



# Singular Values and Singular Vectors

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## Linear Algebra

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# Introduction

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range

null space

eigen value

eigen vector

transpose

inverse

symmetric matrix

orthogonal matrix

psd matrix



PCA

low-rank approximation

TLS minimization

pseudoinverse

separable models

optimal rotation

...



$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

# Singular Value

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- $S_{m \times n}$  Non-Square!!
- $\sigma_i = \sqrt{\lambda_i} \quad \lambda_i \in \sigma(S^T S), i = 1, \dots, n$
- $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{m-1} \geq \sigma_m$

## Example

$$S = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$$

$$S^T S = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix} \Rightarrow \lambda(S^T S) = \{360, 90, 0\}$$

$$\Rightarrow \begin{cases} \sigma_1 = \sqrt{360} = 6\sqrt{10} \\ \sigma_2 = \sqrt{90} = 3\sqrt{10} \\ \sigma_3 = 0 \end{cases}$$



## Theorem

$\{v_1, \dots, v_n\}$  are orthonormal eigenvectors of matrix  $S^T S$  then singular values of matrix  $S$  are norm of  $Sv_i$  vectors:

$$\|Sv_i\| = \sigma_i$$

Proof?



## Example

$$S = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} \rightarrow S^T S = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix} \rightarrow \sigma_1 = \sqrt{360}, \sigma_2 = \sqrt{90}, \sigma_3 = 0$$

$$v_1 = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}, v_2 = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}, v_3 = \begin{bmatrix} 2/3 \\ -2/3 \\ 1/3 \end{bmatrix}$$

$$Sv_1 = \begin{bmatrix} 18 \\ 6 \end{bmatrix} \Rightarrow \|Sv_1\| = \sqrt{18^2 + 6^2} = \sigma_1$$

$$Sv_2 = \begin{bmatrix} 3 \\ -9 \end{bmatrix} \Rightarrow \|Sv_2\| = \sqrt{3^2 + (-9)^2} = \sigma_2$$

$$Sv_3 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow \|Sv_3\| = 0 = \sigma_3$$





## Theorem

$\{v_1, \dots, v_n\}$  are orthonormal eigenvectors of matrix  $S^T S$  and  $S$  has  $r$  non-zero singular value:

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0, \quad \sigma_{r+1} = \dots = \sigma_n = 0$$

$\{Sv_1, \dots, Sv_r\}$  is a orthogonal basis for range of  $S$

$\text{rank}(S)=r$

Rank of Matrix = Number of nonzero singular values

How to find  $\{u_1, \dots, u_r\}$  is a orthonormal basis for range of  $S$

# SVD

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- Given any  $m \times n$  matrix  $A$ , algorithm to find matrices  $U$ ,  $V$ , and  $\Sigma$  such that (**always exists**)
- $A = U\Sigma V^T$   $A = U\Sigma V^*$ 
  - $U$  is  $m \times m$  and orthogonal (always real)
  - $\Sigma$  is  $m \times n$  and diagonal with non-negative (always real) called singular values.
  - $V$  is  $n \times n$  and orthogonal (always real)
- Columns of  $U$  are eigenvectors of  $AA^T$  (called the left singular vectors).
- Columns of  $V$  are eigenvectors of  $A^T A$  (called the right singular vectors).
- The non-zero singular values are the positive square roots of non-zero eigenvalues of  $AA^T$  or  $A^T A$ .



- ❑ **Generalization of the spectral decomposition** that applies to all matrices, rather than just normal matrices.
- ❑ Applications:
  - Compute the size of a matrix (in a way that typically makes more sense than norm)
  - Provide a new geometric interpretation of linear transformations
  - Solve optimization problems
  - Construct an “almost inverse” for matrices that do not have an inverse.



| SVD   | Diagonalization                                       | Spectral Decomposition                            |
|---|---|---|
| applies to every single matrix (even rectangular ones).                                       | only applies to matrices with a basis of eigenvectors | only applies to normal matrices                   |
| matrix $\Sigma$ in the middle of the SVD is diagonal (and even has real non-negative entries) | do not guarantee an entrywise non-negative matrix     | do not guarantee an entrywise non-negative matrix |
| It requires two unitary matrices $U$ and $V$  | only required one invertible matrix                   | only required one unitary matrix                  |



- ❑ The  $\sum_i$  are called the **singular values** of  $\mathbf{A}$
- ❑ If  $\mathbf{A}$  is singular, some of the  $\sum_i$  will be 0
- ❑ In general  $\text{rank}(\mathbf{A}) = \text{number of nonzero } \sum_i$
- ❑ SVD is mostly unique (up to permutation of singular values, or if some  $\sum_i$  are equal)



- The SVD is a factorization of a  $m \times n$  matrix into

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

Where  $U$  is a  $m \times m$  orthogonal matrix,  $V^T$  is a  $n \times n$  orthogonal matrix and  $\Sigma$  is a  $m \times n$  diagonal matrix.

