Singular Values and Singular Vectors

Linear Algebra

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Introduction

Introduction

range

null space

eigen value

eigen vector

transpose

inverse

symmetric matrix

orthogonal matrix

psd matrix

S V D

PCA

low-rank approximation

TLS minimization

pseudoinverse

separable models

optimal rotation

...

Introduction

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

Singular Value

Singular value and eigenvalue

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

Example

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

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

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

Singular value and eigenvector

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?

Singular value and eigenvector

Example

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

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

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

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

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

Singular value and Rank

Theorem

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

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

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

$rank(S)=r$

Rank of Matrix = Number of nonzero singular values why???

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

SVD

SVD Introduction

- 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.

Singular Value Decomposition (SVD)

- Given any $m \times n$ matrix **A**, algorithm to find matrices **U**, **V**, and $\sum$ such that (**always exists**)
- $A = U\Sigma V^T$ $A = U\Sigma V^*$

  U is $m \times m$ and orthogonal (always real)

  $\sum$ 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 vectors are the positive square roots of non-zero eigenvalues of AA^T or $A^T A$.

SVD

- The Σ_i are called the singular values of **A**
- If **A** is singular, some of the Σ_i will be 0
- In general *rank*(**A**) = number of nonzero Σ_i
- SVD is mostly unique (up to permutation of singular values, or if some Σ_i are equal)

Columns of V are eigenvectors of $A^T A$

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

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

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 Σ^2 are the eigenvalues of $A^T A$
- Let's call λ the eigenvalues of $A^T A$, then $\sigma_i^2 = \lambda_i$

Columns of U are eigenvectors of AA^T

- In a similar way,

$$AA^T = (U\Sigma V^T)(U\Sigma V^T)^T$$

$$(U\Sigma V^T)(V^T)^T(\Sigma)^T U^T = U\Sigma V^T V \Sigma^T U^T = U\Sigma\Sigma^T U^T$$

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 λ_i of $A^T A$
2. Make a matrix V from the normalized vectors v_i. The columns are called "right singular vectors".

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

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

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

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

Example

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

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

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

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

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

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

SVD for Square Matrix

- The SVD is a factorization of a m x n matrix into

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

Where U is a m x m orthogonal matrix, V^T is a n x n orthogonal matrix and Σ is a m x n diagonal matrix.

For a square matrix (m=n):

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

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

Reduced SVD

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

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

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

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

Reduced SVD

- 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 x m matrix and Σ_R is a m x m matrix

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

In general:

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

U_R is a m x k matrix
Σ_R is a k x k matrix
V_R is a n x k matrix

k = min(m, n)

Reduced SVD

- m > n

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

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

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 x n matrix and Σ_R is a n x n matrix

Reduced SVD

- Let's take a look at the product of $\Sigma^T\Sigma$ where Σ has the singular values of a A, a m x n matrix.

