Task 10. Singular value decomposition (SVD) of the rectangular matrix

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Zadanie 10

Write a program that performs singular value decomposition (SVD) of the rectangular matrix $\mathbf{A}$. Using this decomposition calculate the pseudo-inverse matrix $\mathbf{A}^{+}$.

Singular value decomposition of rectangular matrix $\mathbf{A}_{m\times n}$

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{Tr}$$

- $\mathbf{U}$ orthogonal matrix $m \times m$
- $\mathbf{V}$ orthogonal matrix $n \times n$
- $\boldsymbol{\Sigma}$ diagonal (rectangular) matrix $m \times n$, where the diagonal elements σ_i of $\boldsymbol{\Sigma}$ are non-negative and they are ordered as follows

  $$\sigma_1 \geqslant \sigma_2 \geqslant \ldots \geqslant \sigma_{\min(m,n)} \geqslant 0$$

  σ_i are the singular values of $\mathbf{A}$ matrix
- $j = 1 \min(m, n)$ columns $\mathbf{u}_j$ and $\mathbf{v}_j$ of $\mathbf{U}$ and $\mathbf{V}$ matrices, respectively, satisfy the following relations

$$\mathbf{A}\,\mathbf{v}_j = \sigma_j\mathbf{u}_j, \quad \mathbf{A}^{Tr}\mathbf{u}_j = \sigma_j\mathbf{v}_j, \quad \mathbf{A}^{Tr}\mathbf{A}\,\mathbf{v}_j = \sigma_j^2\mathbf{v}_j, \quad \mathbf{A}\mathbf{A}^{Tr}\mathbf{u}_j = \sigma_j^2\mathbf{u}_j$$

Rectangular diagonal matrix - 4×3 example

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \\ 0 & 0 & 0 \end{pmatrix} \quad \boldsymbol{\Sigma}^{Tr} = \begin{pmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & \sigma_3 & 0 \end{pmatrix}$$

$$\boldsymbol{\Sigma}^{Tr}\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{pmatrix}$$

$$\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{Tr} = \begin{pmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & 0 \\ 0 & 0 & \sigma_3^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

SVD - derivations (1)

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n}\,\mathbf{V}^{Tr}_{n\times n} \quad \Big| \cdot \mathbf{V}_{n\times n} \qquad (\mathbf{V}^{Tr}\mathbf{V} = \mathbf{1})$$

$$\mathbf{A}_{m\times n}\,\mathbf{V}_{n\times n} = \mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n}$$

$$\sum_{k=1}^{n} A_{ik} V_{kj} = \underbrace{\sum_{\ell=1}^{\min(m,n)} U_{i\ell}\sigma_\ell\delta_{\ell j}}_{U_{ij}\sigma_j} \qquad i = 1,\ldots,m,\ j = 1,\ldots,n$$

$$\Downarrow$$

$$\mathbf{A}\mathbf{v}_j = \sigma_j\mathbf{u}_j, \quad j = 1,\ldots,\min(m,n)$$

$\mathbf{v}_j$ and $\mathbf{u}_j$ are the columns of $\mathbf{V}$ and $\mathbf{U}$ matrices, respectively

SVD - derivations (2)

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n}\,\mathbf{V}^{Tr}_{n\times n}$$

$$\mathbf{A}^{Tr}_{n\times m} = (\mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n}\,\mathbf{V}^{Tr}_{n\times n})^{Tr} = (\mathbf{V}^{Tr}_{n\times n})^{Tr}(\mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n})^{Tr}$$

$$= \mathbf{V}_{n\times n}\,\mathbf{\Sigma}^{Tr}_{n\times m}\mathbf{U}^{Tr}_{m\times m}$$

$$\mathbf{A}^{Tr}_{n\times m} = \mathbf{V}_{n\times n}\,\mathbf{\Sigma}^{Tr}_{n\times m}\mathbf{U}^{Tr}_{m\times m} \qquad |\cdot\mathbf{U}_{m\times m} \qquad (\mathbf{U}^{Tr}\mathbf{U} = \mathbf{1})$$

$$\mathbf{A}^{Tr}_{n\times m}\,\mathbf{U}_{m\times m} = \mathbf{V}_{n\times n}\,\mathbf{\Sigma}^{Tr}_{n\times m}$$

$$\sum_{k=1}^{m}(\mathbf{A}^{Tr})_{ik}U_{kj} = \underbrace{\sum_{\ell=1}^{\min(m,n)} V_{i\ell}\sigma_\ell\delta_{\ell j}}_{V_{ij}\sigma_j} \qquad i = 1,\ldots,n,\; j = 1,\ldots,m$$

$$\Downarrow$$

$$\mathbf{A}^{Tr}\mathbf{u}_j = \sigma_j\mathbf{v}_j, \quad j = 1,\ldots,\min(m,n)$$

$\mathbf{v}_j$ and $\mathbf{u}_j$ are the columns of **V** and **U** matrices, respectively

SVD - derivations (3)

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\boldsymbol{\Sigma}_{m\times n}\mathbf{V}^{Tr}_{n\times n} \qquad \mathbf{A}^{Tr}_{n\times m} = \mathbf{V}_{n\times n}\boldsymbol{\Sigma}^{Tr}_{n\times m}\mathbf{U}^{Tr}_{m\times m}$$

$$\mathbf{A}^{Tr}\mathbf{A} = \mathbf{V}\boldsymbol{\Sigma}^{Tr}\underbrace{\mathbf{U}^{Tr}\mathbf{U}}_{\mathbf{1}}\boldsymbol{\Sigma}\mathbf{V}^{Tr} = \mathbf{V}\boldsymbol{\Sigma}^{Tr}\boldsymbol{\Sigma}\mathbf{V}^{Tr}$$

$$\mathbf{A}^{Tr}\mathbf{A} = \mathbf{V}\boldsymbol{\Sigma}^{Tr}\boldsymbol{\Sigma}\mathbf{V}^{Tr} \quad |\cdot\mathbf{V}$$

$$(\mathbf{A}^{Tr}\mathbf{A})_{n\times n}\mathbf{V}_{n\times n} = \mathbf{V}_{n\times n}(\boldsymbol{\Sigma}^{Tr}\boldsymbol{\Sigma})_{n\times n}$$

$$\sum_{k=1}^{n}(\mathbf{A}^{Tr}\mathbf{A})_{ik}V_{kj} = \underbrace{\sum_{\ell=1}^{\min(m,n)} V_{i\ell}\sigma_\ell^2\delta_{\ell j}}_{V_{ij}\sigma_j^2}$$

$$\Downarrow$$

$$\mathbf{A}^{Tr}\mathbf{A}\,\mathbf{v}_j = \sigma_j^2\,\mathbf{v}_j, \qquad j = 1,\ldots,\min(m,n)$$