For a square matrix ( $m=n$ ):

$$A = \begin{pmatrix} \vdots & \cdots & \vdots \\ u_1 & \cdots & u_n \\ \vdots & \cdots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} \cdots & v_1^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_n^T & \cdots \end{pmatrix}$$

$$A = \begin{pmatrix} \vdots & \cdots & \vdots \\ u_1 & \cdots & u_n \\ \vdots & \cdots & \vdots \end{pmatrix} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \begin{pmatrix} \vdots & \cdots & \vdots \\ v_1 & \cdots & v_n \\ \vdots & \cdots & \vdots \end{pmatrix}^T$$



$$\begin{aligned}
 [Sv_1 \quad \dots \quad Sv_r \quad 0 \quad \dots \quad 0]_{m \times n} &= [\sigma_1 u_1 \quad \dots \quad \sigma_r u_r \quad 0 \quad \dots \quad 0]_{m \times n} \\
 [Sv_1 \quad \dots \quad Sv_r \quad Sv_{r+1} \quad \dots \quad Sv_n]_{m \times n} &= [\sigma_1 u_1 \quad \dots \quad \sigma_r u_r \quad 0 \quad \dots \quad 0]_{m \times n}
 \end{aligned}$$

$$S[v_1 \quad \dots \quad v_n] = [u_1 \quad \dots \quad u_m] \left[ \begin{array}{ccc|c} \sigma_1 & \dots & 0 & 0 \\ \vdots & & \vdots & \\ 0 & \dots & \sigma_r & \\ \hline & & & 0 \end{array} \right]$$

$$S_{m \times n} V_{n \times n} = U_{m \times m} \Sigma_{m \times n}$$

$$S = U \Sigma V^T$$





□ what happens when  $A$  is not a square matrix?

□  $n > m$

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

$$= \begin{pmatrix} \vdots & \cdots & \vdots \\ u_1 & \cdots & u_m \\ \vdots & \cdots & \vdots \end{pmatrix}_{m \times m} \begin{pmatrix} \sigma_1 & & & 0 & & \\ & \ddots & & & \ddots & \\ & & \sigma_m & & & \\ & & & & & 0 \end{pmatrix}_{m \times n} \begin{pmatrix} \cdots & v_1^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_m^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_n^T & \cdots \end{pmatrix}_{n \times n}$$

We can instead rewrite the above as:

$$A = U\Sigma_R V_R^T$$

where  $V_R$  is  $n \times m$  matrix and  $\Sigma_R$  is a  $m \times m$  matrix

**In general:**

$$A = U_R \Sigma_R V_R^T$$

Now  $U$  and  $V$  are not orthogonal.  
But their columns are orthonormal.

$U_R$  is a  $m \times k$  matrix  
 $\Sigma_R$  is a  $k \times k$  matrix  
 $V_R$  is a  $n \times k$  matrix

$k = \min(m, n)$



□  $m > n$

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

$$= \begin{pmatrix} \vdots & \cdots & \vdots & \cdots & \vdots \\ u_1 & \cdots & u_n & \cdots & u_m \\ \vdots & \cdots & \vdots & \cdots & \vdots \end{pmatrix}_{m \times m} \begin{pmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_n & & \\ 0 & \cdots & 0 & \cdots & \\ \vdots & \ddots & \vdots & \ddots & \\ 0 & \cdots & 0 & \cdots & \end{pmatrix}_{m \times n} \begin{pmatrix} \cdots & v_1^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_n^T & \cdots \end{pmatrix}_{n \times n}$$

We can instead rewrite the above as:

$$A = U\Sigma_R V_R^T$$

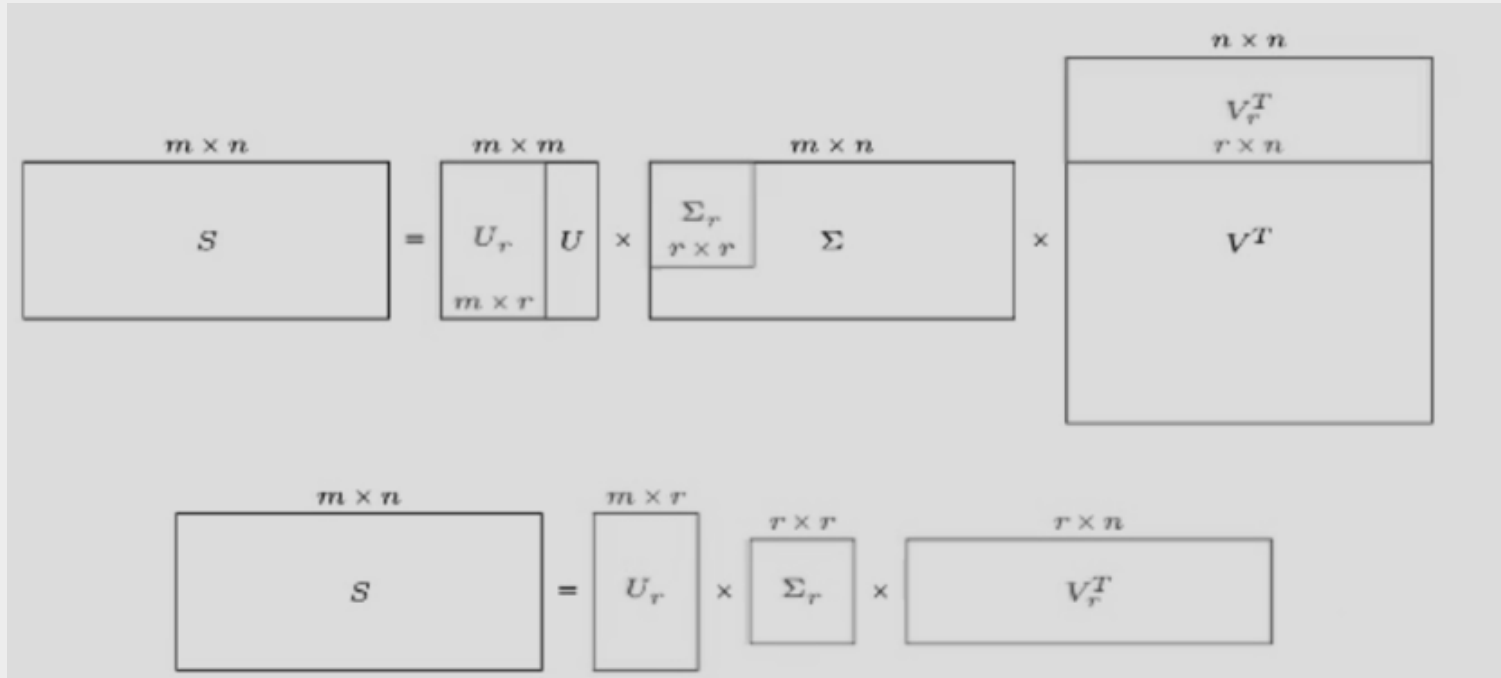
Now U and V are not orthogonal.  
But their columns are orthonormal.