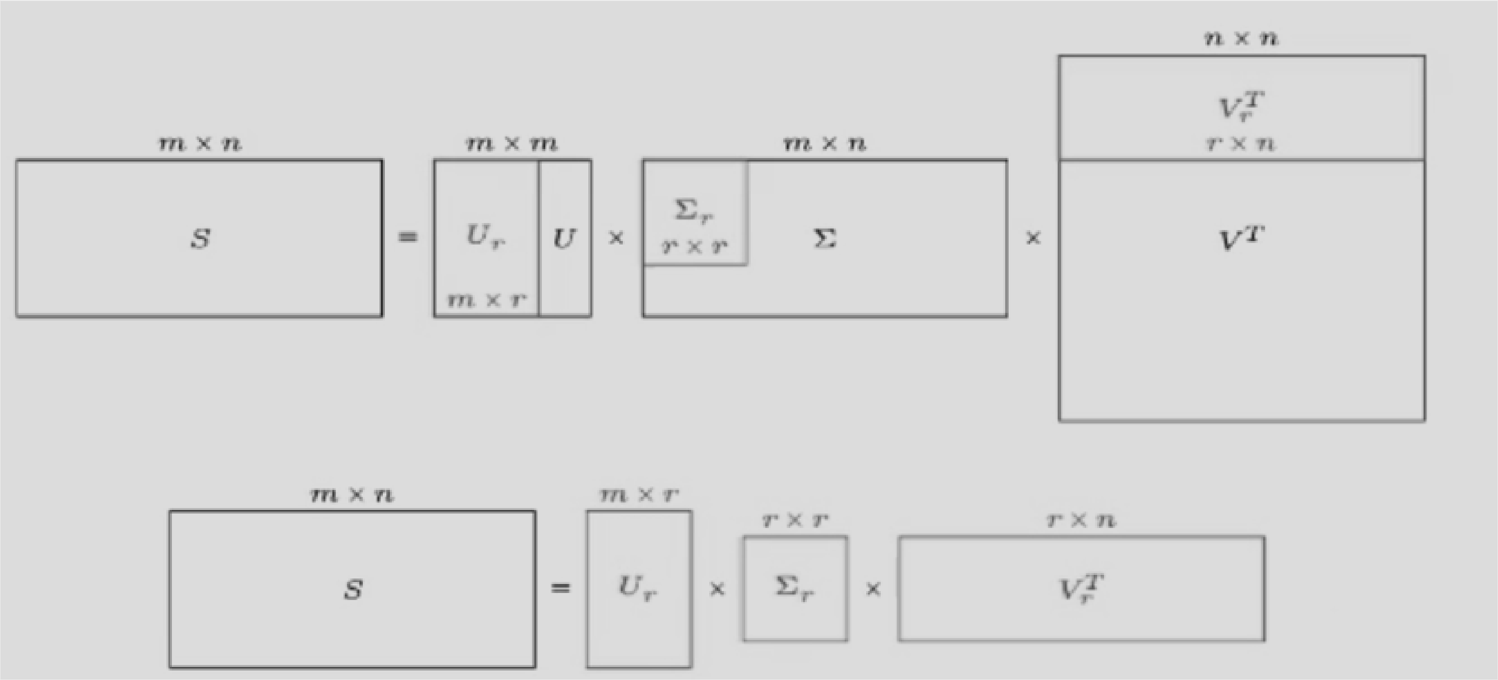
  - **m > n:**

$$\Sigma^T\Sigma = \begin{pmatrix} \sigma_1 & & & 0 & & \\ & \ddots & & & \ddots & \\ & & \sigma_n & & & 0 \end{pmatrix}_{n\times m} \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}_{m\times n} = \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{pmatrix}_{n\times n}$$

  - **n > m:**

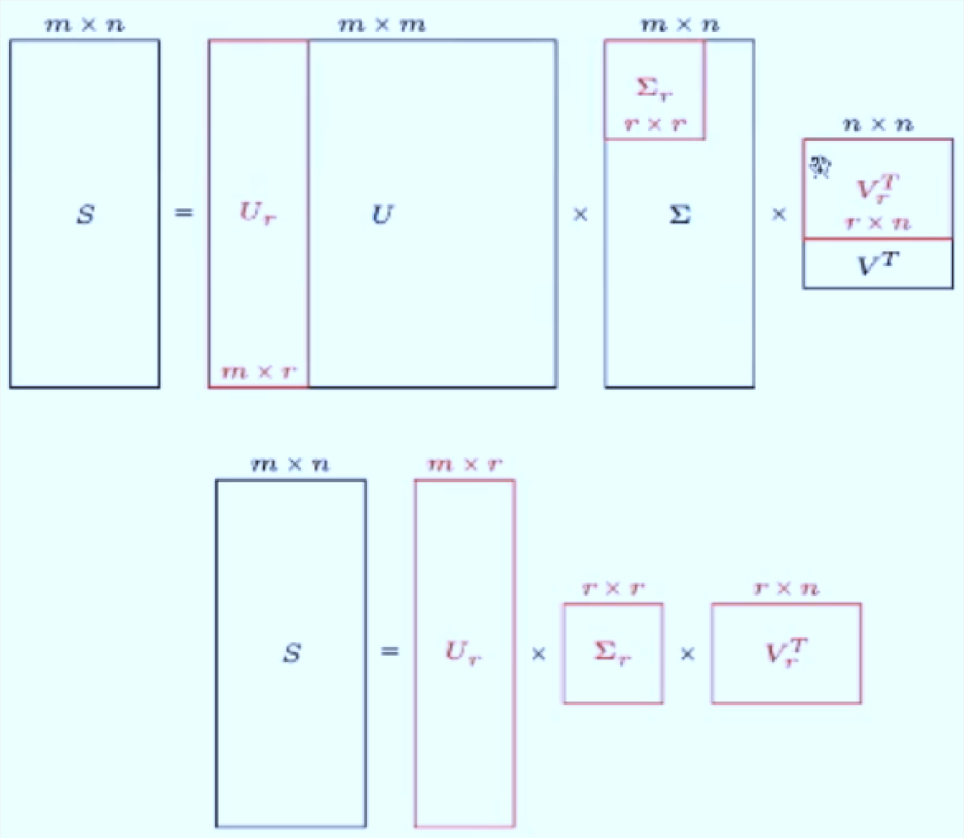
$$\Sigma^T\Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_m \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}_{n\times m} \begin{pmatrix} \sigma_1 & & & 0 & & \\ & \ddots & & & \ddots & \\ & & \sigma_m & & & 0 \end{pmatrix}_{m\times n} = \begin{pmatrix} \sigma_1^2 & & & 0 & & \\ & \ddots & & & \ddots & \\ & & \sigma_m^2 & & & 0 \\ 0 & & & 0 & & \\ & \ddots & & & \ddots & \\ & & 0 & & & 0 \end{pmatrix}_{n\times n}$$