Column $\mathbf{v}_j$ is the eigenvector of the square and symmetric matrix $\mathbf{A}^{Tr}\mathbf{A}$ corresponding to eigenvalue σ_j^2

SVD - derivations (4)

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\,\mathbf{\Sigma}_{m\times n}\,\mathbf{V}^{Tr}_{n\times n} \qquad \mathbf{A}^{Tr}_{n\times m} = \mathbf{V}_{n\times n}\,\mathbf{\Sigma}^{Tr}_{n\times m}\mathbf{U}^{Tr}_{m\times m}$$

$$\mathbf{A}\mathbf{A}^{Tr} = \mathbf{U}\mathbf{\Sigma}\underbrace{\mathbf{V}^{Tr}\mathbf{V}}_{\mathbf{1}}\mathbf{\Sigma}^{Tr}\mathbf{U}^{Tr} = \mathbf{U}\mathbf{\Sigma}\mathbf{\Sigma}^{Tr}\mathbf{U}^{Tr}$$

$$\mathbf{A}\mathbf{A}^{Tr} = \mathbf{U}\mathbf{\Sigma}\mathbf{\Sigma}^{Tr}\mathbf{U}^{Tr} \quad \big| \cdot \mathbf{U}$$

$$(\mathbf{A}\mathbf{A}^{Tr})_{m\times m}\mathbf{U}_{m\times m} = \mathbf{U}_{m\times m}(\mathbf{\Sigma}\mathbf{\Sigma}^{Tr})_{m\times m}$$

$$\sum_{k=1}^{m}(\mathbf{A}\mathbf{A}^{Tr})_{ik}U_{kj} = \underbrace{\sum_{\ell=1}^{\min(m,n)} U_{i\ell}\sigma_\ell^2\delta_{\ell j}}_{U_{ij}\sigma_j^2}$$

$$\Downarrow$$

$$\mathbf{A}\mathbf{A}^{Tr}\,\mathbf{u}_j = \sigma_j^2\,\mathbf{u}_j, \qquad j = 1,\ldots,\min(m,n)$$

Column $\mathbf{u}_j$ is the eigenvectors of square and symmetric matrix $\mathbf{A}\mathbf{A}^{Tr}$ corresponding to eigenvalue σ_j^2

Singular value decomposition of rectangular matrix $\mathbf{A}_{m \times n}$

Applications of SVD

- Euclidean norm

$$\|\mathbf{A}\|_2 = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \sigma_{\max}$$

- Rank of a matrix is equal to the number of non-zero singular values. Numerical rank of the matrix is the number of singular values that are larger than the assumed threshold value (close to zero).

Singular value decomposition of rectangular matrix $\mathbf{A}_{m \times n}$

Applications of SVD

- Condition number of the (square or rectangular) matrix

$$\mathrm{cond}(\mathbf{A}) = \sigma_{\mathrm{max}} / \sigma_{\mathrm{min}}$$

- Solution of the overdetermined system of linear equations $\mathbf{Ax} \approx \mathbf{b}$ by means of least squares. Namely, the solution that minimizes the Euclidean norm of **Ax**-**b**, i.e. $(\|\mathbf{Ax} - \mathbf{b}\|_2)^2 = \min$, is the following

$$\mathbf{x} = \sum_{\sigma_i > 0} \frac{\mathbf{u}_i^{Tr} \mathbf{b}}{\sigma_i} \mathbf{v}_i$$

  where σ_i are non-zero singular values of matrix **A**. SVD allows in a controllable way to find the solution of badly conditioned problems just by omitting very low singular values; this makes the solution less sensitive to the perturbations of the input data.

Singular value decomposition of rectangular matrix $\mathbf{A}_{m\times n}$

We are going to define pseudo-inverse of general rectangular matrix, but first, we have to define pseudo-inverse of the number and pseudo-inverse of the diagonal matrix

- Pseudo-inverse of the number

$$\sigma^+ = \begin{cases} 1/\sigma & \sigma \neq 0 \\ 0 & \sigma = 0 \end{cases}$$

- Pseudo-inverse of the diagonal rectangular matrix $\mathbf{\Sigma}_{m\times n}$ is the diagonal rectangular matrix $\mathbf{\Sigma}^+_{n\times m}$, in which the diagonal elements are the pseudo-inverse numbers σ_1^+, σ_2^+,...,$\sigma^+_{\min(m,n)}$ of the corresponding diagonal elements of $\mathbf{\Sigma}$ matrix

Pseudo-inverse of diagonal matrix $\boldsymbol{\Sigma}$ - example 4×3

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \\ 0 & 0 & 0 \end{pmatrix} \quad \Rightarrow \quad \boldsymbol{\Sigma}^+ = \begin{pmatrix} \frac{1}{\sigma_1} & 0 & 0 & 0 \\ 0 & \frac{1}{\sigma_2} & 0 & 0 \\ 0 & 0 & \frac{1}{\sigma_3} & 0 \end{pmatrix}$$

where it is assumed that $\sigma_i \neq 0, \ i = 1, 2, 3$

$$\boldsymbol{\Sigma}\boldsymbol{\Sigma}^+ = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \boldsymbol{\Sigma}^+\boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Pseudo-inverse of matrix $\mathbf{A}_{m\times n}$