where  $U_R$  is  $m \times n$  matrix and  $\Sigma_R$  is a  $n \times n$  matrix



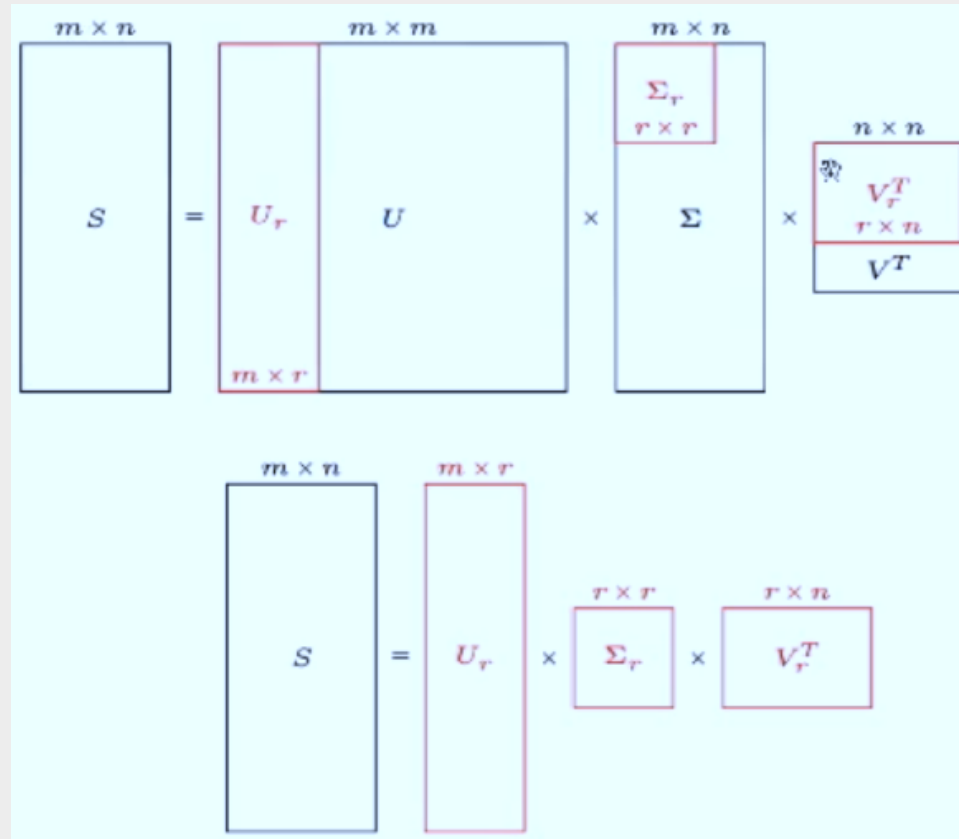


## Wide Matrix





## □ Tall Matrix





- Assume  $A$  with singular value decomposition  $A = U\Sigma V^T$ . Let's take a look at the eigenpairs corresponding to  $A^T A$ :

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

Hence  $A^T A = V\Sigma^2 V^T$

- Recall that columns of  $V$  are all linear independent (orthogonal matrix), then from diagonalization ( $B = XDX^{-1}$ ), we get:
  - The columns of  $V$  are the eigenvectors of the matrix  $A^T A$
  - The diagonal entries of  $\Sigma^2$  are the eigenvalues of  $A^T A$
- Let's call  $\lambda$  the eigenvalues of  $A^T A$ , then  $\sigma_i^2 = \lambda_i$