- Wide Matrix


$m \times n$
S
$=$
$m \times m$
U_r
U
$m \times r$
$\times$
$m \times n$
Σ_r
$r \times r$
Σ
$\times$
$n \times n$
V_r^T
$r \times n$
V^T
$m \times n$
S
$=$
$m \times r$
U_r
$\times$
$r \times r$
Σ_r
$\times$
$r \times n$
V_r^T

Reduced SVD

- Tall Matrix



SVD Comparison

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 Σ 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

Unitary Freedom of PSD Decompositions

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

a. There exists a unitary matrix $U \in \mathcal{M}_m(\mathbb{F})$ such that $C = UB$,

b. $B^*B = C^*C$,

c. $(B\mathbf{v}).(B\mathbf{w}) = (C\mathbf{v}).(C\mathbf{w})$ for all $\mathbf{v}, \mathbf{w} \in \mathbb{F}^n$, and

d. $||B\mathbf{v}|| = ||C\mathbf{v}||$ for all $\mathbf{v} \in \mathbb{F}^n$.

Example

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

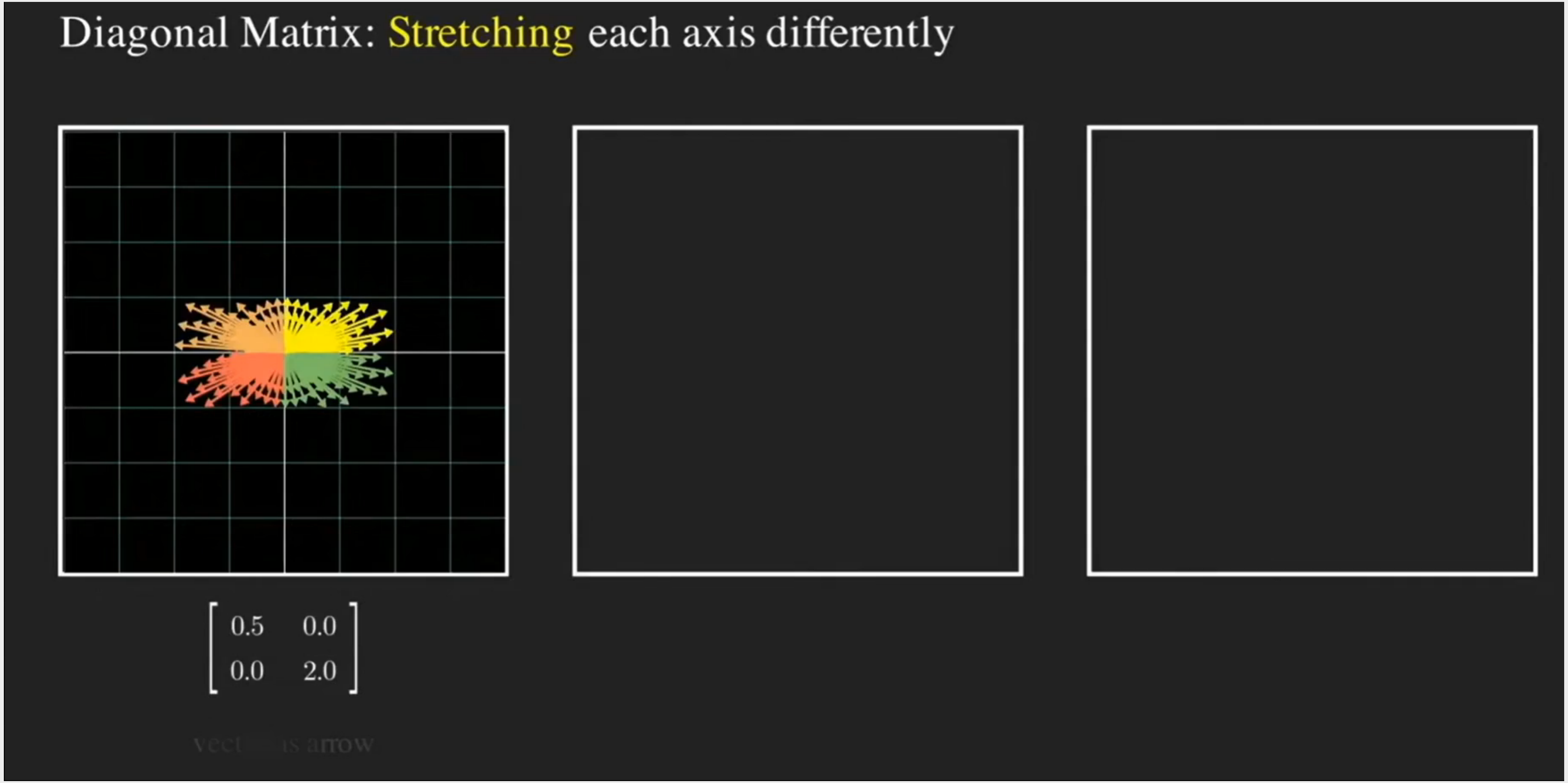
$$\begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \\ 3 & 2 & 1 \end{bmatrix}$$

SVD Proof

- 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.

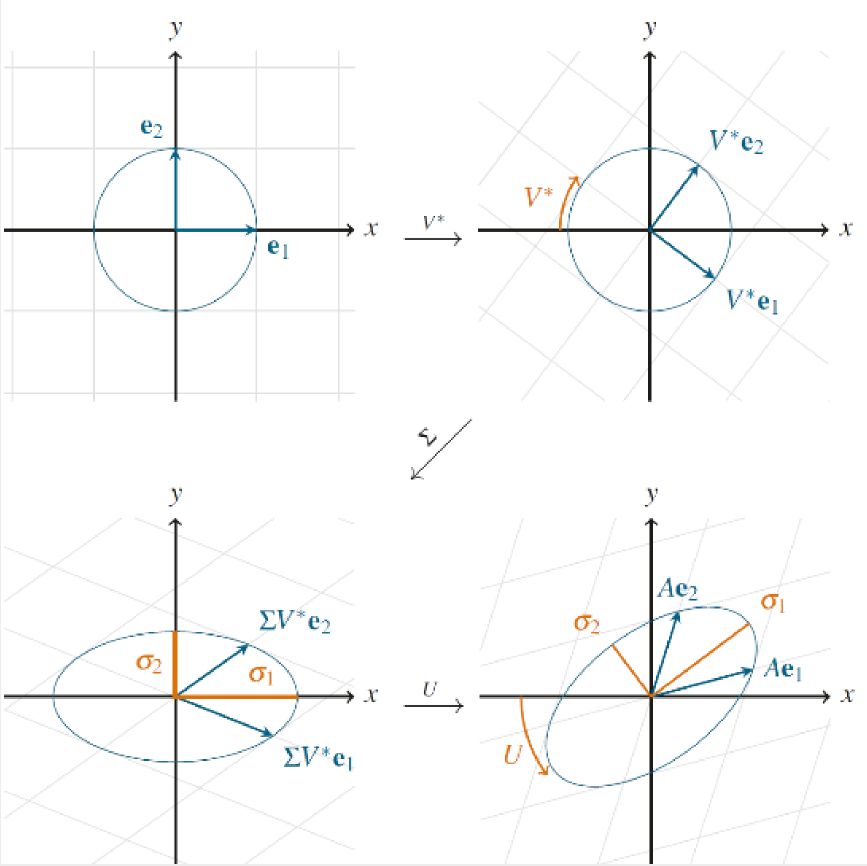
- Proof SVD in another view!!

