}\, m_{ij} & \sum_{j=}^{n} \sum_{i=1}^{p} v_{j2} u_{i2}\, m_{ij} & \cdots & \sum_{j=}^{n} \sum_{i=1}^{p} v_{jn} u_{i2}\, m_{ij} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{j=}^{n} \sum_{i=1}^{p} v_{j1} u_{ip}\, m_{ij} & \sum_{j=}^{n} \sum_{i=1}^{p} v_{j2} u_{ip}\, m_{ij} & \cdots & \sum_{j=}^{n} \sum_{i=1}^{p} v_{jn} u_{ip}\, m_{ij} \end{pmatrix}_{p\times n}$$

It is difficult to calculate

$$\sum_{j=}^{n} \sum_{i=1}^{p} v_{jk} u_{ih}\, m_{ij}$$

However, we can understand that the matrix of $\boldsymbol{\Sigma}$ should be $p \times n$, and

$$\sum_{j=}^{n} \sum_{i=1}^{p} v_{jk} u_{ih}\, m_{ij} = \gamma_i \delta_{ij}$$

Function δ_{ij} is Kronecker delta. Kronecker delta Kronecker delta is following binary variable.

$$\delta_{ij} = \begin{Bmatrix} 1\ (i = j) \\ 0\ (i \neq j) \end{Bmatrix}$$

An example.

There is a matrix of $\boldsymbol{U_1}^T \boldsymbol{U_1}$

$$\boldsymbol{U_1}^T \boldsymbol{U_1} = \begin{pmatrix} \boldsymbol{u_1}^T \\ \boldsymbol{u_2}^T \\ \vdots \\ \boldsymbol{u_p}^T \end{pmatrix} (\boldsymbol{u_1} \quad \boldsymbol{u_2} \quad \cdots \quad \boldsymbol{u_p}) = \begin{pmatrix} \boldsymbol{u_1}^T \boldsymbol{u_1} & \boldsymbol{u_1}^T \boldsymbol{u_2} & \cdots & \boldsymbol{u_1}^T \boldsymbol{u_p} \\ \boldsymbol{u_2}^T \boldsymbol{u_1} & \boldsymbol{u_2}^T \boldsymbol{u_2} & \cdots & \boldsymbol{u_2}^T \boldsymbol{u_p} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{u_p}^T \boldsymbol{u_1} & \boldsymbol{u_p}^T \boldsymbol{u_2} & \cdots & \boldsymbol{u_p}^T \boldsymbol{u_p} \end{pmatrix}$$

When the factor of the matrix is as follow,

$$\boldsymbol{u_i}^T \boldsymbol{u_j} = \delta_{ij}$$

We can express the matrix as follow.

$$\boldsymbol{U_1}^T \boldsymbol{U_1} = \begin{pmatrix} \delta_{11} & \delta_{12} & \cdots & \delta_{1p} \\ \delta_{21} & \delta_{22} & \cdots & \delta_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \delta_{p1} & \delta_{p2} & \cdots & \delta_{pp} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}_{p \times p}$$

$$\boldsymbol{U}^T \boldsymbol{MV} = \begin{pmatrix} \gamma_1 \delta_{11} & \delta_{12} & \cdots & \delta_{1p} & \delta_{1p+1} & \cdots & \delta_{1n} \\ \delta_{21} & \gamma_2 \delta_{22} & \cdots & \delta_{2p} & \delta_{2p+1} & \cdots & \delta_{2n} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ \delta_{p1} & \delta_{p2} & \cdots & \gamma_p \delta_{pp} & \delta_{pp+1} & \cdots & \delta_{pn} \end{pmatrix}_{p \times n} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \gamma_p & 0 & \cdots & 0 \end{pmatrix}_{p \times n}$$

The name of γ is single value.

When we multiply $\boldsymbol{U}$ from left $\boldsymbol{V}^T$ from right,

$$\gamma_i = \sqrt{\lambda_1}$$

$$\boldsymbol{UU}^T \boldsymbol{MVV}^T = \boldsymbol{U} \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \gamma_p & 0 & \cdots & 0 \end{pmatrix}_{p \times n} \boldsymbol{V}^T = \boldsymbol{U \Sigma V}^T$$

$$\boldsymbol{UU}^T \boldsymbol{MVV}^T = \boldsymbol{IMI} = \boldsymbol{M}$$

$$\boldsymbol{M} = \boldsymbol{U \Sigma V}^T$$

This is singular value decomposition. We can obtain left singular operator as orthogonal projection operator for diagonalization of $\boldsymbol{MM}^T$ and can obtain right singular operator as operator for diagonalization of $\boldsymbol{M}^T \boldsymbol{M}$. This the conclusion of this paragraph. However, we have to prove the adequacy of hypothesis that there exist $\boldsymbol{U}$ and $\boldsymbol{V}$

