

Singular Values and Singular Vectors

Linear Algebra

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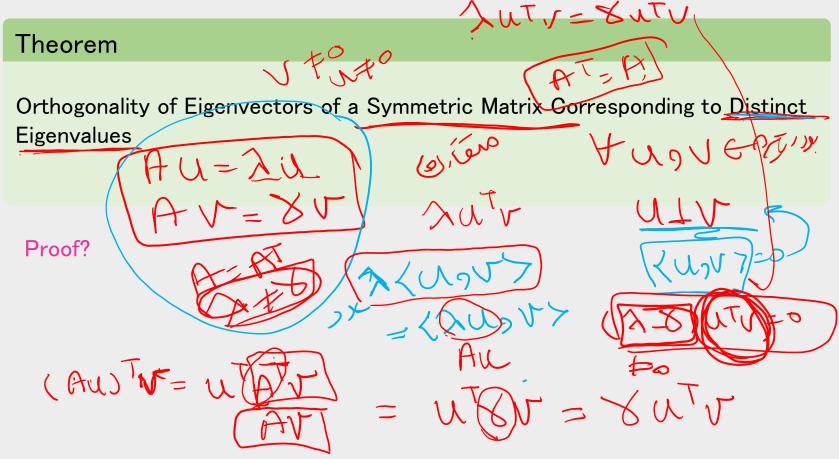
Introduction



range null space -PCA eigen value **Low-rank** approximation eigen vector TLS minimization transpose pseudoinverse inverse separable models symmetric matrix optimal rotation orthogonal matrix psd matrix 🐧

REVIEW: Eigenvectors of a Symmetric Matrix



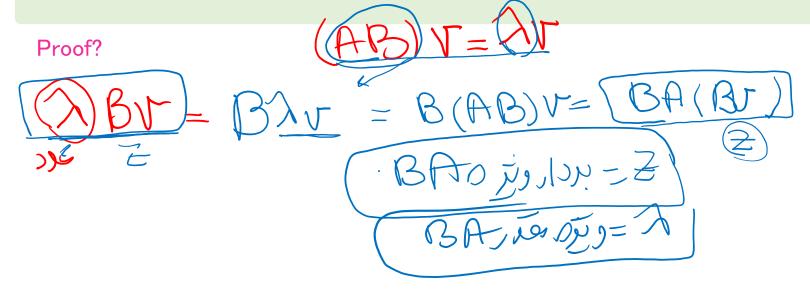


REVIEW: Eigenvalues



Theorem

The nonzero Eigenvalues of AB equal to the nonzero eigenvalues of BA.



Introduction



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

Singular Value



\square $S_{m \times n}$ Non-Square!!

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{m-1} \geq \sigma_m$$

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 eigenvalue



Theorem

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

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

Proof?

Singular value and eigenvalue



Example

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

$$v_{1} = \begin{bmatrix} 1/3 \\ 2/3 \\ 2/3 \end{bmatrix}, v_{2} = \begin{bmatrix} -2/3 \\ -1/3 \\ 2/3 \end{bmatrix}, v_{3} = \begin{bmatrix} 2/3 \\ -2/3 \\ 1/3 \end{bmatrix}$$

$$Sv_{1} = \begin{bmatrix} 18 \\ 6 \end{bmatrix} \Rightarrow ||Sv_{1}|| = \sqrt{18^{2} + 6^{2}} = \sigma_{1}$$

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

$$Sv_{3} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow ||Sv_{3}|| = 0 = \sigma_{3}$$

Singular value and Rank



Theorem

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

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

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

$$rank(S)=r$$

Rank of Matrix = Number of nonzero singular values

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

Singular Value Decomposition (SVD)



- □ Given any m×n matrix A, algorithm to find matrices U, V, and ∑ such that (always exists)

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

 \sum is $m \times n$ and diagonal with non-negative (always real) called <u>singular</u> values.

V is $n \times n$ and orthogonal (always real)

- \Box Columns of U are eigenvectors of AA^T (called the left singular vectors).
- \Box Columns of V are eigenvectors of A^TA (called the right singular vectors).
- The non-zero singular vectors are the positive square roots of non-zero eigenvalues of AA^T or A^TA .

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)
- o Provide a new geometric interpretation of linear transformations
- Solve optimization problems
- Construct an "almost inverse" for matrices that do not have an inverse.

SVD Comparison



SVD	Diagonalization	Spectral decomposition	Schur triangularization
applies to every single matrix (even rectangular ones).	only applies to matrices with a basis of eigenvectors	only applies to normal matrices	only applies to square matrices
matrix ∑ 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	only results in an upper triangular middle piece
It requires two unitary matrices U and V	only required one invertible matrix	only required one unitary matrix	only required one unitary matrix

SVD



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

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):

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

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



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

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

$$S[v_1 \quad \dots \quad v_n] = \begin{bmatrix} u_1 & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & & \vdots & 0 \\ 0 & \dots & \sigma_r & 0 \end{bmatrix}$$

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

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



what happens when A is not a square matrix?