Having SVD decomposition of matrix $\mathbf{A}$

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\,\boldsymbol{\Sigma}_{m\times n}\,\mathbf{V}^{Tr}_{n\times n}$$

we can define pseudo-inverse of matrix $\mathbf{A}$ as follows

$$\mathbf{A}^{+}_{n\times m} = \mathbf{V}_{n\times n}\,\boldsymbol{\Sigma}^{+}_{n\times m}\,\mathbf{U}^{Tr}_{m\times m}$$

Assuming $m \geqslant n$ and $\sigma_{\min} > 0$ we can show that pseudo-inverse matrix behaves **almost** as inverse matrix

$$\mathbf{A}^{+}\mathbf{A} = \mathbf{V}\,\boldsymbol{\Sigma}^{+}\,\underbrace{\mathbf{U}^{Tr}\,\mathbf{U}}_{\mathbf{1}}\,\boldsymbol{\Sigma}\,\mathbf{V}^{Tr} = \mathbf{V}\,\underbrace{\boldsymbol{\Sigma}^{+}\,\boldsymbol{\Sigma}}_{\mathbf{1}}\,\mathbf{V}^{Tr} = \mathbf{V}\mathbf{V}^{Tr} = \mathbf{1}_{n\times n}$$

$$\mathbf{A}\mathbf{A}^{+} = \mathbf{U}\,\boldsymbol{\Sigma}\,\underbrace{\mathbf{V}^{Tr}\,\mathbf{V}}_{\mathbf{1}}\,\boldsymbol{\Sigma}^{+}\,\mathbf{U}^{Tr} = \mathbf{U}\,\underbrace{\boldsymbol{\Sigma}\,\boldsymbol{\Sigma}^{+}}_{\tilde{\mathbf{1}}}\,\mathbf{U}^{Tr} = \mathbf{U}\tilde{\mathbf{1}}\mathbf{U}^{Tr} = \tilde{\mathbf{1}}_{m\times m}$$

$$\tilde{\mathbf{1}} = \begin{pmatrix} \mathbf{1}_{n\times n} & \mathbf{0}_{n\times(m-n)} \\ \mathbf{0}_{(m-n)\times n} & \mathbf{0}_{(m-n)\times(m-n)} \end{pmatrix}_{m\times m}$$

Singular value decomposition of rectangular matrix $\mathbf{A}_{m \times n}$

To be translated

Zastosowania SVD

- Przybliżanie macierzy przez macierz o mniejszym rzędzie:

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \sigma_1 \boldsymbol{E}_1 + \sigma_2 \boldsymbol{E}_2 + \ldots + \sigma_n \boldsymbol{E}_n$$

Każda macierz $\boldsymbol{E}_i = \underline{u}_i \boldsymbol{v}_i^T$ jest rzędu 1.

Zwarte przybliżenie macierzy $\boldsymbol{A}$ – suma z pominięciem wyrazów odpowiadających małym wartościom σ_i.

Jeśli $\boldsymbol{A}$ jest przybliżona przez sumę zbudowaną przy pomocy k największych wartości szczególnych, to otrzymujemy przybliżenie $\boldsymbol{A}$ najlepsze w sensie normy Frobeniusa (norma euklidesowa macierzy traktowanej jako wektor w przestrzeni $\mathcal{R}^{mn}$).

Takie przybliżenie jest przydatne przy przetwarzaniu obrazów, kompresji danych, kryptografii, itp.

Method for SVD of the matrix $\mathbf{A}_{m\times n}$, where $m \geqslant n$

$$\mathbf{A}_{m\times n} = \mathbf{U}_{m\times m}\mathbf{\Sigma}_{m\times n}\mathbf{V}^{Tr}_{n\times n}$$

1. Perform decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $\mathbf{P}$ and $\mathbf{Q}$ are orthogonal matrices, whereas $\mathbf{J}$ is the two-diagonal matrix
2. Perform SVD of the matrix $\mathbf{J}_{m\times n} = \mathbf{X}_{m\times m}\mathbf{\Sigma}_{m\times n}\mathbf{Y}^{Tr}_{n\times n}$, where $\mathbf{X}$ and $\mathbf{Y}$ are orthogonal matrices; matrix $\mathbf{J}$ possesses the same singular values as matrix $\mathbf{A}$
3. Calculate orthogonal matrices $\mathbf{U}$ and $\mathbf{V}$

$$\begin{aligned}\mathbf{A} = \mathbf{PJQ}^{Tr} &= \mathbf{P}(\mathbf{X\Sigma Y}^{Tr})\mathbf{Q}^{Tr} \\ &= (\mathbf{PX})\mathbf{\Sigma}(\mathbf{QY})^{Tr},\end{aligned}$$

thus

$$\mathbf{U} = \mathbf{PX} \qquad \mathbf{V} = \mathbf{QY}$$

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

Two-diagonal matrix

$$J = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & \cdot & \cdot & \cdot & 0 \\ & \alpha_2 & \beta_2 & 0 & \cdot & \cdot & \cdot \\ & 0 & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \\ & & & & & \cdot & \beta_{n-1} \\ & & & & & & \alpha_n \\ & & & 0 & & & \end{pmatrix} \begin{matrix} \\ \\ \\ \\ \\ \\ \\ \}\,(m-n)\times n \end{matrix}.$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

Procedure uses Hausholder matrices

- We construct consecutive matrices $\mathbf{A}^{(1)}$, $\mathbf{A}^{(3/2)}$, ... $\mathbf{A}^{(k)}$, $\mathbf{A}^{(k+1/2)}$, ... $\mathbf{A}^{(n)}$, $\mathbf{A}^{(n+1/2)}$

$$\mathbf{A}^{(1)} = \mathbf{A}$$
$$\mathbf{A}^{(k+1/2)} = \mathbf{P}^{(k)}\mathbf{A}^{(k)}, \quad k = 1, 2, \ldots, n$$
$$\mathbf{A}^{(k+1)} = \mathbf{A}^{(k+1/2)}\mathbf{Q}^{(k)}, \quad k = 1, 2, \ldots, n-1, \text{ in factupto } n-2.$$

Note that $\mathbf{J} = \mathbf{A}^{(n+1/2)}$, but $\mathbf{J}$ can be cinstructed in the other way...