Proof

First step

$$\boldsymbol{U} = (\boldsymbol{u_1} \quad \boldsymbol{u_2} \quad \cdots \quad \boldsymbol{u_p})$$
$$\boldsymbol{U}^T\boldsymbol{M}\boldsymbol{M}^T\boldsymbol{U} = \boldsymbol{\Lambda}$$

Multiply $\boldsymbol{U}$ from left to both side

$$\boldsymbol{U}\boldsymbol{U}^T\boldsymbol{M}\boldsymbol{M}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{\Lambda}$$
$$\boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{I}$$
$$\boldsymbol{M}\boldsymbol{M}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{\Lambda} = (\boldsymbol{u_1} \quad \boldsymbol{u_2} \quad \cdots \quad \boldsymbol{u_p})\begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p \end{pmatrix} = (\lambda_1\boldsymbol{u_1} \quad \lambda_2\boldsymbol{u_2} \quad \cdots \quad \lambda_p\boldsymbol{u_p})$$
$$\therefore \quad \boldsymbol{M}\boldsymbol{M}^T\boldsymbol{u_i} = \lambda_i\boldsymbol{u_i} = {\gamma_i}^2\boldsymbol{u_i}$$

Similarly,

$$\boldsymbol{V} = (\boldsymbol{v_1} \quad \boldsymbol{v_2} \quad \cdots \quad \boldsymbol{v_n})$$
$$\boldsymbol{V}^T\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{V} = \boldsymbol{L^2}$$
$$\boldsymbol{L^2} = \begin{pmatrix} {l_1}^2 & 0 & \cdots & 0 \\ 0 & {l_2}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & {l_n}^2 \end{pmatrix}$$

Multiply $\boldsymbol{V}$ from left to both side

$$\boldsymbol{V}\boldsymbol{V}^T\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{V} = \mathbf{V}\boldsymbol{L^2}$$
$$\boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{I}$$
$$\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{V} = (\boldsymbol{v_1} \quad \boldsymbol{v_2} \quad \cdots \quad \boldsymbol{v_n})\begin{pmatrix} {l_1}^2 & 0 & \cdots & 0 \\ 0 & {l_2}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & {l_n}^2 \end{pmatrix} = \left({l_1}^2\boldsymbol{v_1} \quad {l_2}^2\boldsymbol{v_2} \quad \cdots \quad {l_n}^2\boldsymbol{v_n}\right)$$
$$\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{v_j} = {l_j}^2\boldsymbol{v_j}$$

When we replace γ_i to l_1,

$$\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{V} = (\boldsymbol{v_1} \quad \boldsymbol{v_2} \quad \cdots \quad \boldsymbol{v_n})\begin{pmatrix} {\gamma_1}^2 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & {\gamma_2}^2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & {\gamma_p}^2 & 0 & \cdots & 0 \end{pmatrix} = \left({\gamma_1}^2\boldsymbol{v_1} \quad {\gamma_2}^2\boldsymbol{v_2} \quad \cdots \quad {\gamma_p}^2\boldsymbol{v_p} \quad 0\boldsymbol{v_{p+1}} \quad \cdots \quad 0\boldsymbol{v_n}\right)$$
$$\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{v_j} = {\gamma_j}^2\boldsymbol{v_j} \quad \text{for j} = 1\sim\text{p}$$
$$\boldsymbol{M}^T\boldsymbol{M}\boldsymbol{v_j} = 0, \boldsymbol{v_j} = 0 \quad \text{for j} = p + 1\sim\text{n}$$

Proof of existence of $\boldsymbol{U}$ and $\boldsymbol{V}$

Existence of $\boldsymbol{V}$ is trivial because $\boldsymbol{V}$ is orthogonal projection operator of symmetric matrix.