- In a similar way,

$$AA^T = (U\Sigma V^T)(U\Sigma V^T)^T \\ (U\Sigma V^T)(V^T)^T(\Sigma)^T U^T = U\Sigma \mathbf{V^T V} \Sigma^T U^T = U\Sigma\Sigma^T U^T$$

Hence  $AA^T = U\Sigma^2 U^T$

- Recall that columns of  $U$  are all linear independent (orthogonal matrix), then from diagonalization ( $B = XDX^{-1}$ ), we get:
  - The columns of  $U$  are the eigenvectors of the matrix  $AA^T$

# How can we compute an SVD of a matrix $A$ ?



1. Evaluate the  $n$  eigenvectors  $v_i$  and eigenvalues  $\lambda_i$  of  $A^T A$
2. Make a matrix  $V$  from the normalized vectors  $v_i$ . The columns are called “right singular vectors”.

$$V = \begin{pmatrix} \vdots & \cdots & \vdots \\ v_1 & \cdots & v_n \\ \vdots & \cdots & \vdots \end{pmatrix}$$

3. Make a diagonal matrix from the square roots of the eigenvalues.

$$\Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix} \quad \sigma_i = \sqrt{\lambda_i} \quad \text{and} \quad \sigma_1 \geq \sigma_2 \geq \cdots$$

4. Find  $U$ :  $A = U\Sigma V^T \Rightarrow U\Sigma = AV \Rightarrow U = AV\Sigma^{-1}$ . The columns are called “left singular values”.



# How can we compute an SVD of a matrix A?



## Example

$$S = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix} \rightarrow S^T S = \begin{bmatrix} 9 & -9 \\ -9 & 9 \end{bmatrix}, \text{rank}(S) = 1$$

$$\Delta(\lambda) = \lambda^2 - 18\lambda = 0 \Rightarrow \sigma_1 = \sqrt{18}, \sigma_2 = 0 \Rightarrow \Sigma = \begin{bmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$v_1 = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}, v_2 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \Rightarrow V = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$Sv_1 = \begin{bmatrix} 2/\sqrt{2} \\ -4/\sqrt{2} \\ 4/\sqrt{2} \end{bmatrix} \Rightarrow u_1 = \frac{1}{\sigma_1} Sv_1 = \frac{1}{3\sqrt{2}} \begin{bmatrix} 2/\sqrt{2} \\ -4/\sqrt{2} \\ 4/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 1/3 \\ -2/3 \\ 2/3 \end{bmatrix}$$

$$u_2 = \begin{bmatrix} 2/3 \\ 2/3 \\ 1/3 \end{bmatrix}, u_3 = \begin{bmatrix} -2/3 \\ 1/3 \\ 2/3 \end{bmatrix} \Rightarrow U = \frac{1}{3} \begin{bmatrix} 1 & 2 & -2 \\ -2 & 2 & 1 \\ 2 & 1 & 2 \end{bmatrix}$$

$$S = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & -2 \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 1 & 2 & -2 \\ -2 & 2 & 1 \\ 2 & 1 & 2 \end{bmatrix} \begin{bmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = U\Sigma V^T$$



## □ Unitary Freedom of PSD Decompositions

Suppose  $B, C \in \mathcal{M}_{m,n}(\mathbb{F})$ . The following are equivalent:

- There exists a unitary matrix  $U \in \mathcal{M}_m(\mathbb{F})$  such that  $C = UB$ .
- $B^*B = C^*C$ ,
- $(B\mathbf{v}) \cdot (B\mathbf{w}) = (C\mathbf{v}) \cdot (C\mathbf{w})$  for all  $\mathbf{v}, \mathbf{w} \in \mathbb{F}^n$ , and
- $\|B\mathbf{v}\| = \|C\mathbf{v}\|$  for all  $\mathbf{v} \in \mathbb{F}^n$ .

## Example

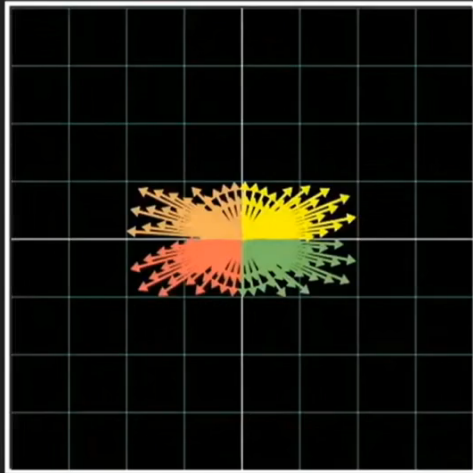
$$\begin{bmatrix} 3 & 2 \\ -2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix}$$



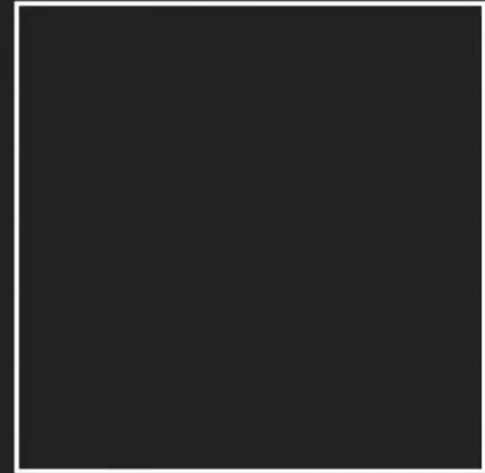
- If  $m \neq n$  then  $A^*A, AA^*$  have different sizes, but they still have essentially the same eigenvalues—whichever one is larger just has some extra 0 eigenvalues.
- The same is actually true of  $AB$  and  $BA$  for any  $A$  and  $B$ .
- **Proof SVD in another view!!**