Review


Diagonal Matrix: Stretching each axis differently
0.5 0.0
0.0 2.0

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

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 x n rectangular matrix where m > n:

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

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

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

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

In general, rank$(A_k) = k$

Conclusion

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

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

Then

a. $\{u_1, u_2, \ldots, u_r\}$ is an orthonormal basis of range(A),

b. $\{u_{r+1}, u_{r+2}, \ldots, u_m\}$ is an orthonormal basis of null(A^*),

c. $\{v_1, v_2, \ldots, v_r\}$ is an orthonormal basis of range(A^*), and

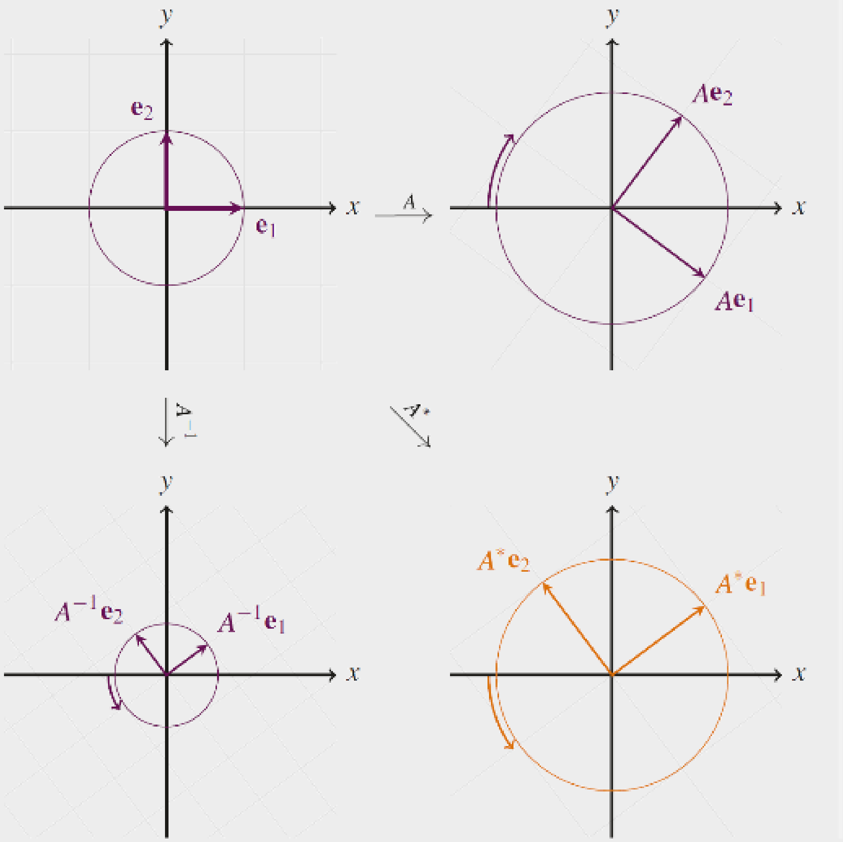
d. $\{v_{r+1}, v_{r+2}, \ldots, v_n\}$ is an orthonormal basis of null(A)