$$\boldsymbol{w_j} = \frac{1}{\gamma_j}\boldsymbol{v_j}$$
$$\boldsymbol{v_i}\boldsymbol{v_j} = \delta_{ij}$$

$$\boldsymbol{w_i w_j} = \frac{1}{\gamma_i\gamma_j}\boldsymbol{v_i v_j} = \frac{1}{\gamma_i\gamma_j}\delta_{ij}$$

$$\boldsymbol{w_i} \perp \boldsymbol{w_j}\ (i \neq j)$$

$$\boldsymbol{V} = (\boldsymbol{v_1} \quad \boldsymbol{v_2} \quad \cdots \quad \boldsymbol{v_p} \quad \boldsymbol{v_{p+1}} \quad \cdots \quad \boldsymbol{v_n})$$

$$\boldsymbol{W} = (\boldsymbol{w_1} \quad \boldsymbol{w_2} \quad \cdots \quad \boldsymbol{w_p})$$

$$\boldsymbol{W^T} = \begin{pmatrix} \boldsymbol{w_1}^T \\ \boldsymbol{w_2}^T \\ \vdots \\ \boldsymbol{w_p}^{\boldsymbol{T}} \end{pmatrix}$$

$$\boldsymbol{L} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_p \end{pmatrix}$$

$$\boldsymbol{W}^T\boldsymbol{LV} = \boldsymbol{W}^T\boldsymbol{L}(\boldsymbol{v_1} \quad \boldsymbol{v_2} \quad \cdots \quad \boldsymbol{v_p} \quad \boldsymbol{v_{p+1}} \quad \cdots \quad \boldsymbol{v_n})$$

$$= \boldsymbol{W}^T(\gamma_1\boldsymbol{w_1} \quad \gamma_2\boldsymbol{w_2} \quad \cdots \quad \gamma_p\boldsymbol{w_p} \quad 0 \quad \cdots \quad 0)$$

$$= \begin{pmatrix} \boldsymbol{w_1}^T \\ \boldsymbol{w_2}^T \\ \vdots \\ \boldsymbol{w_p}^{\boldsymbol{T}} \end{pmatrix}(\gamma_1\boldsymbol{w_1} \quad \gamma_2\boldsymbol{w_2} \quad \cdots \quad \gamma_p\boldsymbol{w_p} \quad 0 \quad \cdots \quad 0)$$

$$= \begin{pmatrix} \gamma_1\boldsymbol{w_1}^T\boldsymbol{w_1} & \gamma_2\boldsymbol{w_1}^T\boldsymbol{w_2} & \cdots & \gamma_p\boldsymbol{w_1}^T\boldsymbol{w_p} & 0\boldsymbol{w_1}^T & \cdots & 0\boldsymbol{w_1}^T \\ \gamma_1\boldsymbol{w_2}^T\boldsymbol{w_1} & \gamma_2\boldsymbol{w_2}^T\boldsymbol{w_2} & \cdots & \gamma_p\boldsymbol{w_2}^T\boldsymbol{w_p} & 0\boldsymbol{w_2}^T & \cdots & 0\boldsymbol{w_2}^T \\ \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots \\ \gamma_1\boldsymbol{w_p}^T\boldsymbol{w_1} & \gamma_2\boldsymbol{w_p}^T\boldsymbol{w_2} & \cdots & \gamma_p\boldsymbol{w_2}^T\boldsymbol{w_p} & 0\boldsymbol{w_p}^T & \cdots & 0\boldsymbol{w_p}^T \end{pmatrix}$$

$$= \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & \gamma_p & 0 & \cdots & 0 \end{pmatrix}$$

$$\because \quad \boldsymbol{w_i}^T\boldsymbol{w_j} = \delta_{ij} \quad \boldsymbol{w_i} \perp \boldsymbol{w_j} \qquad \text{iii}$$

Q.E.D

We could demonstrate that there exist left singular operator and right singular operator for all matrix and we can denote $\mathrm{U} = \boldsymbol{W}$

Conclusively

$$\boldsymbol{M} = \boldsymbol{U\Sigma V}^T$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & \gamma_p & 0 & \cdots & 0 \end{pmatrix}_{p\times n}$$

We discussed only the case when $p < n$. In the case when $p > n$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_n \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}_{p\times n}$$

Formula 72

In several case, $\boldsymbol{M}$ is positive semidefinite (eigenvalue include 0.). The number of positive singular value is rank (r). $r \leq p$

In such case $r < p$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \gamma_r & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}_{p\times n}$$

More generally, $\boldsymbol{\Sigma}$ can be expressed as follow

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{S}_{r,r} & \boldsymbol{O}_{r.n-r} \\ \boldsymbol{O}_{m-r,r} & \boldsymbol{O}_{m-r,n-r} \end{pmatrix}$$

$$\boldsymbol{S}_{r,r}\text{: diagonal } matrix,\ \ diag(\gamma_1 \quad \cdots \quad \gamma_r)$$

$$diag(\quad)\text{ is diagonal components}$$

$$\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_r > 0$$

$$\boldsymbol{O}_{i,j} = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}_{i\times j}$$

Application of singular value decomposition

$$\boldsymbol{M} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

This matrix is linearly dependent (not independent), because third column and third row are real number times of second column and second row. From this we can judge that rank of the matrix is 2, because number of linearly independent column and row is 2. However, judgement of number of rank difficult from dataset is generally difficult, because we cannot notice the dependency of the row or column, when a row or column is linear combination of other rows or columns. In addition to this, similar samples are often included in data set, and many data are approximately the same. In such case, we obtain several very small singular values which is approximately 0.