## Diagonal Matrix: **Stretching** each axis differently



$$\begin{bmatrix} 0.5 & 0.0 \\ 0.0 & 2.0 \end{bmatrix}$$

vector is arrow

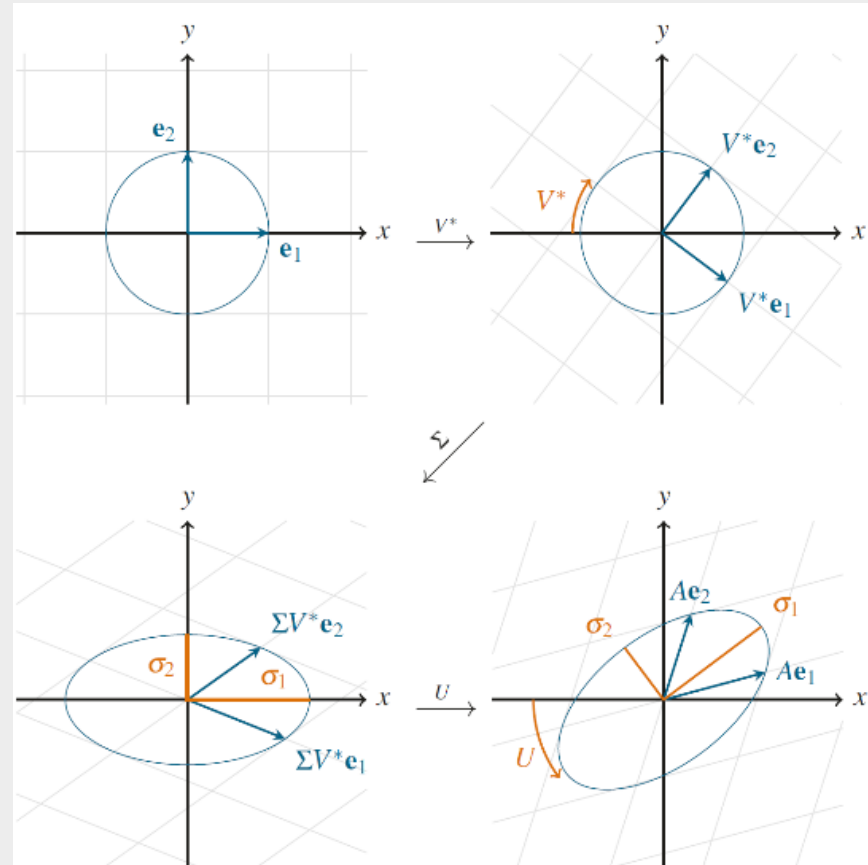


# Geometric Interpretation and the Fundamental Subspaces



$$A = U\Sigma V^*$$

The product of a matrix's singular values equals the absolute value of its determinant



# Determining the rank of a matrix



□ Suppose  $A$  is a  $m \times n$  rectangular matrix where  $m > n$ :

$$A = \begin{pmatrix} \vdots & \cdots & \vdots & \cdots & \vdots \\ u_1 & \cdots & u_n & \cdots & u_m \\ \vdots & \cdots & \vdots & \cdots & \vdots \end{pmatrix}_{m \times m} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}_{m \times n} \begin{pmatrix} \cdots & v_1^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_n^T & \cdots \end{pmatrix}_{n \times n}$$

$$A = \begin{pmatrix} \vdots & \cdots & \vdots \\ u_1 & \cdots & u_n \\ \vdots & \cdots & \vdots \end{pmatrix} \begin{pmatrix} \cdots & \sigma_1 v_1^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & \sigma_n v_n^T & \cdots \end{pmatrix} = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_n u_n v_n^T$$

$$A = \sum_{i=1}^n \sigma_i u_i v_i^T$$

$$A_1 = \sigma_1 u_1 v_1^T \text{ what is } \text{rank}(A_1) = ?$$

In general,  $\text{rank}(A_k) = k$



- Let  $A \in \mathcal{M}_{m,n}$  be a matrix with  $\text{rank}(A) = r$  and the singular value decomposition  $A = U\Sigma V^T$ , where

$$U = [u_1 \mid u_2 \mid \dots \mid u_m] \text{ and } V = [v_1 \mid v_2 \mid \dots \mid v_n]$$

Then

- $\{u_1, u_2, \dots, u_r\}$  is an orthonormal basis of  $\text{range}(A)$ ,
- $\{u_{r+1}, u_{r+2}, \dots, u_m\}$  is an orthonormal basis of  $\text{null}(A^*)$ ,
- $\{v_1, v_2, \dots, v_r\}$  is an orthonormal basis of  $\text{range}(A^*)$ , and
- $\{v_{r+1}, v_{r+2}, \dots, v_n\}$  is an orthonormal basis of  $\text{null}(A)$

