Singular Value Decomposition
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1. Introduction

Singular value decomposition (SVD) is a matrix factorization technique. It can be done for both real and complex matrices. Singular value decomposition has a lot of applications in machine learning. It can be used to detect hidden structures in data and also determing the similarity of two samples. SVD is commonly used in principal component analysis.

2. Mathematical Formulation

In machine learning, we will mostly be dealing with real matrices. Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be a real matrix. According to the singular value decomposition theorem, there always exists a unique decomposition of $\mathbf{A}$ of the form

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top \tag{2.1}$$

where $\mathbf{U} \in \mathbb{R}^{m \times r}$ is the left singular matrix, $\mathbf{V} \in \mathbb{R}^{n \times r}$ is the right singular matrix and $\mathbf{\Sigma} \in \mathbb{R}^{r \times r}$ is a diagonal matrix containing the singular values along its diagonal. Here r is the rank of $\mathbf{A}$.

$\mathbf{U}$ and $\mathbf{V}$ are column orthonormal, i.e.,

$$\mathbf{U}^\top\mathbf{U} = \mathbf{I}_r \tag{2.2}$$

$$\mathbf{V}^\top\mathbf{V} = \mathbf{I}_r \tag{2.3}$$

Moreover, the entries of $\mathbf{\Sigma}$ (singular values) are positive and are in decreasing order, i.e.,

$$\text{If } \mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_r \end{pmatrix} \tag{2.4}$$

$$\text{then } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0 \tag{2.5}$$

Now,

$$\mathbf{A}\mathbf{A}^\top = \left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)\left(\mathbf{V}\mathbf{\Sigma}^\top\mathbf{U}^\top\right) \tag{2.6}$$

$$= \mathbf{U}\mathbf{\Sigma}\left(\mathbf{V}^\top\mathbf{V}\right)\mathbf{\Sigma}\mathbf{U}^\top \tag{2.7}$$

$$= \mathbf{U}\mathbf{\Sigma}^2\mathbf{U}^\top \tag{2.8}$$

$$\implies \mathbf{A}\mathbf{A}^\top\mathbf{U} = \mathbf{U}\mathbf{\Sigma}^2 \tag{2.9}$$

$$\text{Similarly, } \mathbf{A}^\top\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{\Sigma}^2 \tag{2.10}$$

Thus, the columns of $\mathbf{U}$ are the eigenvectors of $\mathbf{A}\mathbf{A}^\top$ and the columns of $\mathbf{V}$ are the eigenvectors of $\mathbf{A}^\top\mathbf{A}$. Moreover, $\mathbf{\Sigma}^2$ contains the non-zero eigenvalues of $\mathbf{A}\mathbf{A}^\top$ (which are the same as those of $\mathbf{A}^\top\mathbf{A}$) and thus, $\mathbf{\Sigma}$ contains the square roots of the non-zero eigenvalues of $\mathbf{A}\mathbf{A}^\top$ also known as the singular values of $\mathbf{A}$.

3. Questions

Let

$$\mathbf{A} = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} \tag{3.1}$$

i) Find $\mathbf{A}\mathbf{A}^\top$ and $\mathbf{A}^\top\mathbf{A}$
ii) Find the eigenvalues of the above matrices
iii) Find the eigenvectors of the above matrices
iv) Find the singular values of $\mathbf{A}$
v) Thus, write the singular value decomposition of $\mathbf{A}$

4. Answers

i)

$$\mathbf{A} = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} \tag{4.1}$$

$$\mathbf{A}^\top = \begin{pmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{pmatrix} \tag{4.2}$$

$$\mathbf{A}\mathbf{A}^\top = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} \begin{pmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{pmatrix} = \begin{pmatrix} 17 & 8 \\ 8 & 17 \end{pmatrix} \tag{4.3}$$

$$\mathbf{A}^\top\mathbf{A} = \begin{pmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} = \begin{pmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{pmatrix} \tag{4.4}$$

ii) The eigen values of $\mathbf{A}\mathbf{A}^\top$ are the solutions to

$$\begin{vmatrix} 17-\lambda & 8 \\ 8 & 17-\lambda \end{vmatrix} = 0 \tag{4.5}$$

$$\implies (17-\lambda)^2 = 8^2 \tag{4.6}$$

$$\implies 17-\lambda = \pm 8 \tag{4.7}$$

$$\implies \lambda = 25, 9 \tag{4.8}$$

Similarly, the eigen values of $\mathbf{A}^\top\mathbf{A}$ are the solutions to

$$\begin{vmatrix} 13-\lambda & 12 & 2 \\ 12 & 13-\lambda & -2 \\ 2 & -2 & 8-\lambda \end{vmatrix} = 0 \tag{4.9}$$

$$\implies \lambda = 25, 9, 0 \tag{4.10}$$

iii) The eigenvector of $\mathbf{A}\mathbf{A}^\top$ corresponding to λ is given by

$$\begin{pmatrix} 17-\lambda & 8 \\ 8 & 17-\lambda \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \mathbf{O} \tag{4.11}$$

$$\implies (17-\lambda)v_1 + 8v_2 = 0 \tag{4.12}$$

$$8v_1 + (17-\lambda)v_2 = 0 \tag{4.13}$$

$$\implies \frac{v_1}{v_2} = \frac{8}{\lambda - 17} \tag{4.14}$$

Thus, the normalized eigenvectors of $\mathbf{A}\mathbf{A}^\top$ are

$$\mathbf{v}_{\lambda=25} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad \mathbf{v}_{\lambda=9} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \tag{4.15}$$

Similarly, the normalized eigenvectors of $\mathbf{A}^\top\mathbf{A}$ (corresponding to non-zero eigenvalues) are

$$\mathbf{v}_{\lambda=25} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix} \qquad \mathbf{v}_{\lambda=9} = \frac{1}{\sqrt{18}}\begin{pmatrix}1\\-1\\4\end{pmatrix} \tag{4.16}$$

iv) The singular values of $\mathbf{A}$ are the square roots of the above obtained eigenvalues.

$$\sigma_1 = \sqrt{25} = 5 \tag{4.17}$$

$$\sigma_2 = \sqrt{9} = 3 \tag{4.18}$$

v) We can now write $\mathbf{U}, \mathbf{V}, \mathbf{\Sigma}$ as

$$\mathbf{U} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix} \tag{4.19}$$

$$\mathbf{V} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{18}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{18}}\\ 0 & \frac{4}{\sqrt{18}}\end{pmatrix} \tag{4.20}$$

$$\mathbf{\Sigma} = \begin{pmatrix}5 & 0\\ 0 & 3\end{pmatrix} \tag{4.21}$$

Therefore, the decomposition is given by

$$\begin{pmatrix}3 & 2 & 2\\ 2 & 3 & -2\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}5 & 0\\ 0 & 3\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{18}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{18}}\\ 0 & \frac{4}{\sqrt{18}}\end{pmatrix}^\top \tag{4.22}$$