$\boldsymbol{\Sigma}$ is as follow

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_p & 0 & \cdots & 0 \end{pmatrix}_{p\times n}$$

$$diag(\gamma_1 \quad \cdots \quad \gamma_p)$$

$$\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_p \geq 0$$

The analysts should judge the singular values are 0 or not 0, comparing the singular values to other singular values, considering the purpose of analysis, drawing their experience and referring previous works. The work the analysts is judgement of threshold, which is S in following inequality

$$\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_r \geq S \geq \gamma_{r+1} \geq \cdots \geq \gamma_{r'} > 0$$

Then following $\boldsymbol{\Sigma}$ is determined.

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \gamma_r & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}_{p\times n}$$

In case of following matrix

$$\boldsymbol{M} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\boldsymbol{M^T} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\boldsymbol{MM^T} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}\begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix} = \begin{pmatrix} 16 & 0 & 0 \\ 0 & 2 & -2 \\ 0 & -2 & 2 \end{pmatrix}$$

固有方程式

$$\begin{vmatrix} 16-\lambda & 0 & 0 \\ 0 & 2-\lambda & -2 \\ 0 & -2 & 2-\lambda \end{vmatrix} = 0$$

$$(16-\lambda)(2-\lambda)(2-\lambda) - 4(16-\lambda) = 0$$

$$(\lambda - 16)(\lambda - 4)\lambda = 0$$

From this we can judge the rank of the matrix as 3－1=2.

Eigenvector　belonging eigenvalue16

$$\begin{pmatrix} 16 & 0 & 0 \\ 0 & 2 & -2 \\ 0 & -2 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 16\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\begin{pmatrix} 16x_1 \\ 2x_2 - 2x_3 \\ -2x_2 + 2x_3 \end{pmatrix} = \begin{pmatrix} 16x_1 \\ 16x_2 \\ 16x_3 \end{pmatrix}$$

$$14x_2 + 2x_3 = 0$$

$$2x_2 + 14x_3 = 0$$
$$x_2 = x_3 = 0$$
$$\boldsymbol{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$
Eigenvector belonging eigenvalue 4
$$\begin{pmatrix} 16 & 0 & 0 \\ 0 & 2 & -2 \\ 0 & -2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 4 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$
$$\begin{pmatrix} 16x_1 \\ 2x_2 - 2x_3 \\ -2x_2 + 2x_3 \end{pmatrix} = \begin{pmatrix} 4x_1 \\ 4x_2 \\ 4x_3 \end{pmatrix}$$
$$12x_1 = 0$$
$$-2x_2 - 2x_3 = 0$$
$$-2x_2 - 2x_3 = 0$$
$$x_1 = 0, \qquad x_2 = -x_3$$
$$\boldsymbol{e}_2 = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$
Eigenvector belonging eigenvalue 0
$$\begin{pmatrix} 16 & 0 & 0 \\ 0 & 2 & -2 \\ 0 & -2 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$
$$\begin{pmatrix} 16x_1 \\ 2x_2 - 2x_3 \\ -2x_2 + 2x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$
$$x_1 = 0$$
$$2x_2 - 2x_3 = 0$$
$$-2x_2 + 2x_3 = 0$$
$$x_1 = 0, \qquad x_2 = x_3$$
$$\boldsymbol{e}_3 = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$
Result of singular value decomposition is as follow.

Left singular operator is $\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{-\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$.

Right singular operator is $\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{-\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}^T$

$$\boldsymbol{\Sigma} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Confirmation of adequacy of the result

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{-\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & -\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} 4 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

This is means that left singular operator equals to right singular operator in singular value decomposition. This is understandable when we consider power method of symmetric matrix.