- Symmetric and orthogonal Hauseholder matrices $\mathbf{P}^{(k)}$ and $\mathbf{Q}^{(k)}$

$$\mathbf{P}^{(k)} = \mathbf{1} - 2\mathbf{x}^{(k)}(\mathbf{x}^{(k)})^{Tr}, \quad (\mathbf{x}^{(k)})^{Tr}\mathbf{x}^{(k)} = 1$$
$$\mathbf{Q}^{(k)} = \mathbf{1} - 2\mathbf{y}^{(k)}(\mathbf{y}^{(k)})^{Tr}, \quad (\mathbf{y}^{(k)})^{Tr}\mathbf{y}^{(k)} = 1$$

are constructed in order to make zeros in the columns and rows of $\mathbf{A}^{(k+1/2)}$ and $\mathbf{A}^{(k+1)}$, respectively, i.e.

$$\mathbf{P}^{(k)}: \quad A^{(k+1/2)}_{ik} = 0, \quad i = k+1, \ldots, m$$
$$\mathbf{Q}^{(k)}: \quad A^{(k+1)}_{kj} = 0, \quad j = k+2, \ldots, n$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

Almost two-diagonal matrix

$$A^{(k+1)} = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & \cdot & \cdot & & & & & \\ 0 & \alpha_2 & \beta_2 & 0 & \cdot & & & & & \\ \cdot & 0 & \cdot & \cdot & \cdot & & & \mathbf{0} & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & & & \\ & & & & \alpha_k & \beta_k & & & & \\ & & & & & x & x & \cdot & \cdot & \cdot \\ & & \mathbf{0} & & & x & x & \cdot & \cdot & \cdot \\ & & & & & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & & & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

Calculation of the unit vector $\mathbf{x}^{(k)}$ and the diagonal element α_k

$$s_k = \sqrt{\sum_{i=k}^{m} |A^{(k)}_{ik}|^2}$$

$$\alpha_k = -s_k \,\mathrm{sign}(A^{(k)}_{kk})$$

$$x^{(k)}_i = 0, \quad i < k$$

$$x^{(k)}_k = \sqrt{\frac{1}{2}\left(1 + \frac{|A^{(k)}_{kk}|}{s_k}\right)}$$

$$x^{(k)}_i = c_k\, A^{(k)}_{i,k}, \quad i = k+1, \ldots, m$$

where

$$c_k = \frac{\mathrm{sign}(A^{(k)}_{kk})}{2 s_k\, x^{(k)}_k}$$

If $s_k = 0$, then $\alpha_k = 0$ i $\mathbf{x}^{(k)} = \mathbf{0}$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

Calculation of the unit vector $\mathbf{y}^{(k)}$ and the off-diagonal element β_k

$$t_k = \sqrt{\sum_{j=k+1}^{n} |A_{kj}^{(k+1/2)}|^2}$$

$$\beta_k = -t_k \,\mathrm{sign}(A_{k,k+1}^{(k+1/2)})$$

$$y_j^{(k)} = 0, \quad j \leqslant k$$

$$y_{k+1}^{(k)} = \sqrt{\frac{1}{2}\left(1 + \frac{|A_{k,k+1}^{(k+1/2)}|}{t_k}\right)}$$

$$y_j^{(k)} = d_k\, A_{k,j}^{(k+1/2)}, \quad j = k+2, \ldots, n$$

where

$$d_k = \frac{\mathrm{sign}(A_{k,k+1}^{(k+1/2)})}{2t_k\, y_{k+1}^{(k)}}$$

If $t_k = 0$, then $\beta_k = 0$ i $\mathbf{y}^{(k)} = \mathbf{0}$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

$$
\begin{aligned}
\mathbf{A}^{(1)} &= \mathbf{A} \\
\mathbf{A}^{(k+1/2)} &= \mathbf{P}^{(k)}\mathbf{A}^{(k)}, \quad k = 1, 2, \ldots, n \\
\mathbf{A}^{(k+1)} &= \mathbf{A}^{(k+1/2)}\mathbf{Q}^{(k)}, \quad k = 1, 2, \ldots, n-1. \\
\mathbf{A}^{(n+1/2)} &= \mathbf{J}
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\mathbf{A}^{(3/2)} &= \mathbf{P}^{(1)}\mathbf{A}^{(1)} \\
\mathbf{A}^{(2)} &= \mathbf{P}^{(1)}\mathbf{A}^{(1)}\mathbf{Q}^{(1)} \\
\mathbf{A}^{(5/2)} &= \mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}^{(1)}\mathbf{Q}^{(1)} \\
\mathbf{A}^{(3)} &= \mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}^{(1)}\mathbf{Q}^{(1)}\mathbf{Q}^{(2)} \\
&\vdots \\
\mathbf{A}^{(n+1/2)} &= \mathbf{P}^{(n)}\ldots\mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}^{(1)}\mathbf{Q}^{(1)}\mathbf{Q}^{(2)}\ldots\mathbf{Q}^{(n-1)}
\end{aligned}
$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

$$\mathbf{A}^{(1)} = \mathbf{A}$$
$$\mathbf{A}^{(k+1/2)} = \mathbf{P}^{(k)}\mathbf{A}^{(k)}, \quad k = 1, 2, \ldots, n$$
$$\mathbf{A}^{(k+1)} = \mathbf{A}^{(k+1/2)}\mathbf{Q}^{(k)}, \quad k = 1, 2, \ldots, n-1.$$
$$\mathbf{A}^{(n+1/2)} = \mathbf{J}$$

