

Lecture 4 - *The Singular Value Decomposition (SVD)*

OBJECTIVE:

The SVD is a matrix factorization that has many applications:

e.g., information retrieval, least-squares problems, image processing

It is so important that we introduce it at this early stage.

◇ GEOMETRIC INTERPRETATION

The SVD is motivated by the following geometric fact:

The image of the unit sphere under any $m \times n$ matrix is a hyperellipse.

Note 1. An “ellipse” is a 2D object $\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1\right)$.

In 3D, it is called an “ellipsoid” $\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1\right)$.

The generalization to m dimensions is called a hyper-ellipse.

(Even the unit sphere in m dimensions is more accurately called a hypersphere!)

The sphere maps into the hyperellipse by stretching the sphere by (possibly zero) factors

$$\sigma_1, \sigma_2, \dots, \sigma_m$$

in orthogonal directions

$$\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_m \in \mathbb{R}^m.$$

It is convenient to take the \mathbf{u}_i to be unit vectors.

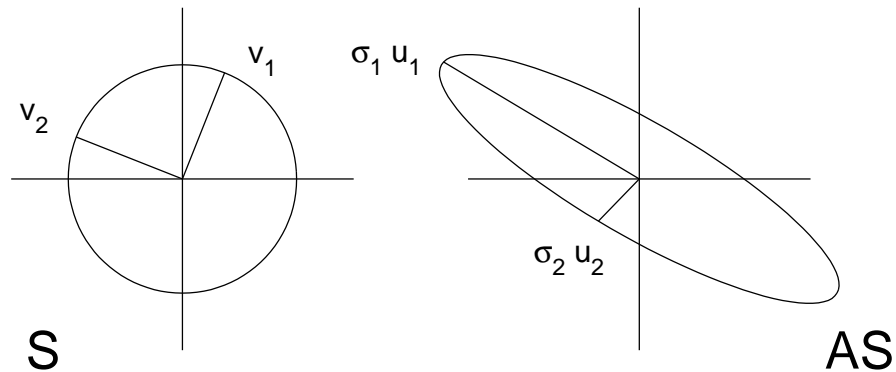
Then, the vectors $\{\sigma_i \mathbf{u}_i\}_{i=1}^m$ can be viewed as the *principal semi-axes* of the hyperellipse with lengths

$$\sigma_1, \sigma_2, \dots, \sigma_m$$

If \mathbf{A} has rank r , then exactly r of the lengths σ_i will be nonzero. In particular, if $m \geq n$, then at most n of the σ_i will be nonzero.

These facts are not obvious, but for now just assume they are true!

Here is the basic picture:



Let S be the unit sphere in \mathbb{R}^n .

Choose any $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $m \geq n$.

For simplicity, let $\text{rank}(\mathbf{A}) = n$ (full rank).

The image \mathbf{AS} is a hyperellipse in \mathbb{R}^m with the following properties:

1. The n *singular values* $\sigma_1, \sigma_2, \dots, \sigma_n$ of \mathbf{A} are the lengths of the principal semi-axes of \mathbf{AS} . By convention, we assume the σ_i are ordered in descending order.

i.e., $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$
(why $\sigma_i > 0$?)

2. The set of unit vectors $\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n\}$ are the n *left singular vectors* of \mathbf{A} . They are the directions of the principal semi-axes of \mathbf{AS} corresponding to the n singular values.

$\therefore \sigma_i \mathbf{u}_i$ is the i^{th} largest principal semi-axes of \mathbf{AS} .

3. The set of unit vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ are the n *right singular vectors* of \mathbf{A} . They are the “pre-images” of the \mathbf{u}_i numbered accordingly.

i.e., $\mathbf{A}\mathbf{v}_j = \sigma_j \mathbf{u}_j$

(why “left” and “right” will be explained below)

◇ REDUCED SVD

The equations relating the right singular values $\{\mathbf{v}_j\}$ and the left singular vectors $\{\mathbf{u}_j\}$ are

$$\mathbf{A}\mathbf{v}_j = \sigma_j\mathbf{u}_j \quad j = 1, 2, \dots, n$$

i.e.,

$$\begin{aligned} [\mathbf{A}] \left[\begin{array}{c|c|c|c} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_n \end{array} \right] \\ = \left[\begin{array}{c|c|c|c} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_n \end{array} \right] \left[\begin{array}{cccc} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{array} \right] \end{aligned}$$