In symmetric matrix,

$$\boldsymbol{M}\boldsymbol{M}^T = \boldsymbol{M}^T\boldsymbol{M} = \boldsymbol{M}^2$$

Matrix $\boldsymbol{M}$ is decompose as follow.

$$\boldsymbol{M} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$

Using power method of symmetric matrix

$$\boldsymbol{M}\boldsymbol{M}^T = \boldsymbol{M}^T\boldsymbol{M} = \boldsymbol{M}^2 = \boldsymbol{U}\boldsymbol{\Lambda}^2\boldsymbol{U}^T$$

From this we can accept that diagonalization of symmetric matrix is a specific case of right singular decomposition in which left singular operator equals to right singular operator.

Figure 61 is illustrating the procedure of singular value decomposition. In this illustration the matrix $\boldsymbol{M}$ is transformation of unit circle and yellow vector (A) to inclined ellipse and yellow vector (D). When there exists inverse matrix $\boldsymbol{M}^{-1}$, inverse operation is multiplication of $\boldsymbol{M}^{-1}$. However, there are several conditions for existence of inverse matrix. Particularly, non-square matrix has no inverse matrix. Singular value decomposition provides alternative detour root of inverse operation. Matrix $\boldsymbol{V}^T$ is rotation, matrix $\boldsymbol{\Sigma}$ is expansion and contraction, and $\boldsymbol{U}$ is rotation.

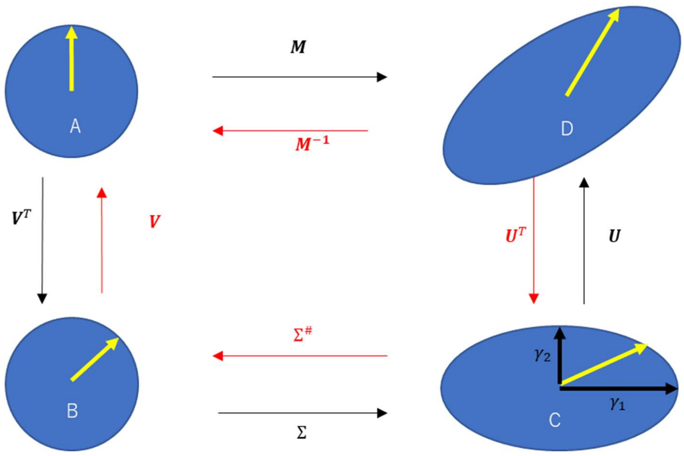

Fig. 61 Procedure of singular value decomposition and inverse operation.

The process A → D is expressed as follow

$$\boldsymbol{MA} = \boldsymbol{D}$$

The process D → A is expressed as follow

$$\boldsymbol{M}^{-1}\boldsymbol{MA} = \boldsymbol{M}^{-1}\boldsymbol{D}$$

$$\boldsymbol{A} = \boldsymbol{M}^{-1}\boldsymbol{D}$$

However, we cannot obtain $\boldsymbol{M}^{-1}$. The alternative route of $\boldsymbol{M}$ is $\boldsymbol{V}^T \to \boldsymbol{\Sigma} \to \boldsymbol{U}$. This is expressed as

$$\boldsymbol{M} = \boldsymbol{U\Sigma V}^T$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \gamma_r & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}_{p \times n}$$

Converse route is $\boldsymbol{U}^T \to \boldsymbol{\Sigma} \to \boldsymbol{V}$. This procedure is expressed as follow

$$\boldsymbol{M}^* = \boldsymbol{V\Sigma}^{\#}\boldsymbol{U}^T$$

$$\boldsymbol{\Sigma}^{\#} = \begin{pmatrix} \frac{1}{\gamma_1} & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\gamma_2} & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \frac{1}{\gamma_r} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{pmatrix}_{n \times p}$$

$$\boldsymbol{M}^*\text{: Alternative motrix for inverse matrix (pseudo} - \text{inverse matrix)}$$

$$\boldsymbol{A} = \boldsymbol{M}^*\boldsymbol{D}$$

Pseudo-inverse matrix has similar function as singular value decomposition. Let clarify the relation between pseudo-inverse matrix and singular value decomposition. The formula of pseudo-inverse matrix is as follow

$$\boldsymbol{M}^{\#} = (\boldsymbol{M}^T\boldsymbol{M})^{-1}\boldsymbol{M}^T$$

Using diagonalization of symmetric matrix

$$\boldsymbol{M}^T\boldsymbol{M} = \boldsymbol{V}\boldsymbol{\Sigma}^2\boldsymbol{V}^T$$