$$\Downarrow$$

$$\left(\mathbf{P}^{(n)}\right)^{Tr} \mid \quad \mathbf{J} = \mathbf{P}^{(n)}\ldots\mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}\mathbf{Q}^{(1)}\mathbf{Q}^{(2)}\ldots\mathbf{Q}^{(n-1)} \quad \mid \left(\mathbf{Q}^{(n-1)}\right)^{Tr}$$
$$\left(\mathbf{P}^{(n-1)}\right)^{Tr} \mid \quad \mathbf{P}^{(n)}\mathbf{J}\mathbf{Q}^{(n-1)} = \mathbf{P}^{(n-1)}\ldots\mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}\mathbf{Q}^{(1)}\mathbf{Q}^{(2)}\ldots\mathbf{Q}^{(n-2)} \quad \mid \left(\mathbf{Q}^{(n-2)}\right)^{Tr}$$
$$\mathbf{P}^{(n-1)}\mathbf{P}^{(n)}\mathbf{J}\mathbf{Q}^{(n-1)}\mathbf{Q}^{(n-2)} = \mathbf{P}^{(n-2)}\ldots\mathbf{P}^{(2)}\mathbf{P}^{(1)}\mathbf{A}\mathbf{Q}^{(1)}\mathbf{Q}^{(2)}\ldots\mathbf{Q}^{(n-3)}$$
$$\vdots$$
$$\mathbf{P}^{(2)}\ldots\mathbf{P}^{(n-1)}\mathbf{P}^{(n)}\mathbf{J}\mathbf{Q}^{(n-1)}\mathbf{Q}^{(n-2)}\ldots\mathbf{Q}^{(2)} = \mathbf{P}^{(1)}\mathbf{A}\mathbf{Q}^{(1)}$$
$$\underbrace{\mathbf{P}^{(1)}\mathbf{P}^{(2)}\ldots\mathbf{P}^{(n-1)}\mathbf{P}^{(n)}}_{\mathbf{P}}\,\mathbf{J}\,\underbrace{\mathbf{Q}^{(n-1)}\mathbf{Q}^{(n-2)}\ldots\mathbf{Q}^{(2)}\mathbf{Q}^{(1)}}_{\mathbf{Q}^{Tr}} = \mathbf{A}$$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

Decomposition $\mathbf{A}_{m\times n} = \mathbf{P}_{m\times m}\mathbf{J}_{m\times n}\mathbf{Q}^{Tr}_{n\times n}$, where $m \geqslant n$

$$\mathbf{A}^{(1)} = \mathbf{A}$$

$$\mathbf{A}^{(k+1/2)} = \mathbf{P}^{(k)}\mathbf{A}^{(k)}, \quad k = 1, 2, \ldots, n$$

$$\mathbf{A}^{(k+1)} = \mathbf{A}^{(k+1/2)}\mathbf{Q}^{(k)}, \quad k = 1, 2, \ldots, n-1.$$

$$\mathbf{A}^{(n+1/2)} = \mathbf{J}$$

$$\Downarrow$$

Orthogonal matrices

$$\mathbf{P} = \mathbf{P}^{(1)}\,\mathbf{P}^{(2)}\ldots\mathbf{P}^{(n)}$$

$$\mathbf{Q}^{Tr} = \mathbf{Q}^{(n-1)}\ldots\mathbf{Q}^{(2)}\,\mathbf{Q}^{(1)}$$

In addition to $\mathbf{x}^{(k)}$ and $\mathbf{y}^{(k)}$ we have also calculated digonal α_k elements and off-diagonal elements β_k of two-diagonal matrix $\mathbf{J}$

G. Golub, W. Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, J. SIAM Numer. Anal. B 2, 205-224 (1965).

SVD of two-diagonal matrix $\mathbf{J}_{m\times n} = \mathbf{X}_{m\times m}\mathbf{\Sigma}_{m\times n}\mathbf{Y}^{Tr}_{n\times n}$

1. Find eigenvalues λ_i of the symmetric three-diagonal matrix $\mathbf{K}_{n\times n} = \mathbf{J}^{Tr}\mathbf{J}$, where $\lambda_{n-i+1} = \sigma_i^2$ and $\sigma_1 \geqslant \sigma_2 \geqslant \ldots \geqslant \sigma_n$
2. Find eigenvectors $\mathbf{y}_i$ of matrix $\mathbf{K}$, where $\mathbf{K}\mathbf{y}_i = \sigma_i^2\mathbf{y}_i$; $\mathbf{y}_i$ is i-th column of the matrix $\mathbf{Y}$
   (zobacz zad. 9)
3. Find first n columns $\mathbf{x}_j$ of matrix $\mathbf{X}$

$$\mathbf{x}_j = \frac{1}{\sigma_j}\mathbf{J}\,\mathbf{y}_j, \quad \sigma_j > 0$$

There may be some problems in 2. and 3., when $\sigma_j \sim 0$...

Eigenvalues of symmetric and three-diagonal matrix $\mathbf{K}$

Symmetric and three-diagonal matrix

$$\mathbf{K}_{n\times n} = \begin{pmatrix} c_1 & b_2 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ b_2 & c_2 & b_3 & 0 & \dots & \dots & \dots & \dots & 0 \\ 0 & b_3 & c_3 & b_4 & 0 & \dots & \dots & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ 0 & \dots & 0 & b_k & c_k & b_{k+1} & 0 & \dots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & 0 & b_{n-2} & c_{n-2} & b_{n-1} & 0 \\ 0 & \dots & \dots & \dots & \dots & 0 & b_{n-1} & c_{n-1} & b_n \\ 0 & \dots & \dots & \dots & \dots & \dots & 0 & b_n & c_n \end{pmatrix}$$

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

Eigenvalues of symmetric and three-diagonal matrix **K**

Denotations

- $\mathbf{c} = [c_1, c_2, \ldots, c_n]^{Tr}$ - vector containing diagonal elements of matrix $\mathbf{K}_{n\times n}$
- $\mathbf{b} = [0, b_2, \ldots, b_n]^{Tr}$ - vector containing off-diagonal elements of matrix $\mathbf{K}_{n\times n}$

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

Eigenvalues of symmetric and three-diagonal matrix **K**

Theorem:
Eigenvalues λ_i of matrix **K** are within range $[\lambda_{min}, \lambda_{max}]$, where $(b_1 = b_{n+1} = 0)$

$$\lambda_{min} = \min_{i=1,\ldots,n} \left[c_i - (|b_i| + |b_{i+1}|)\right]$$
$$\lambda_{max} = \max_{i=1,\ldots,n} \left[c_i + (|b_i| + |b_{i+1}|)\right],$$

