Singular Value Decomposition

Note Title 5/2/2012

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

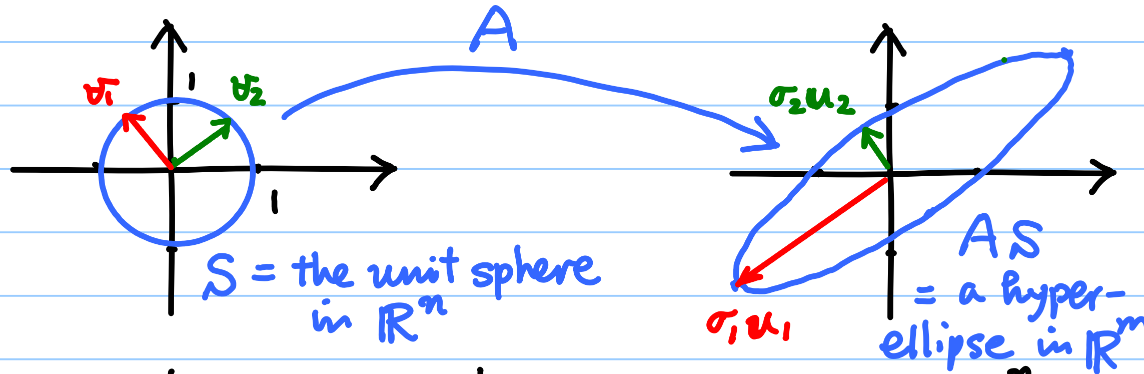
- SVD can be a concepual tool in linear algebra
  $\Rightarrow$ via SVD, we can check:
  - a given matrix is near singular
  - rank of the matrix
  - etc.

- $\exists$ 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 huge matrix fast!

☆ 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 hyperellipse."



ONB = orthonormal basis

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

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

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

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

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

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

i.e., at most n of σ_i's are nonzero.

For simplicity, let's assume $m \geq n$ and 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 hyperellipse AS

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

Def. The n left singular vectors of A

$\overset{\text{def}}{\Longleftrightarrow}$ $\{u_1, \cdots, u_n\}$: the unit vectors in $\mathbb{R}^m$ along the principal semiaxes of AS.

So, $\sigma_i u_i$ is the ith largest principal semiaxis of AS.

Def. The n right singular vectors of A

$\overset{\text{def}}{\Longleftrightarrow}$ $\{v_1, \cdots, v_n\} \in S$: the preimages of the principal semiaxes of AS, i.e.,

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

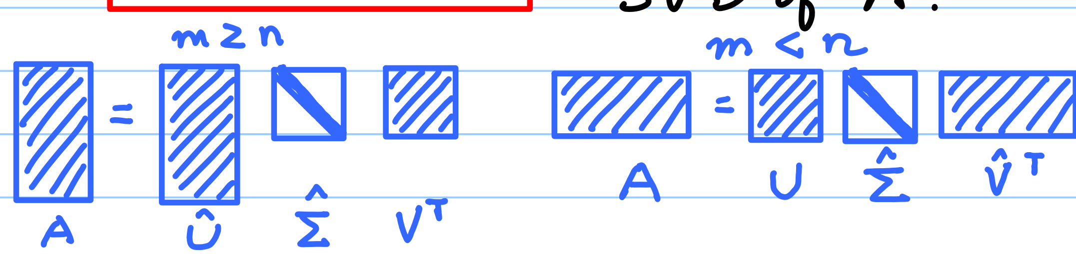
☆ Reduced SVD

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

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

Since V is an orthogonal matrix,

$$\boxed{A = \hat{U} \hat{\Sigma} V^T}$$ The reduced SVD of A.



☆ Full SVD

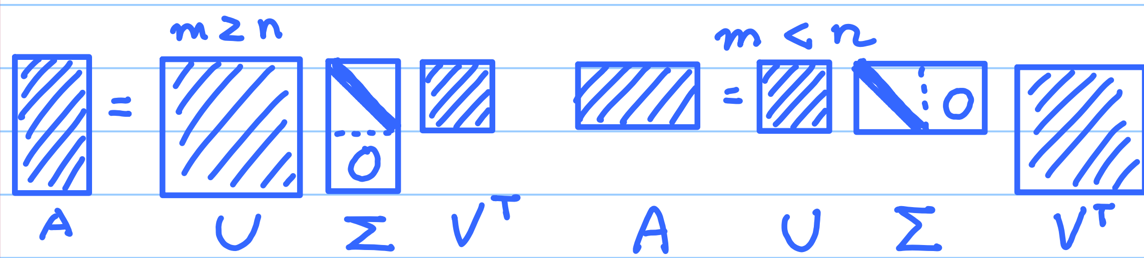
Note $\hat{U} \in \mathbb{R}^{m \times n}$ in the reduced SVD with $m \geq n$.

$\Rightarrow$ 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.

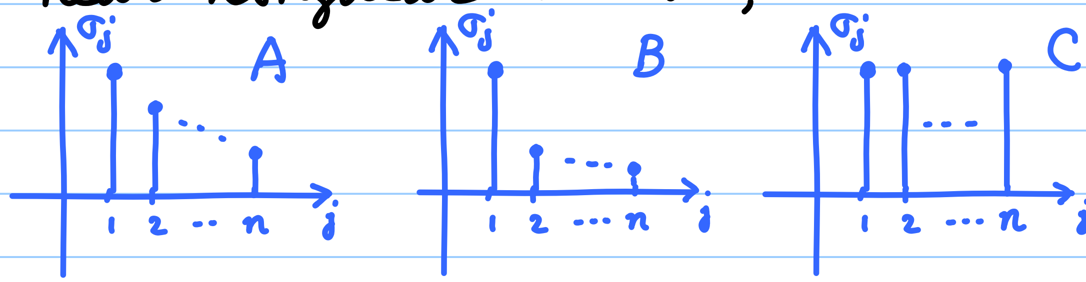
So,

$$\Sigma = \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \\ \hline & & 0 & & \end{bmatrix} \text{ or } \left[\begin{array}{cccccc|c} \sigma_1 & & & & & & \\ & \ddots & & & & & \\ & & \sigma_r & & & & 0 \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & \end{array}\right]$$

$m \geq n$ $\qquad$ $m \leq n$

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

However, we can gain more info by checking the distibution 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

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

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

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

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

$$= [u_1 \cdots u_r \ 0 \cdots 0] \begin{bmatrix} u_1^T \\ \vdots \\ u_m^T \end{bmatrix}$$

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

reduced version.

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

<u>The Moore-Penrose Conditions</u>

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 $X = A^+$.