$$(\boldsymbol{M}^T\boldsymbol{M})^{-1} = \boldsymbol{V}^{T^{-1}}\boldsymbol{\Sigma}^{-2}\boldsymbol{V}^{-1} = \boldsymbol{V}\boldsymbol{\Sigma}^{-2}\boldsymbol{V}^T$$

$$\boldsymbol{M}^T = (\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T)^T = \boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{U}^T$$

$$\boldsymbol{M}^{\#} = (\boldsymbol{M}^T\boldsymbol{M})^{-1}\boldsymbol{M}^T = \boldsymbol{V}\boldsymbol{\Sigma}^{-2}\boldsymbol{V}^T\,\boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{U}^T = \boldsymbol{V}\boldsymbol{\Sigma}^{-1}\boldsymbol{U}^T$$

$$\boldsymbol{M}^* = \boldsymbol{M}^{\#}$$

We could confirm that inverse operation of singular value decomposition is pseudo-inverse matrix. This means that when we consider small singular value as 0, we can decrease the rank for approximate calculation. This is the base of Principle component analysis.

Exercises for clear understanding

Exercise I. Singular value decomposition of 2×2 matrix

$$\boldsymbol{A} = \begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix}$$

Calculation of singular value and left singular operator

$$\boldsymbol{A}\boldsymbol{A}^{\boldsymbol{T}} = \begin{pmatrix} 0 & -2 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -2 & 0 \end{pmatrix} = \begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}$$

Eigenvalue and eigenvector

$$\begin{vmatrix} 4-\lambda & 0 \\ 0 & 1-\lambda \end{vmatrix} = 0$$

$$(4-\lambda)(1-\lambda) = 0$$

$$\lambda = 4, 1$$

Eigenvector for $\lambda = 4$

$$\begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 4\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$x_1 = x_1$$

$$x_2 = 4x_2$$

$$x_1 = t \text{ and } x_2 = 0、$$

$$\begin{pmatrix}1\\0\end{pmatrix}$$

Eigenvector for $\lambda = 1$

$$\begin{pmatrix}4 & 0\\0 & 1\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix} = 1\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$4x_1 = x_1$$

$$x_2 = x_2$$

$$x_1 = 0 \text{ and } x_2 = t$$

$$\begin{pmatrix}0\\1\end{pmatrix}$$

Left singular operator

$$\boldsymbol{U} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

$$\boldsymbol{U^{-1}} = \ \boldsymbol{U}^T = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

Calculation of right singular operator

$$\boldsymbol{A^TA} = \begin{pmatrix}0 & 1\\-2 & 0\end{pmatrix}\begin{pmatrix}0 & -2\\1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 4\end{pmatrix}$$

Eigenvalue and eigenvector

$$\begin{vmatrix}1-\lambda & 0\\0 & 4-\lambda\end{vmatrix} = 0$$

$$(4-\lambda)(1-\lambda) = 0$$

$$\lambda = 4, 1$$

$$\begin{pmatrix}1 & 0\\0 & 4\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix} = 4\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$x_1 = 4x_1$$

$$x_2 = x_2$$

$$\begin{pmatrix}0\\1\end{pmatrix}$$

$$\begin{pmatrix}1 & 0\\0 & 4\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix} = 1\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$x_1 = x_1$$

$$4x_2 = x_2$$

$$x_1 = \mathrm{t}x_1$$

$$x_2 = 0$$

$$\begin{pmatrix}1\\0\end{pmatrix}$$

$$\boldsymbol{V}=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ \boldsymbol{V^{-1}}=\ \boldsymbol{V}^T=\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\gamma_1=\sqrt{\lambda_1}=\sqrt{4}=2$$

$$\gamma_2=\sqrt{\lambda_2}=\sqrt{1}=1$$

$$\boldsymbol{\Sigma}=\begin{pmatrix}2&0\\0&1\end{pmatrix}$$

Confirmation

$$\begin{pmatrix}0&2\\1&0\end{pmatrix}=\boldsymbol{U\Sigma V}^T=\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}2&0\\0&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}=\begin{pmatrix}2&0\\0&1\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}=\begin{pmatrix}0&2\\1&0\end{pmatrix}$$

Exercise II. Singular value decomposition of 2×3 matrix

$$\boldsymbol{A}=\begin{pmatrix}1&0&0\\0&1&1\end{pmatrix}$$

Rank of this matrix is 2

$$\boldsymbol{A}^T=\begin{pmatrix}1&0\\0&1\\0&1\end{pmatrix}$$

Left singular operator

$$\boldsymbol{AA}^T=\begin{pmatrix}1&0&0\\0&1&1\end{pmatrix}\begin{pmatrix}1&0\\0&1\\0&1\end{pmatrix}=\begin{pmatrix}1&0\\0&2\end{pmatrix}$$

