# Singular Value Decomposition

Note Title

- SVD is a matrix factorization that is useful for many applications, e.g., search engines, LS problems, tomographic image reconstruction, ...

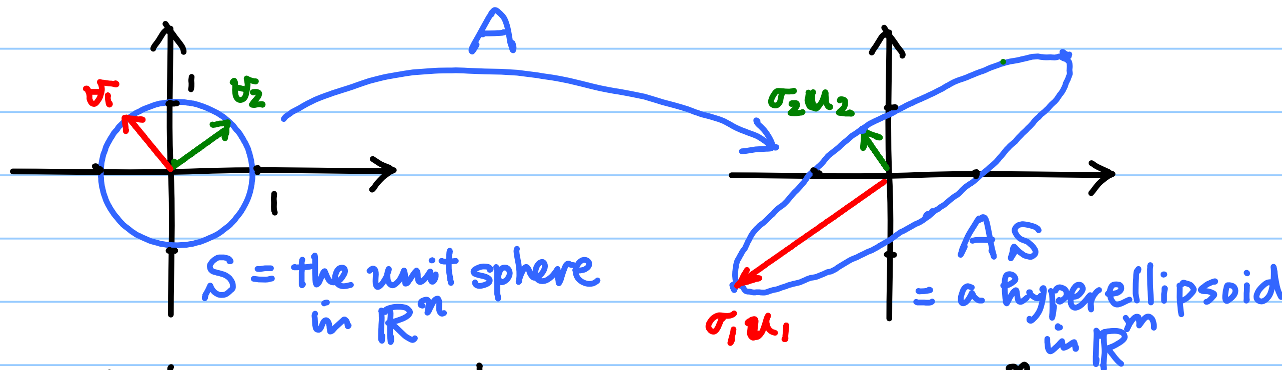
- SVD can be a concepual tool in linear algebra
  ⇒ via SVD, we can check:
  - a given matrix is near singular
  - rank of the matrix
  - etc.

- $\exists$ a numerically stable algorithm to compute the SVD of a given matrix (it's expensive though...)
  In fact, one of the hottest topics in numerical linear algebra is how to compute a good approximation to the SVD of a <u>huge</u> matrix <u>fast</u>!

## ☆ A Geometric Observation

Let $A \in \mathbb{R}^{m \times n}$, and consider how $A$ maps an input vector in $\mathbb{R}^n$ to an output vector in $\mathbb{R}^m$.

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




Let $\{v_1, \cdots, v_n\}$ be an ONB of $\mathbb{R}^n$

Let $\{u_1, \cdots, u_m\}$ be an ONB of $\mathbb{R}^m$

ONB = orthonormal basis

Let $\{\sigma_1, \cdots, \sigma_m\}$ be a set of $m$ scalars with $\sigma_i \geq 0$, $i = 1, \cdots m$.

Then, $\sigma_i u_i$ is the $i$th principal semiaxis with length $\sigma_i$ in $\mathbb{R}^m$.

Now, if $\text{rank}(A) = r$, then exactly $r$ of $\{\sigma_1, \cdots, \sigma_m\}$ are nonzero, and exactly $m-r$ of $\sigma_i$'s are zero.

So, if $\underline{m \geq n}$, then $\underline{\text{rank}(A) \leq n}$. ← full rank if $= n$

i.e., at most $n$ of $\sigma_i$'s are nonzero.

For simplicity, let's assume $m \geq n$ and $\text{rank}(A) = n$ for the time being.

**Def.** The **singular values** of $A$

$\overset{\text{def}}{\Longleftrightarrow}$ The lengths of the $n$ principal semiaxes of the hyperellipsoid $AS$

Our convention: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \underset{\neq}{>} 0$

**Def.** The $n$ **left singular vectors** of $A$
$\overset{\text{def}}{\iff}$ $\{u_1, \cdots, u_n\}$ : the unit vectors in $\mathbb{R}^m$ along the principal semiaxes of $AS$.
So, $\sigma_i u_i$ is the $i$th largest principal semiaxis of $AS$.

**Def.** The $n$ **right singular vectors** of $A$
$\overset{\text{def}}{\iff}$ $\{v_1, \cdots, v_n\} \in S$ : the preimages of the principal semiaxes of $AS$, i.e.,

$$A v_i = \sigma_i u_i \qquad i = 1, \cdots, n.$$

## ☆ Reduced SVD

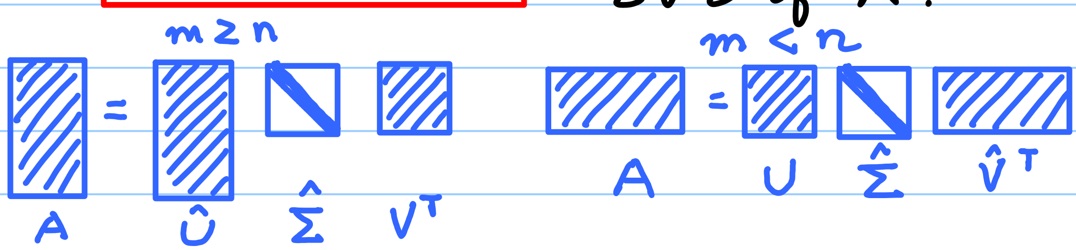
$$m\underset{n}{\begin{bmatrix} A \end{bmatrix}} \underbrace{\begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}}_{n\ =\ V}{}^{n} = m\underbrace{\begin{bmatrix} u_1 & \cdots & u_n \end{bmatrix}}_{n\ =\ \hat{U}} \underbrace{\begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \end{bmatrix}}_{n\ =\ \hat{\Sigma}}{}^{n}$$

$$\Rightarrow \quad \underset{m\times n}{A}\ \underset{n\times n}{V} = \underset{m\times n}{\hat{U}}\ \underset{n\times n}{\hat{\Sigma}}$$

Since $V$ is an orthogonal matrix,

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

The **reduced** SVD of $A$.