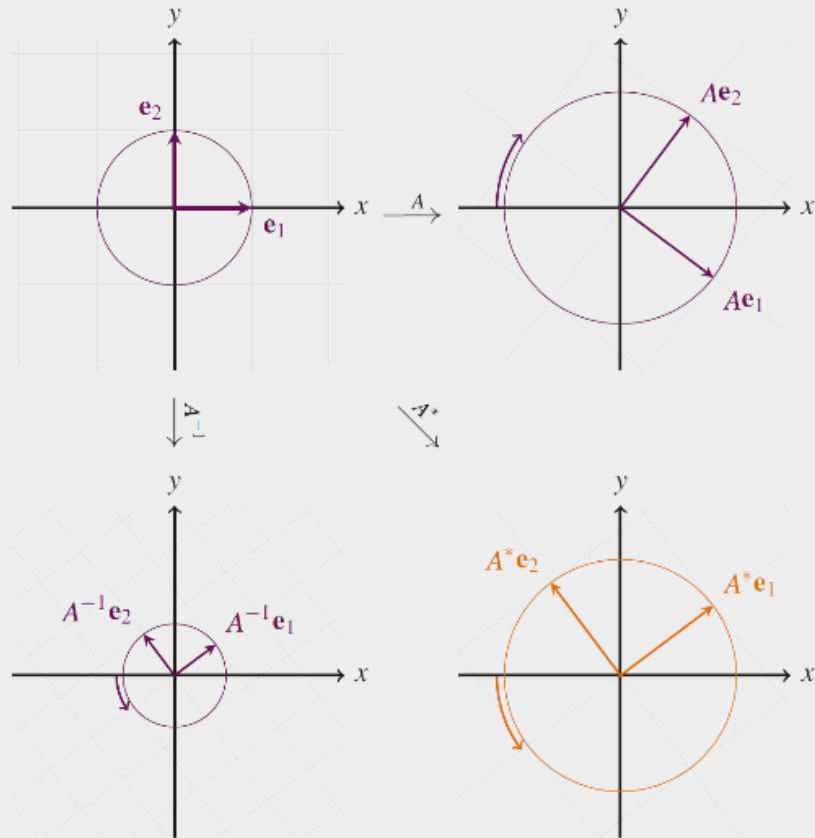


# A Geometric Interpretation

$$A = U\Sigma V^*$$

$$A^* = V\Sigma^*U^*$$

$$A^{-1} = V\Sigma^{-1}U^*$$





# Applications

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- Suppose  $\mathbb{F} = \mathbb{R}$  or  $\mathbb{F} = \mathbb{C}$ , and  $A \in \mathcal{M}_{m,n}(\mathbb{F})$  has  $\text{rank}(A) = r$ . There exist orthonormal sets of vectors  $\{u_j\}_{j=1}^r \subset \mathbb{F}^m$  and  $\{v_j\}_{j=1}^r \subset \mathbb{F}^n$  such that

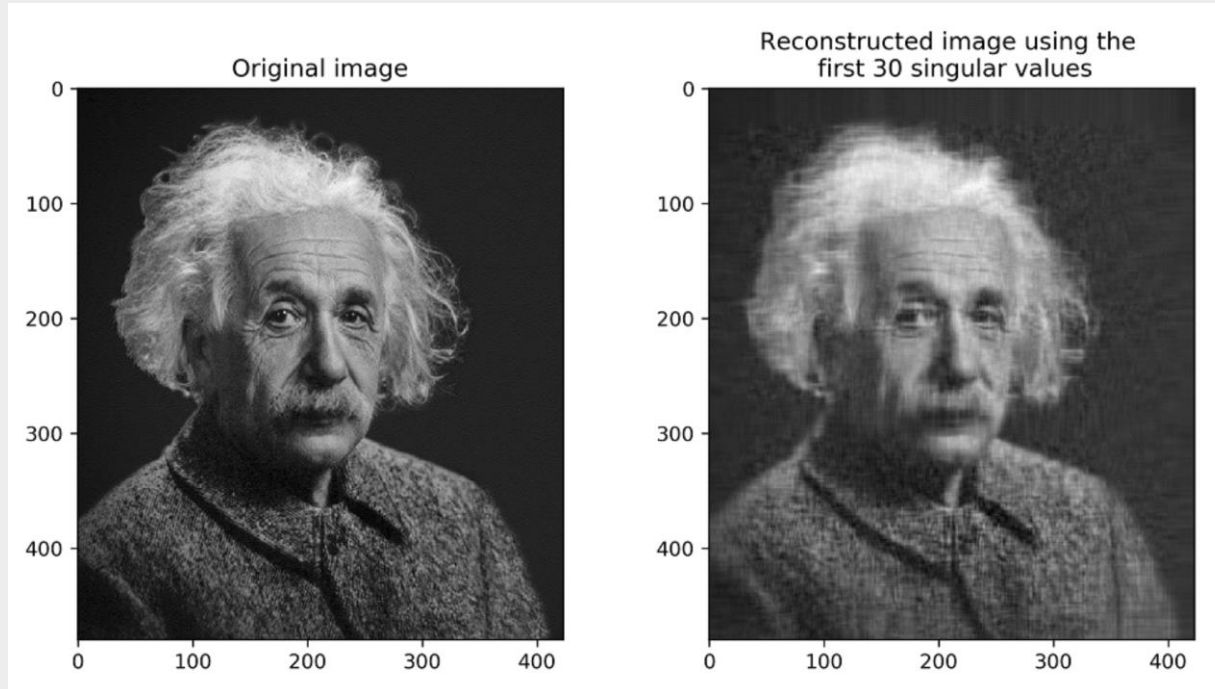
$$A = \sum_{i=1}^r \sigma_i u_i v_i^*,$$

where  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$  are the non-zero singular values of  $A$ .