Eigenvalue is $\lambda=2,1$ and singular value $\gamma_1=\sqrt{2}$, and $\gamma_1=1$.
Eigenvector

$$\begin{pmatrix}1&0\\0&2\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix}=2\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$x_1=2x_1$$

$$2x_2=2x_2$$

$$x_1=0,x_2=t$$

$$\begin{pmatrix}1&0\\0&2\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix}=\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$x_1=x_1$$

$$2x_2=x_2$$

$$x_1=1,x_2=0$$

$$\boldsymbol{U}=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ \boldsymbol{U^{-1}}=\ \boldsymbol{U}^T=\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

Right singular operator

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

Eigenvalue and eigenvector

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ 0 & 1-\lambda & 1 \\ 0 & 1 & 1-\lambda \end{vmatrix} = 0$$

$$(1-\lambda)^3 - (1-\lambda) = 0$$

$$(1-\lambda)\{(1-\lambda)^2 - 1\} = 0$$

$$\lambda(1-\lambda)(2-\lambda) = 0$$

$$\lambda = 2, 1, 0$$

Rank of $\boldsymbol{A}$ is 2

Eigenvector for $\lambda = 2$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$x_1 = 2x_1$$

$$x_2 + x_3 = 2x_2$$

$$x_2 + x_3 = 2x_3$$

$$\begin{pmatrix} 0 \\ t \\ t \end{pmatrix}$$

$$\mathrm{t} = \frac{1}{\sqrt{2}}$$

$$\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

Eigenvector for $\lambda = 1$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 1 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$x_1 = x_1$$

$$x_2 + x_3 = x_2$$

$$x_2 + x_3 = x_3$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

Eigen vector for $\lambda = 0$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$x_1 = x_1$$

$$x_2 + x_3 = 0$$

$$x_2 + x_3 = 0$$

$$\begin{pmatrix} 0 \\ t \\ -t \end{pmatrix}$$

$$\mathrm{t} = \frac{1}{\sqrt{2}}$$

$$\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

Right singular operator

$$\boldsymbol{V} = \begin{pmatrix} 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\boldsymbol{V}^T = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \end{pmatrix}$$

Conformation

$$\boldsymbol{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} = \boldsymbol{U\Sigma V^T} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

Exercise III. Pseudo-inverse matrix of upper 2 ×3 matrix

At first, we try to calculate directly by following equation.

$$\boldsymbol{A}^{\#} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$$

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{vmatrix} = 0$$

We cannot calculate inverse matrix of $\boldsymbol{A}^T\boldsymbol{A}$**,** because the determinant is 0. So, we try to calculate Pseudo-inverse matrix of upper 2 ×3 matrix by singular value decomposition

$$\boldsymbol{A}^{\#} = \boldsymbol{V}\boldsymbol{\Sigma}^{\#}\boldsymbol{U}^T$$

$$\boldsymbol{V}=\begin{pmatrix}0 & 1 & 0\\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}}\end{pmatrix}$$

$$\boldsymbol{\Sigma}^{\#}=\begin{pmatrix}\frac{1}{\sqrt{2}} & 0\\ 0 & 1\end{pmatrix}$$

$$\boldsymbol{U}^{T}=\boldsymbol{U}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$\boldsymbol{A}^{\#}=\boldsymbol{V}\boldsymbol{\Sigma}^{\#}\boldsymbol{U}^{T}=\begin{pmatrix}0 & 1 & 0\\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$=\begin{pmatrix}0 & 1\\ \frac{1}{2} & 0\\ \frac{1}{2} & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & \frac{1}{2}\\ 0 & \frac{1}{2}\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}$$

Confirmation

$$\boldsymbol{A}\boldsymbol{A}^{\#}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$\boldsymbol{A}^{\#}\boldsymbol{A}=\begin{pmatrix}1 & 0\\ 0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 1\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 1\\ 0 & 0 & 0\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}$$