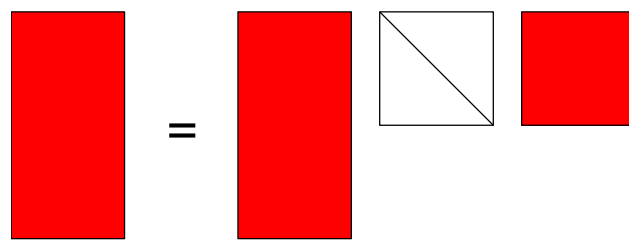
or

$$\mathbf{A}\mathbf{V} = \hat{\mathbf{U}}\hat{\mathbf{\Sigma}}$$

Note 2. $\hat{\Sigma} \in \mathbb{R}^{n \times n}$ is diagonal with positive entries.
 $\hat{\mathbf{U}} \in \mathbb{R}^{m \times n}$ with orthonormal columns.
 $\mathbf{V} \in \mathbb{R}^{n \times n}$ with orthonormal columns.
 $(\Rightarrow \mathbf{V}$ is orthogonal so $\mathbf{V}^{-1} = \mathbf{V}^T)$

$$\therefore \mathbf{A} = \hat{\mathbf{U}} \hat{\Sigma} \mathbf{V}^T$$

This factorization is called the *reduced SVD* of \mathbf{A} .
 (We'll see why "reduced" in a minute.)



\mathbf{A}
 $\hat{\mathbf{U}}$
 $\hat{\Sigma}$
 \mathbf{V}^T

◇ FULL SVD

In practice, SVD is mostly used in its reduced form. But, theoretically, there is a “full SVD” that is more standard.

The idea of the full SVD is as follows:

$\hat{\mathbf{U}}$ is made up of n orthonormal vectors in \mathbb{R}^m .

So, unless $m = n$, this cannot be a basis for \mathbb{R}^m , and $\hat{\mathbf{U}}$ cannot be orthogonal.

But, we can make $\hat{\mathbf{U}}$ orthogonal by adding $m - n$ additional orthonormal columns.

Let's suppose we do this and call the result \mathbf{U} .

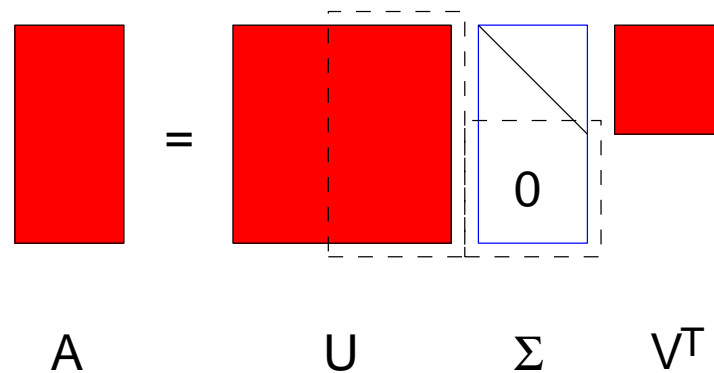
But, if we replace $\hat{\mathbf{U}}$ by \mathbf{U} , we will have to change $\hat{\Sigma}$ as well

→ for the factorization not to change, we must multiply the last $m - n$ columns of \mathbf{U} by 0.

This leads to the full SVD

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{V} \in \mathbb{R}^{n \times n}$ are both orthogonal, and $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$.



In this framework, we no longer need to assume \mathbf{A} has full rank.

If $\text{rank}(\mathbf{A}) = r < n$, only r singular vectors of \mathbf{A} are determined by the geometry of the hyperellipse and we will have to add $m - r$ orthonormal columns to \mathbf{U} and $n - r$ orthonormal columns to \mathbf{V} . $\mathbf{\Sigma}$ will have r positive diagonal entries.

Alternatively, in this case it is possible to further reduce the reduced SVD of \mathbf{A} by letting $\hat{\mathbf{U}} \in \mathbb{R}^{m \times r}$, $\hat{\mathbf{\Sigma}} \in \mathbb{R}^{r \times r}$, and $\hat{\mathbf{V}}^T \in \mathbb{R}^{r \times n}$.

◇ FORMAL DEFINITION OF SVD

Given $\mathbf{A} \in \mathbb{R}^{m \times n}$, the SVD of \mathbf{A} is a factorization of the form

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{V} \in \mathbb{R}^{n \times n}$ are orthogonal, and $\mathbf{\Sigma} \in \mathbb{R}^{n \times n}$ is “diagonal”.

Note 3. 1. *There is no assumption that $m \geq n$ or that \mathbf{A} has full rank.*

2. *All diagonal elements of $\mathbf{\Sigma}$ are non-negative and in non-increasing order:*

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0$$

where $p = \min(m, n)$

3. *$\mathbf{\Sigma}$ has the same shape as \mathbf{A} , but \mathbf{U} , \mathbf{V} are square.*

◇ EXISTENCE AND UNIQUENESS OF THE SVD

Theorem 1. *Every matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ has singular value decomposition $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$.*

Furthermore, the singular values $\{\sigma_j\}$ are uniquely determined.

If \mathbf{A} is square and $\sigma_i \neq \sigma_j$ for all $i \neq j$, the left singular vectors $\{\mathbf{u}_j\}$ and the right singular vectors $\{\mathbf{v}_j\}$ are uniquely determined to within a factor of ± 1 .