- ❑ Suppose you want to find best rank- $k$  approximation to  $\mathbf{A}$ 
  - Answer: set all but the largest  $k$  singular values to zero
- ❑ Can form compact representation by eliminating columns of  $\mathbf{U}$  and  $\mathbf{V}$  corresponding to zeroed  $\Sigma_i$

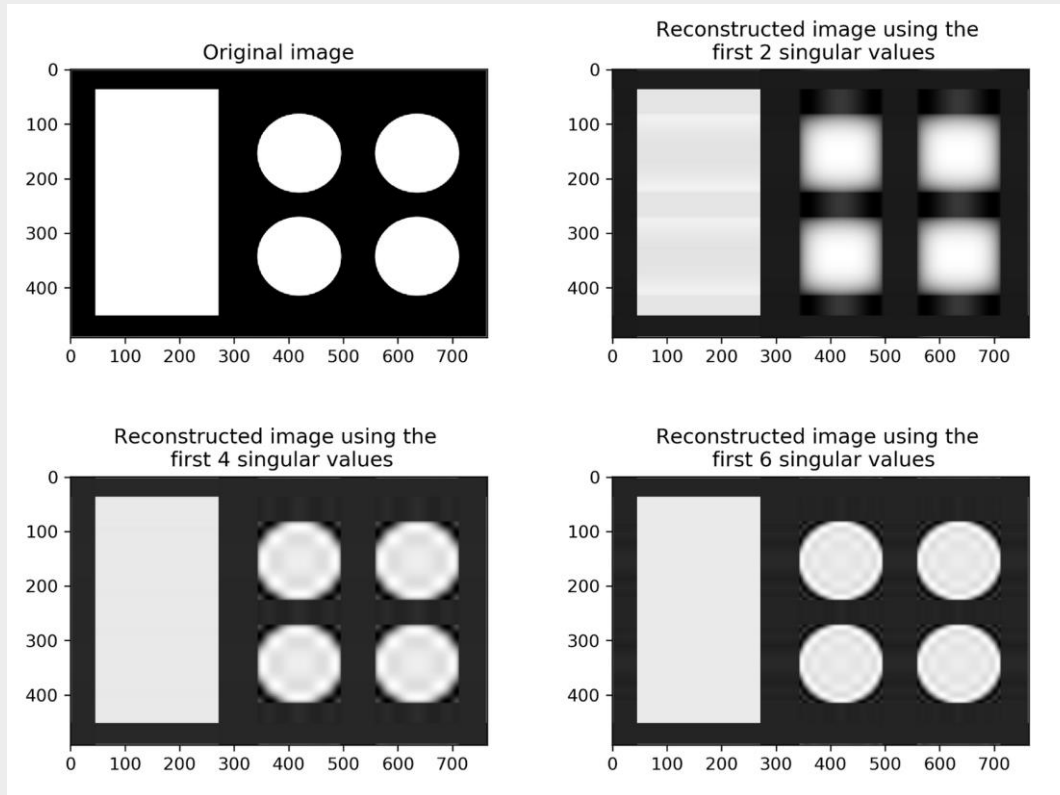
# Application: Dimensionality Reduction



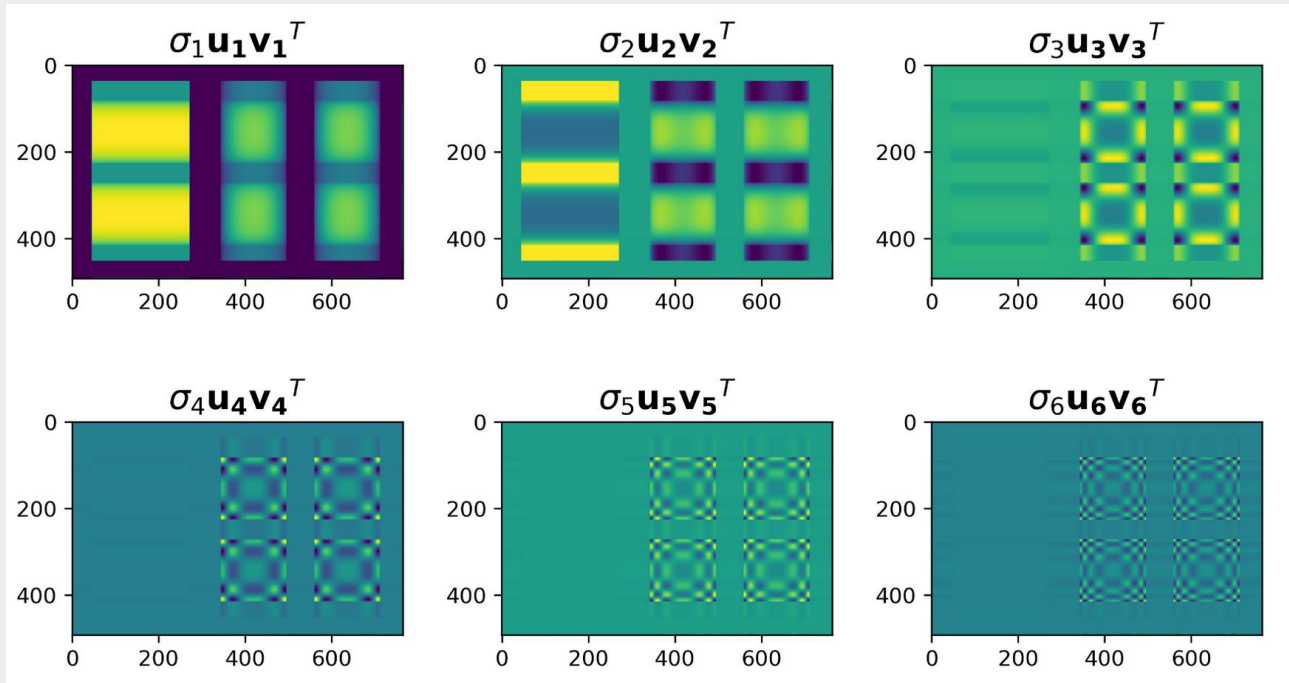
# Application: Dimensionality Reduction



# Application: Dimensionality Reduction



# Application: Dimensionality Reduction



## Low Rank Approximation of Image







- If  $A \in \mathcal{M}_n$  is positive semidefinite then its singular values equals its eigenvalues.



- ❑ Why is SVD so useful?
- ❑  $A^{-1} = V\Sigma^{-1}U^{-1} = V\Sigma^{-1}U^T$ 
  - Using fact that inverse = transpose for orthogonal matrices
  - Since  $\Sigma$  is diagonal,  $\Sigma^{-1}$  also diagonal with reciprocals of entries of  $\Sigma$
- ❑ This fails when some  $\Sigma_i$  are 0
  - It's *supposed* to fail – singular matrix
- ❑ Pseudoinverse: if  $\Sigma_i = 0$ , set  $\frac{1}{\Sigma_i}$  to 0 (!)
  - “Closest” matrix to inverse
  - Defined for all (even non-square, singular, etc.) matrices
  - Equal to  $(A^T A)^{-1} A^T$  if  $A^T A$  invertible



- ❑ Problem:  
if  $A$  is rank-deficient,  $\Sigma$  is not invertible.
- ❑ How to fix it:  
Define the Pseudo Inverse
- ❑ Pseudo Inverse of a diagonal matrix:

$$(\Sigma^+)_i = \begin{cases} \frac{1}{\sigma_i}, & \text{if } \sigma_i \neq 0 \\ 0, & \text{if } \sigma_i = 0 \end{cases}$$