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

Eigenvalues of symmetric and three-diagonal matrix **K**

Theorem (∼Sturm):
We have (∼Sturm) sequence

$$q_1(\lambda) = c_1 - \lambda$$
$$q_i(\lambda) = (c_i - \lambda) - b_i^2/q_{i-1}(\lambda), \quad i = 2, \ldots, n$$

Quantity $a(\lambda)$ is the number of negativeelements of the sequence $\{q_i(\lambda)\}_{i=1}^n$. At the same time $a(\lambda)$ is equal to the number of eigenvalues of matrix **K** smaller than λ

Remark: if $q_{i-1} = 0$, then $q_i(\lambda) = (c_i - \lambda) - |b_i|/\epsilon_{mach}$, where ϵ_{mach} is the smallest number ϵ for which $1 + \epsilon > 1$.

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

Eigenvalues of symmetric and three-diagonal matrix $\mathbf{K}$

Bisection that finds eigenvalues $\lambda_k \in [\lambda_{min}, \lambda_{max}]$,
$k = n, n-1, \ldots, 1$ of matrix $\mathbf{K}$. Let $\lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$.
At the beginning $x_l = \lambda_{min}$, $x_u = \lambda_{max}$

1. If $x_u - x_l < \epsilon$, then we stop bisection
2. Calculate the middle point (bisection) $x = (x_l + x_u)/2$
3. If $a(x) < k$ then $x_l = x$, otherwise $x_u = x$

Remarks:

- It is possible to calculate **precisely** all the eigenvalues [1]
- As a byproduct of calculation of a given eigenvalues, we can also collect the information about the positions of the other eigenvalues, i.e. we may shrink the ranges in which the other eigenvalues are to be found (see next page)

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

[1] Well, there are some problems for $\lambda_k \sim 0$

Eigenvalues of symmetric and three-diagonal matrix $\mathbf{K}$

Modified bisection

- Vector $\mathbf{w} = [w_1, \ldots, w_n]^{Tr}$ contains current lower bounds of the eigenvalues
- Vector $\mathbf{x} = [x_1, \ldots, x_n]^{Tr}$ contains current upper bounds of the eigenvalues, in the end of the procedure it will contain eigenvalues
- At the beginning $w_i = \lambda_{min}$, $x_i = \lambda_{max}$.
- Bisection for $k = n, \ldots, 1$, where $\lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$.
  1. $x_l = w_k$, $x_u = x_k$, if $x_u - x_l < \epsilon$, then we stop
  2. Calculate the middle point (bisection) $x_k = (x_l + x_u)/2$
  3. If $a(x_k) < k$ then $x_l = x_k$, otherwise $x_u = x_k$.
     By the way if $a(x_k) < k$, then x_k is also the upper bound for the eigenvalues $\lambda_1, \ldots, \lambda_a$, and at the same time it is the lower bound for eigenvalues $\lambda_{a+1}, \lambda_{a+2} \ldots, \lambda_k$.
     - It means that for $i = 1, \ldots, a$ if $x_i > x_k$, then $x_i = x_k$.
     - It also means that for $i = a + 1, \ldots, k$ if $w_i < x_k$, then $w_i = x_k$.

W. Barth, R. S. Martin and J. H. Wilkinson, *Calculation of the Eigenvalues of a Symmetric Tridiagonal Matrix by the Method of Bisection*, Numerische Mathematik 9, 386-393 (1967) .

TO DO

1. Read from the input real matrix $\mathbf{A}_{m\times n}$, where $m > n$
2. Calculate matrices $\mathbf{U}_{m\times m}$, $\mathbf{\Sigma}_{m\times n}$ $\mathbf{V}_{n\times n}$
3. Check $\mathbf{A} = \mathbf{U\Sigma V}^{Tr}$
4. Calculate pseudo-inverse matrix $\mathbf{A}^{+} = \mathbf{V\Sigma}^{+}\mathbf{U}^{Tr}$, where

$$\mathbf{A}^{+}_{n\times m},\ \mathbf{V}_{n\times n},\ \mathbf{\Sigma}^{+}_{n\times m},\ \mathbf{U}^{Tr}_{m\times m}$$

5. Check $\mathbf{A}^{+}\mathbf{A} = \mathbf{1}_{n\times n}$ ($\mathbf{AA}^{+} = \mathbf{1}_{m\times m}$?), also check $\mathbf{\Sigma}^{+}\mathbf{\Sigma}$ and $\mathbf{\Sigma\Sigma}^{+}$)
6. Note that for the most of the applications we need only at most first n columns of $\mathbf{U}$ matrix

Examples

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}$$

$$\mathbf{A}_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \\ 4 & 6 & 5 \end{pmatrix} \quad \mathbf{A}_3 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \\ 4 & 5 & 6 \end{pmatrix}$$

$$\mathbf{A}_4 = \begin{pmatrix} 21 & 0 & 770 & 0 & 50666 \\ 0 & 770 & 0 & 50666 & 0 \\ 770 & 0 & 50666 & 0 & 3956810 \\ 0 & 50666 & 0 & 3956810 & 0 \\ 50666 & 0 & 3956810 & 0 & 335462666 \end{pmatrix}$$

Dodatek: Równość wartości szczególnych macierzy $\mathbf{J}$ i $\mathbf{A}$

Mamy następujące rozkłady macierzy

$$\mathbf{A} = \mathbf{U\Sigma V}^{Tr}, \qquad \mathbf{A} = \mathbf{PJQ}^{Tr}, \qquad \mathbf{J} = \mathbf{X\Sigma' Y}^{Tr}.$$

Pokażemy, że $\mathbf{\Sigma} = \mathbf{\Sigma}'$:

$$\mathbf{P}^{Tr} \times \mid \quad \mathbf{PJQ}^{Tr} = \mathbf{U\Sigma V}^{Tr} \quad \mid \times \mathbf{Q}$$

$$\mathbf{J} = \mathbf{P}^{Tr}\mathbf{U\Sigma V}^{Tr}\mathbf{Q}$$

Ponieważ $\mathbf{P}^{Tr}\mathbf{U}$ i $\mathbf{V}^{Tr}\mathbf{Q}$ są macierzami ortogonalnymi, to uzyskaliśmy rozkład SVD macierzy $\mathbf{J}$, więc z jednoznaczności[1] SVD mamy w szczególności $\mathbf{\Sigma}' = \mathbf{\Sigma}$.