A Geometric Interpretation

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

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

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



Applications

Orthogonal Rank-One Sum Decomposition

- 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

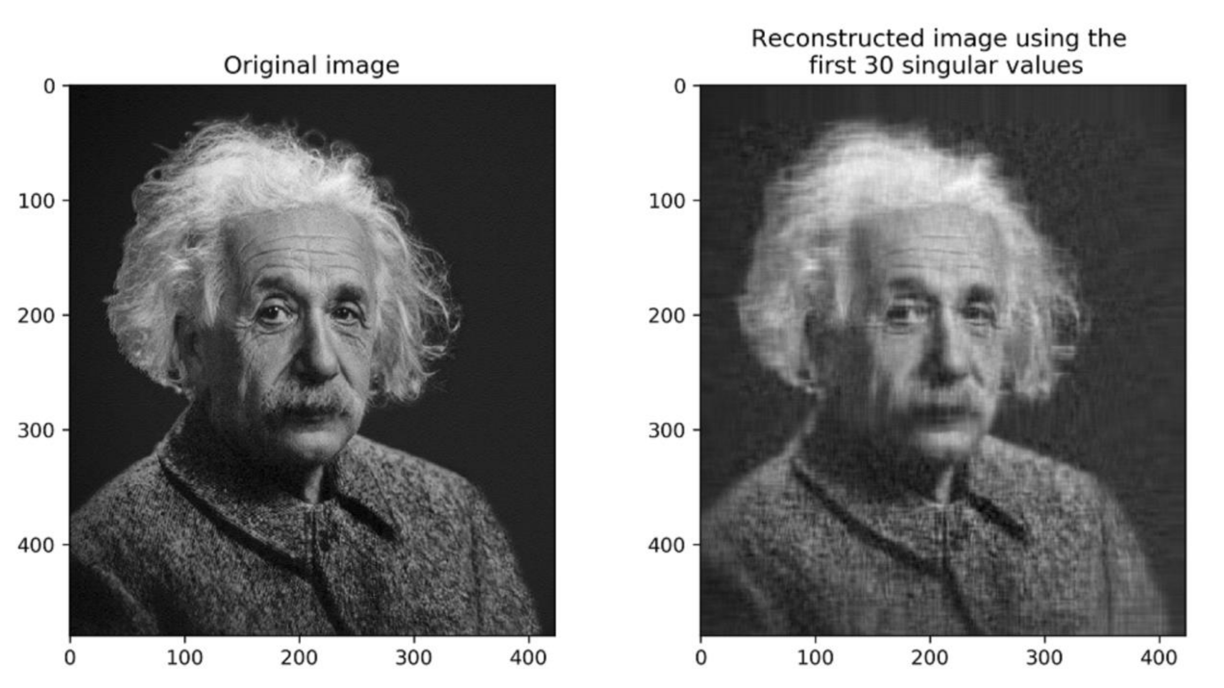
$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^*,$$