- ❑ Pseudo Inverse of a matrix  $A$ :  
$$A^+ = V\Sigma^+U^T$$



- If a matrix  $A$  has the singular value decomposition

$$A = U W V^T$$

then the pseudo-inverse or Moore–Penrose inverse of  $A$  is

$$A^+ = V^T W^{-1} U$$

- If  $A$  is ‘tall’ ( $m > n$ ) and has full rank

$$A^+ = (A^T A)^{-1} A^T$$

(it gives the least-squares

solution  $x_{lsq} = A^+ b$ )

- If  $A$  is ‘short’ ( $n > m$ ) and has full rank

$$A^+ = A^T (A A^T)^{-1}$$

(it gives the least-norm solution  $x_{l-n}$

$= A^+ b$ )

- In general,  $x_{pinv} = A^+ b$  is the minimum-norm, least-square solution.



- One common definition for the norm of a matrix is the Frobenius norm:

$$\|A\|_F^2 = \sum_{i=1:m} \sum_{j=1:n} a_{ij}^2$$

- Frobenius norm can be computed from SVD

$$\|A\|_F^2 = \sum_{i=1:p} \Sigma_i^2 \quad \text{where } p = \min(n, m)$$

- So changes to a matrix can be evaluated by looking at changes to singular values



□ 2-norm:

$$\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} = \sigma_1$$



$$\square \mathbf{x}^* = \mathbf{A}^{-1}\mathbf{b} = (\mathbf{U}\mathbf{D}\mathbf{V}^T)^{-1}\mathbf{b},$$

$$(\mathbf{U}\mathbf{D}\mathbf{V}^T)^{-1} = \mathbf{V}^{-T} \mathbf{D}^{-1} \mathbf{U}^{-1}$$

Moore-Penrose pseudoinverse

$$\mathbf{x}^* = \mathbf{A}^{-1}\mathbf{b} = \boxed{\mathbf{V}\mathbf{D}^{-1}\mathbf{U}^T}\mathbf{b}$$

- Invert the diagonal entries in  $\mathbf{D}$  that are nonzero, but leave the other diagonal entries alone as zeros.