Exercise IV. Singular value decomposition of 3×4 matrix

$$\boldsymbol{A}=\begin{pmatrix}2 & 2 & 2 & 2\\ 1 & -1 & 1 & -1\\ -1 & 1 & -1 & 1\end{pmatrix}$$

$$\boldsymbol{A}\boldsymbol{A}^{T}=\begin{pmatrix}2 & 2 & 2 & 2\\ 1 & -1 & 1 & -1\\ -1 & 1 & -1 & 1\end{pmatrix}\begin{pmatrix}2 & 1 & -1\\ 2 & -1 & 1\\ 2 & 1 & -1\\ 2 & -1 & 1\end{pmatrix}=\begin{pmatrix}16 & 0 & 0\\ 0 & 4 & -4\\ 0 & -4 & 4\end{pmatrix}=4\begin{pmatrix}4 & 0 & 0\\ 0 & 1 & -1\\ 0 & -1 & 1\end{pmatrix}$$

$$\boldsymbol{A}^{T}\boldsymbol{A}=\begin{pmatrix}2 & 1 & -1\\ 2 & -1 & 1\\ 2 & 1 & -1\\ 2 & -1 & 1\end{pmatrix}\begin{pmatrix}2 & 2 & 2 & 2\\ 1 & -1 & 1 & -1\\ -1 & 1 & -1 & 1\end{pmatrix}=\begin{pmatrix}6 & 0 & 6 & 0\\ 0 & 6 & 0 & 6\\ 6 & 0 & 6 & 0\\ 0 & 6 & 0 & 6\end{pmatrix}$$

Left singular operator

Singular value

$$\begin{vmatrix}4-\lambda & 0 & 0\\ 0 & 1-\lambda & -1\\ 0 & -1 & 1-\lambda\end{vmatrix}=0$$

$$(4-\lambda)(1-\lambda)^2-(4-\lambda)=0$$

$$(4-\lambda)((1-\lambda)^2-1)=0$$

$$\lambda(4-\lambda)(2-\lambda)=0$$

$$\lambda_1=4\times 4, \lambda_2=4\times 2, \lambda_3=0$$

Rank r=2

$$\gamma_1=4, \gamma_2=2\sqrt{2}$$

$$\Sigma=\begin{pmatrix}4 & 0 & 0 & 0\\ 0 & 2\sqrt{2} & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}$$

Eigenvector

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

$$4x_1=4x_1$$

$$x_2-x_3=4x_2$$

$$-x_2+x_3=4x_3$$

$$-x_3=3x_2$$

$$-x_2=3x_3$$

Eigenvector $\begin{pmatrix}1\\ 0\\ 0\end{pmatrix}$

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

$$4x_1=2x_1$$

$$x_2-x_3=2x_2$$

$$-x_2+x_3=2x_3$$

$$-x_3=x_2$$

$$-x_2=x_3$$

Eigenvector $\begin{pmatrix}0\\ \frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}$

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

$$4x_1=0$$

$$x_2-x_3=0$$

$$-x_2+x_3=0$$

$$x_2=x_3$$

$$x_3=x_2$$

$$\text{Eigenvector} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\boldsymbol{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

Right singular operator

$$\begin{vmatrix} 6-\lambda & 0 & 6 & 0 \\ 0 & 6-\lambda & 0 & 6 \\ 6 & 0 & 6-\lambda & 0 \\ 0 & 6 & 0 & 6-\lambda \end{vmatrix} = 0$$

$$(6-\lambda)^4 + 6^4 - 2 \times 6^2(6-\lambda)^2 = 0$$

$$((6-\lambda)^2)^2 - 2 \times 6^2(6-\lambda)^2 + (6^2)^2 = 0$$

$$((6-\lambda)^2 - 6^2)^2 = 0$$

$$(\lambda^2 - 12\lambda)^2 = 0$$

$$\lambda = 12, 0$$

$$\begin{pmatrix} 6 & 0 & 6 & 0 \\ 0 & 6 & 0 & 6 \\ 6 & 0 & 6 & 0 \\ 0 & 6 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = 12 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

$$6x_1 + 6x_3 = 12x_1$$

$$6x_2 + 6x_4 = 12x_4$$

$$x_1 = x_3$$

$$x_2 = x_4$$

$$\text{Eigenvector} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}$$

$$\begin{pmatrix} 6 & 0 & 6 & 0 \\ 0 & 6 & 0 & 6 \\ 6 & 0 & 6 & 0 \\ 0 & 6 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = 0$$

$$6x_1 + 6x_3 = 0$$

$$6x_2 + 6x_4 = 0$$

$$x_1 = -x_3$$

$$x_2 = -x_4$$

$$\text{Eigenvector} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

Right singular operator

$$\boldsymbol{V} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Confirmation

$$\boldsymbol{A} = \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix} = \boldsymbol{U\Sigma}\mathbf{V}^{T}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}^{T}$$

$$\begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 2 & 2 & 2 & 2 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix}$$