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

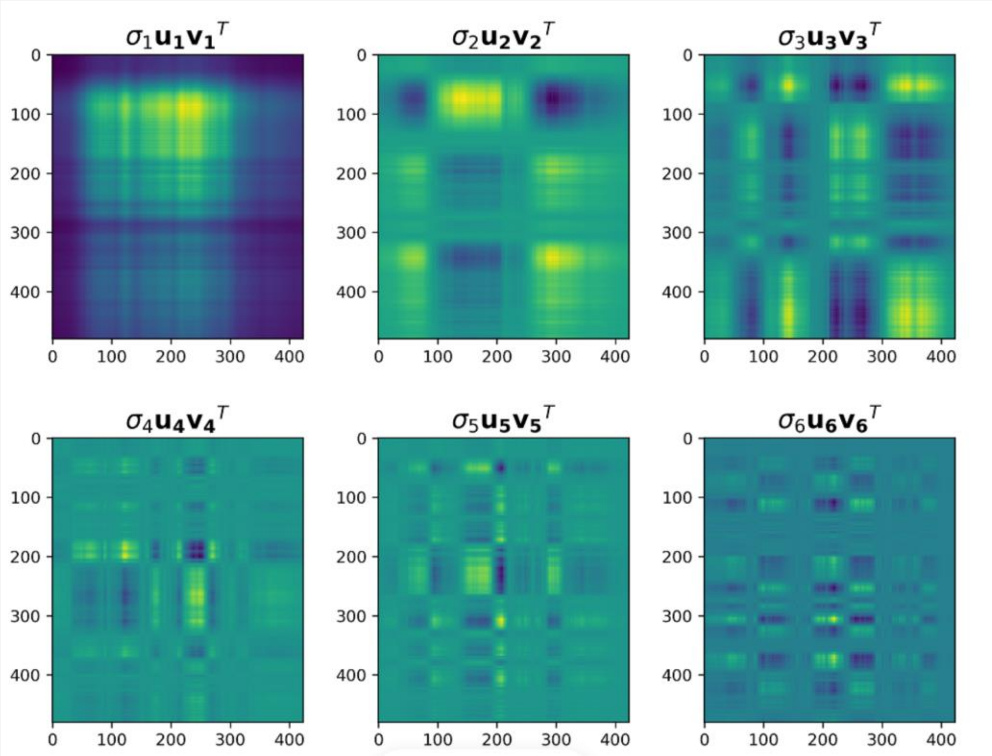
SVD and Matrix Similarity

- Suppose you want to find best rank−k approximation to **A**
  - Answer: set all but the largest k singular values to zero
- Can form compact representation by eliminating columns of **U** and **V** corresponding to zeroed Σ_i