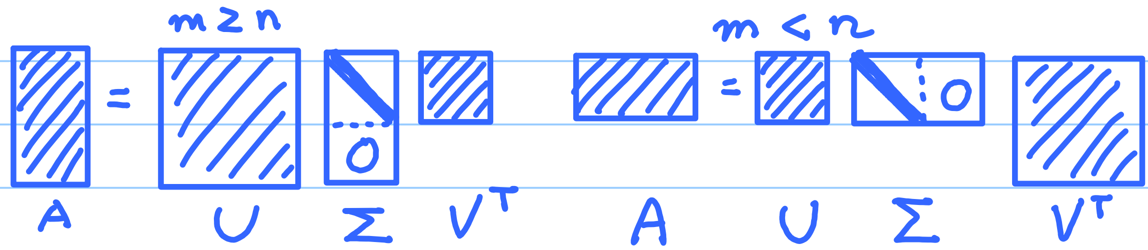
## ☆ Full SVD

Note $\hat{U} \in \mathbb{R}^{m\times n}$ in the reduced SVD with $m \geq n$.

$\Rightarrow$ The column vectors of $\hat{U}$ do not form an ONB of $\mathbb{R}^m$ unless $m = n$.

$\Rightarrow$ Remedy : adjoin $m-n$ ON vectors to $\hat{U}$ to form an orthogonal matrix $U$.
Then $\hat{\Sigma}$ must be changed to $\Sigma \in \mathbb{R}^{m\times n}$

$$\boxed{A = U \Sigma V^T}$$ The full SVD of A

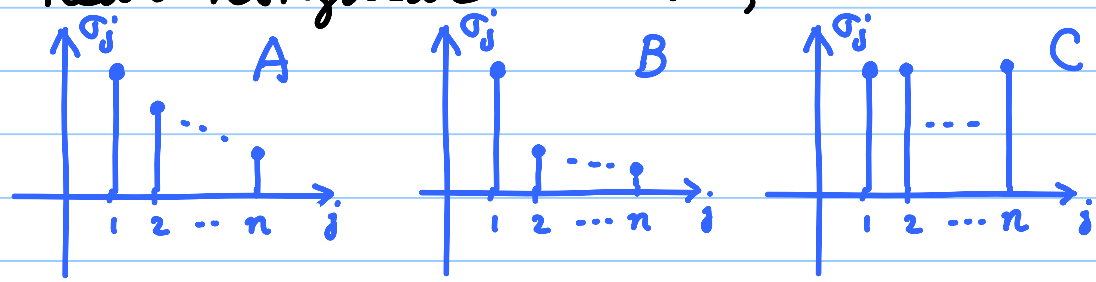



For non-full rank matrices, i.e., $\text{rank}(A) = r < \min(m, n)$,
$\exists$ only $r$ positive singular values.
So,

$$\Sigma = \underbrace{\left[\begin{array}{ccccc} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \\ \hline & & O & & \end{array}\right]}_{m \geq n} \quad \text{or} \quad \underbrace{\left[\begin{array}{cccccc|c} \sigma_1 & & & & & & \\ & \ddots & & & & & \\ & & \sigma_r & & & & O \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \end{array}\right]}_{m \leq n}$$

Let's consider $m = n$ and full rank case.
Theoretically, it's invertible, nonsingular.

However, we can gain more info by checking the distribution of the singular values of $A$ $\Rightarrow$ We can see whether $A$ is near singular or not, etc.




Out of these three scenarios, which matrix do you think behaves best numerically?
$\Rightarrow$ C.

## ☆ Pseudoinverse via SVD

$$\boxed{A^{+} = V \Sigma^{+} U^{T}}$$

where

$$\Sigma^{+} := \underbrace{\left[\begin{array}{ccccc} \frac{1}{\sigma_1} & & & & \\ & \ddots & & & \\ & & \frac{1}{\sigma_r} & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \\ \hline & & O & & \end{array}\right]}_{m \geq n} \quad \text{or} \quad \underbrace{\left[\begin{array}{cccccc|c} \frac{1}{\sigma_1} & & & & & & \\ & \ddots & & & & & \\ & & \frac{1}{\sigma_r} & & & & O \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \end{array}\right]}_{m \leq n}$$

<u>Check</u>: $AA^{+} = U\Sigma V^T V \Sigma^{+} U^T$

$$= U\Sigma\Sigma^{+}U^T$$

$$= U \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \\ & & O & & \end{bmatrix} U^T$$

$$= [\mathbf{u}_1 \cdots \mathbf{u}_r \; \mathbf{0} \cdots \mathbf{0}] \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_m^T \end{bmatrix}$$

$$= \hat{U}\hat{U}^T$$

→ reduced version.

Similarly, $A^{+}A = \hat{V}\hat{V}^T$

## The Moore-Penrose Conditions

For a given matrix $A \in \mathbb{R}^{m\times n}$, if $X \in \mathbb{R}^{n \times m}$ satisfies the following:

$$\begin{cases} (1) & AXA = A \\ (2) & XAX = X \\ (3) & (AX)^T = AX \\ (4) & (XA)^T = XA \end{cases}$$

then $X$ is called the pseudoinverse (or the Moore-Penrose inverse) of $A$ and written as $A^{+}$

$\exists$ many applications using $A^{+}$!

<u>Note</u>: If $\| AX - I_m \|_F \to \min$ then $X = A^{+}$.