[1] SVD nie jest w pełni jednoznaczny, ale dla danej macierzy mamy na pewno jeden zbiór wartości szczególnych.

Dodatek: „Naturalna” metoda rozkładu SVD macierzy $\mathbf{A}_{m\times n}$

„Naturalna” metoda: rozwiązać zagadnienie własne dla mniejszej macierzy symetrycznej

1. $m \geqslant n : \mathbf{A}^{Tr}\mathbf{A}\,\mathbf{v}_j = \sigma_j^2\,\mathbf{v}_j, \quad j = 1, \ldots, n$
2. $m < n : \ \mathbf{A}\mathbf{A}^{Tr}\,\mathbf{u}_k = \sigma_k^2\,\mathbf{u}_k, \quad k = 1, \ldots, m$

Problemy

- Najmniejsze wartości własne, a w konsekwencji σ_i, są narażone na **duże błędy numeryczne**
- Metoda QR ma problem ze zbieżnością, gdy $\sigma_i = \sigma_{i+1}$
- W metodzie QR wykorzystującej ortogonalizację Grama-Schmidta problem, gdy $\sigma_i \approx 0 \Rightarrow$ rozwiązać zagadnienie własne dla $\mathbf{A}^{Tr}\mathbf{A} - s\mathbf{1}$ (albo $\mathbf{A}\mathbf{A}^{Tr} - s\mathbf{1}$), gdzie np. $s = 1$; lepiej zastosować inną metodę rozkładu QR np. używając transformacji Householdera
- Ortogonalizacja Grama-Schmidta (GS) ma swoje dodatkowe problemy... zob. zmodyfikowana metoda GS (MGS)

Dodatek: Rozkład SVD macierzy prostokątnych z wykorzystaniem metody QR

Rozkład SVD macierzy prostokątnej

$$\mathbf{A}_{N\times M} = \mathbf{U}_{N\times N}\mathbf{\Sigma}_{N\times M}\mathbf{V}^{Tr}_{M\times M}$$

Wyznaczamy mniejszą z macierzy ortogonalnych **V** albo **U**, tzn.

1° $N \geqslant M$

$$\left(\mathbf{A}^{Tr}\mathbf{A}\right)\mathbf{v}_k = \sigma_k^2\mathbf{v}_k,\ \ k = 1, ..., M$$

$$\Downarrow$$

$$\mathbf{V} = [\mathbf{v}_1\ \mathbf{v}_2\ \dots\ \mathbf{v}_M]$$

2° $N < M$

$$\left(\mathbf{A}\mathbf{A}^{Tr}\right)\mathbf{u}_j = \sigma_j^2\mathbf{u}_j,\ \ j = 1, ..., N$$

$$\Downarrow$$

$$\mathbf{U} = [\mathbf{u}_1\ \mathbf{u}_2\ \dots\ \mathbf{u}_N]$$

Kolejność kolumn w **V** (albo **U**) jest wyznaczona relacją

$$\sigma_1 > \sigma_2 > \dots > \sigma_r, \quad r = \min(N, M)$$

Jeżeli powyższe równanie własne macierzy symetrycznych $\mathbf{A}^{Tr}\mathbf{A}$ (albo $\mathbf{A}\mathbf{A}^{Tr}$) rozwiązujemy metodą QR z ortogonalizacją Grama-Schmidta, to dla macierzy symetrycznych, kolumny macierzy ortogonalnej $\mathbf{Q} = \mathbf{Q}_1\mathbf{Q}_2 \dots \mathbf{Q}_{k_{max}}$, są wektorami własnymi rozpatrywanej macierzy symetrycznej, tzn. w naszym przypadku $\mathbf{Q} = \mathbf{V}$ (albo $\mathbf{Q} = \mathbf{U}$) o ile kolumny macierzy **Q** zostały przesortowane tak, że $\sigma_1 > \sigma_2 > \sigma_3 > \dots > \sigma_r$. Macierze ortogonalne $\mathbf{Q}_k$ pochodzą z k-tej iteracji metody QR znajdowania wartości własnych macierzy kwadratowych.

Dodatek: Rozkład SVD macierzy prostokątnych z wykorzystaniem metody QR

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Wyznaczamy mniejszą z macierzy ortogonalnych **V** albo **U**, tzn.

1° $N \geqslant M$

$$\left(\mathbf{A}^{Tr}\mathbf{A}\right)\mathbf{v}_k = \sigma_k^2\mathbf{v}_k,\ \ k = 1, ..., M$$

$$\Downarrow$$

$$\mathbf{V} = [\mathbf{v}_1\ \mathbf{v}_2\ ...\ \mathbf{v}_M]$$

2° $N < M$

$$\left(\mathbf{A}\mathbf{A}^{Tr}\right)\mathbf{u}_j = \sigma_j^2\mathbf{u}_j,\ \ j = 1, ..., N$$

$$\Downarrow$$

$$\mathbf{U} = [\mathbf{u}_1\ \mathbf{u}_2\ ...\ \mathbf{u}_N]$$

Kolejność kolumn w **V** (albo **U**) jest wyznaczona relacją

$$\sigma_1 > \sigma_2 > ... > \sigma_r, \quad r = \min(N, M)$$

Jeżeli powyższe równanie własne macierzy symetrycznych $\mathbf{A}^{Tr}\mathbf{A}$ (albo $\mathbf{A}\mathbf{A}^{Tr}$) rozwiązujemy metodą QR z ortogonalizacją Grama-Schmidta, to możemy napotkać na następujące trudności