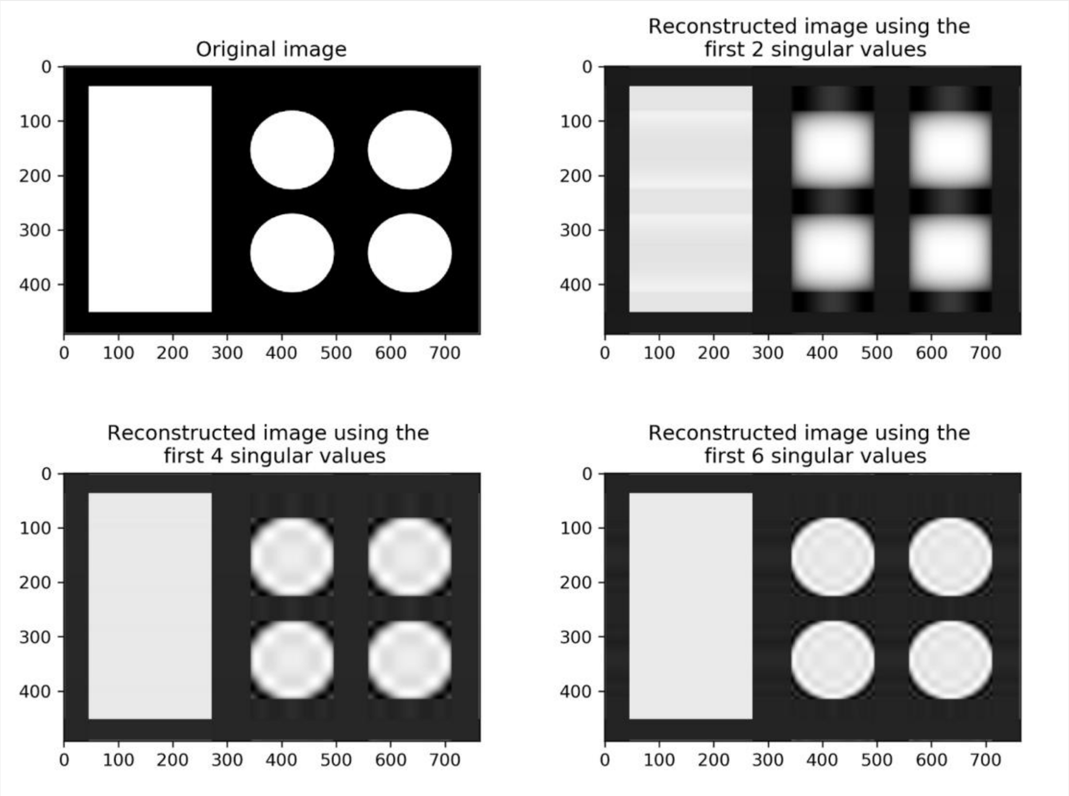
Application: Dimensionality Reduction



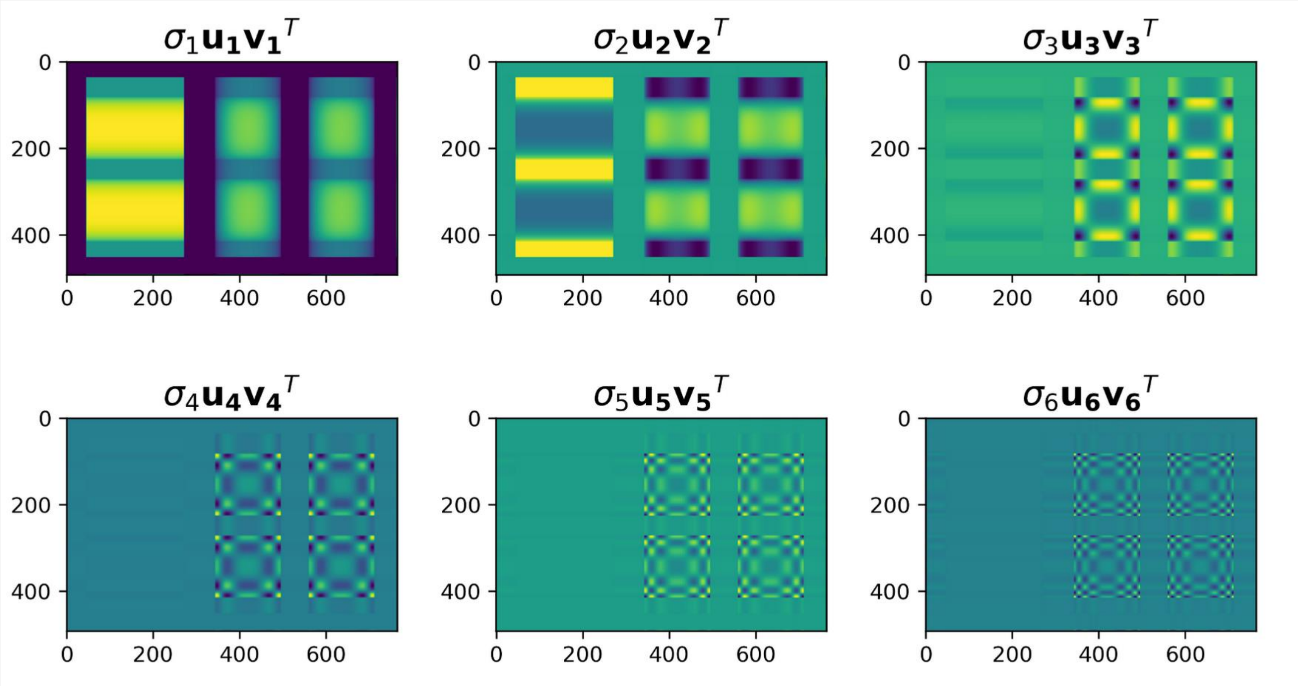
Application: Dimensionality Reduction



Application: Dimensionality Reduction



Application: Dimensionality Reduction




Low Rank Approximation of Image

SVD and PSD

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

SVD and Inverses

- 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 Σ is diagonal, Σ^{-1} also diagonal with reciprocals of entries of Σ
- This fails when some Σ_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 $(A^TA)^{-1}A^T$ if A^TA invertible

Pseudo Inverse

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

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

- Pseudo Inverse of a matrix A:

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

Moore–Penrose inverse (Pseudo Inverse)

- If a matrix A has the singular value decomposition

$$A = UWV^T$$

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

$$A^+ = VW^{-1}U^T$$

1.3 Moore-Penrose Conditions

For a matrix A^+ to be the pseudoinverse of A, it must satisfy the following four **Moore-Penrose conditions:**

1. (MP1) $AA^+A = A$
2. (MP2) $A^+AA^+ = A^+$
3. (MP3) $(AA^+)^T = AA^+$
4. (MP4) $(A^+A)^T = A^+A$

These conditions ensure that A^+ behaves similarly to an inverse, even when A is not invertible.

Pseudo Inverse

$$A^+ = VW^{-1}U^T$$

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

$A^+ = A^T(AA^T)^{-1}$ (it gives the least-norm solution $x_{l-n} = A^+b$)

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

SVD and Least Square

- $x^* = A^{-1}b = (UDV^T)^{-1}b,$

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

Moore–Penrose pseudoinverse

$$x^* = A^{-1}b = \boxed{VD^{-1}U^T} b$$

- Invert the diagonal entries in D that are nonzero, but leave the other diagonal entries alone as zeros.