Singular Value Decomposition

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Singular Value Decomposition (SVD) is a way to decompose any real matrix $A \in \mathbb{R}^{m \times n}$ into a simple form:

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

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ and $\Sigma \in \mathbb{R}^{m \times n}$ is a matrix with only diagonal values. The following proof is based on [Gun].

1 Proof of Existence

1.1 Case $n = m$

Since $A^T A$ is an $n \times n$ positive semi-definite (PSD) matrix, we can diagonalize it as

$$A^T A = V \Lambda V^T = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i \mathbf{v}_i^T = \sum_{i=1}^{n} \sigma_i^2 \mathbf{v}_i \mathbf{v}_i^T,$$

where V is an orthonormal matrix with eigenvectors of $A^T A$ as its column vectors, and Λ is a diagonal matrix with non-negative eigenvalues.

$$V = [\mathbf{v}_1 \, \mathbf{v}_2 \, \cdots \, \mathbf{v}_n]$$

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & \lambda_n \end{bmatrix}, \quad \lambda_i = \sigma_i^2 \geq 0$$

By convention, we permute the eigenvalues in descending order; that is, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

Now, consider the following vectors with m-dimension:

$$\mathbf{u}_i = \frac{A\mathbf{v}_i}{\sigma_i}, \quad 1 \leq i \leq m$$

One can check each $\mathbf{u}_i$ is a unit vector

$$\|\mathbf{u}_i\|^2 = \frac{\mathbf{v}_i^T A^T A \mathbf{v}_i}{\sigma_i^2} = \frac{\mathbf{v}_i^T (\sigma_i^2 \mathbf{v}_i)}{\sigma_i^2} = 1$$

If we define the following matrix

$$U = [\mathbf{u}_1 \, \mathbf{u}_2 \, \cdots \, \mathbf{u}_m]$$

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & \sigma_n \end{bmatrix}$$

We see

$$U = AV\Sigma^{-1} \implies A = U\Sigma V^{-1} = U\Sigma V^T$$

1.2 Case $n \neq m$

If $n \geq m$, since $\sigma_i = 0$ for all $i > m$, we may simply remove the last $n-m$ columns in Σ. The equation above becomes

$$U = AV \begin{bmatrix} \frac{1}{\sigma_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sigma_2} & & \vdots \\ \vdots & & \ddots & \\ 0 & & & \frac{1}{\sigma_m} \\ \vdots & & & \vdots \\ 0 & \cdots & & 0 \end{bmatrix} \implies A = U \begin{bmatrix} \sigma_1 & 0 & \cdots & & & 0 \\ 0 & \sigma_2 & & & & \vdots \\ \vdots & & \ddots & & & \\ 0 & \cdots & & \sigma_m & \cdots & 0 \end{bmatrix} V^T$$

If $n < m$, we can remove the last $m-n$ rows in Σ, leading to

$$U = AV \begin{bmatrix} \frac{1}{\sigma_1} & 0 & \cdots & & & 0 \\ 0 & \frac{1}{\sigma_2} & & & & \vdots \\ \vdots & & \ddots & & & \\ 0 & \cdots & & \frac{1}{\sigma_n} & \cdots & 0 \end{bmatrix} \implies A = U \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & & & \sigma_n \\ \vdots & & & \vdots \\ 0 & \cdots & & 0 \end{bmatrix} V^T$$

Note that the vectors $\{\mathbf{u}_i\}_{i>m}$ are not defined. We replace those undefined vectors by any $n-m$ independent vectors which makes $\{\mathbf{u}_i\}$ span the whole $\mathbb{R}^m$.

References

[Gun] Gregory Gundersen. *Proof of the Singular Value Decomposition*. https://gregorygundersen.com/blog/2018/12/20/svd-proof/. Accessed: 2024-09-13.