1. $\sigma_k = \sigma_{k+1}$ $\Rightarrow$ mogą wystąpić problemy ze zbieżnością metody QR
2. $\sigma_r \approx 0 \Rightarrow$ ortogonalizacja Grama-Schmidta będzie narażona na duże błędy numeryczne lub zupełnie zawiedzie
   Wskazówka: rozwiązać równanie własne dla $\mathbf{A}^{Tr}\mathbf{A} + s\mathbf{1}$ (albo $\mathbf{A}\mathbf{A}^{Tr} + s\mathbf{1}$), gdzie np. $s \sim 1$

Dodatek: Wyznaczenie drugiej (większej) macierzy ortogonalnej

Rozkład SVD macierzy prostokątnej

$$\mathbf{A}_{N\times M} = \mathbf{U}_{N\times N}\mathbf{\Sigma}_{N\times M}\mathbf{V}^{Tr}_{M\times M}$$

1° $N \geqslant M$

Obliczamy M początkowych kolumn macierzy **U** wg wzoru

$$\mathbf{u}_i = \frac{1}{\sigma_i}\mathbf{A}\mathbf{v}_i, \quad \sigma_i > 0$$

$$\mathbf{A}^{Tr}_{M\times N} = \mathbf{V}_{M\times M}\mathbf{\Sigma}^{Tr}_{M\times N}\mathbf{U}^{Tr}_{N\times N}$$

2° $N < M$

Obliczamy N początkowych kolumn macierzy **V** wg wzoru

$$\mathbf{v}_i = \frac{1}{\sigma_i}\mathbf{A}^{Tr}\mathbf{u}_i, \quad \sigma_i > 0$$

Co się dzieje, gdy $\sigma_r = 0$ (lub $\sigma_r \approx 0$) dla $r \leqslant \min(N, M)$?

$$\sigma_r\mathbf{u}_r = \mathbf{A}\mathbf{v}_r, \quad \sigma_r = 0$$

$$\Updownarrow$$

$$\mathbf{A}\mathbf{v}_r = \mathbf{0}$$

$$\sigma_r\mathbf{v}_r = \mathbf{A}^{Tr}\mathbf{u}_r, \quad \sigma_r = 0$$

$$\Updownarrow$$

$$\mathbf{A}^{Tr}\mathbf{u}_r = \mathbf{0}$$

Kolumna $\mathbf{u}_r$ (lub $\mathbf{v}_r$) wyznaczamy z warunków dla $i = 1, 2, ..., r-1$

$$\mathbf{u}_i^{Tr}\mathbf{u}_r = \delta_{ir}$$

$$\mathbf{v}_i^{Tr}\mathbf{v}_r = \delta_{ir}$$

Dodatek: Wyznaczenie drugiej (większej) macierzy ortogonalnej

Rozkład SVD macierzy prostokątnej

$$\mathbf{A}_{N\times M} = \mathbf{U}_{N\times N}\mathbf{\Sigma}_{N\times M}\mathbf{V}^{Tr}_{M\times M}$$

$1^\circ \;\; N \geqslant M$

Obliczamy M początkowych kolumn macierzy **U** wg wzoru

$$\mathbf{u}_i = \frac{1}{\sigma_i}\mathbf{A}\mathbf{v}_i, \quad \sigma_i > 0$$

$$\mathbf{A}^{Tr}_{M\times N} = \mathbf{V}_{M\times M}\mathbf{\Sigma}^{Tr}_{M\times N}\mathbf{U}^{Tr}_{N\times N}$$

$2^\circ \;\; N < M$

Obliczamy N początkowych kolumn macierzy **V** wg wzoru

$$\mathbf{v}_i = \frac{1}{\sigma_i}\mathbf{A}^{Tr}\mathbf{u}_i, \quad \sigma_i > 0$$

Kolumny $\mathbf{u}_i$ (lub $\mathbf{v}_i$), gdzie $i > \min(N, M)$, wyznaczamy z warunków dla $j = 1, 2, ..., i-1$

$$\mathbf{u}_j^{Tr}\mathbf{u}_i = \delta_{ji}, \;\; i = M+1, ..., N$$

$$\mathbf{v}_j^{Tr}\mathbf{v}_i = \delta_{ji}, \;\; i = N+1, ..., M$$

Dodatek: „Uzupełnienie" macierzy ortogonalnej

- $\mathbf{Q}$ jest macierzą kwadratową $n \times n$
- Znamy $m < n$ początkowych kolumn $\mathbf{q}_i$, gdzie $i = 1, \ldots, m$, macierzy $\mathbf{Q}$ spełniających warunki

$$\mathbf{q}_i^{Tr}\mathbf{q}_j = \delta_{ij}, \quad i, j = 1, 2, .., m$$

- Chcemy, żeby cała macierz była ortogonalna tzn., że wszystkie kolumny są wzajemnie otrogonalne i unormowane do 1
  1. Wypełniamy (nieznane) kolumny $\mathbf{q}_k$, gdzie $k > m$ liczbami (pseudo)losowymi, aby uniknąć liniowych zależności (co zrobić jeżeli okaże się, że dana kolumna $\mathbf{q}_k$, gdzie $k > m$, jest jednak liniowo zależna?)
  2. Kolejno dla kolumn $\mathbf{q}_k$, gdzie $k = m + 1, \ldots, n$, dokonujemy ortogonalizacji Grama-Schmidta, tzn.

$$\mathbf{q}'_k = \mathbf{q}_k - \sum_{i=1}^{k-1} (\mathbf{q}_k^{Tr}\mathbf{q}_i)\mathbf{q}_i \qquad \text{ortogonalizacja}$$

$$\mathbf{q}''_k = \frac{\mathbf{q}'_k}{\|\mathbf{q}'_k\|_2} \qquad \text{normalizacja}$$

gdzie

$$\|\mathbf{q}'_k\|_2 = \sqrt{\mathbf{q}'^{Tr}_k \mathbf{q}'_k} = \sqrt{\sum_{i=1}^{n} (q'_{ik})^2}$$