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

$$= \begin{pmatrix} \vdots & \cdots & \vdots \\ u_{1} & \cdots & u_{m} \\ \vdots & \cdots & \vdots \end{pmatrix}_{m \times m} \begin{pmatrix} \sigma_{1} & & & & & \\ & \ddots & & & & \\ & & \sigma_{m} & & & \end{pmatrix}_{m \times n} \begin{pmatrix} \cdots & v_{1}^{T} & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_{m}^{T} & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & v_{n}^{T} & \cdots \end{pmatrix}_{n \times n}$$

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



We can instead rewrite the above as:

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

 $A = U\Sigma_R V_R^T$ 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



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.

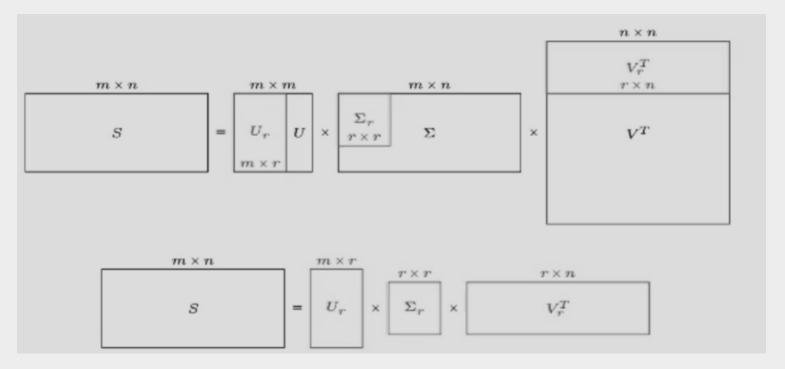
$$\Sigma^{T} \Sigma = \begin{pmatrix} \sigma_{1} & & & & & \\ & \ddots & & & & \\ & & \sigma_{n} & & & & \end{pmatrix}_{n \times m} \begin{pmatrix} \sigma_{1} & & & & \\ & \ddots & & & \\ & & \sigma_{n} & & & \\ & \vdots & \ddots & \vdots & \\ & 0 & \cdots & 0 & \end{pmatrix}_{m \times n} = \begin{pmatrix} \sigma_{1}^{2} & & & \\ & \ddots & & \\ & & \sigma_{n}^{2} \end{pmatrix}_{n \times n}$$

 \circ n \gt m:

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

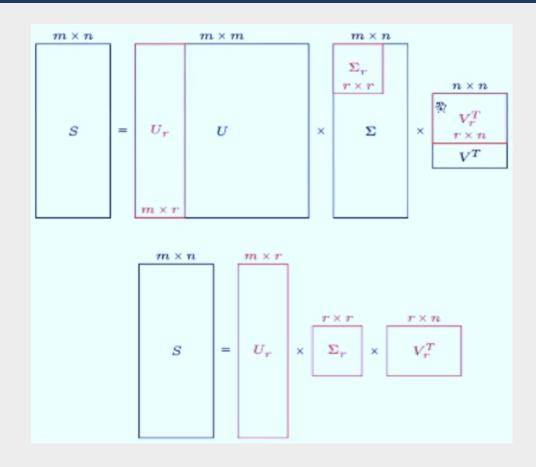


■ Wide Matrix





□ Tall Matrix





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

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

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:
 - \circ The columns of V are the eigenvectors of the matrix A^TA
 - \circ The diagonal entries of Σ^2 are the eigenvalues of A^TA
- \Box Let's call λ the eigenvalues of A^TA , then $\sigma_i^2 = \lambda_i$



☐ In a similar way,

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

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

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



- 1. Evaluate the n eigenvectors v_i and eigenvalues λ_i of A^TA
- 2. Make a matrix V from the normalized vectors v_i . The columns are called "right singular vectors".

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

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

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

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

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

$$\Delta(\lambda) = \lambda^{2} - 18\lambda = 0 \Rightarrow \sigma_{1} = \sqrt{18}, \sigma_{2} = 0 \Rightarrow \Sigma = \begin{bmatrix} 3\sqrt{2} & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

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

$$Sv_{1} = \begin{bmatrix} 2/\sqrt{2} \\ -4/\sqrt{2} \\ 4/\sqrt{2} \end{bmatrix} \Rightarrow u_{1} = \frac{1}{\sigma_{1}} Sv_{1} = \frac{1}{3\sqrt{2}} \begin{bmatrix} 2/\sqrt{2} \\ -4/\sqrt{2} \\ 4/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 1/3 \\ -2/3 \\ 2/3 \end{bmatrix}$$

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

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

Lemma



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

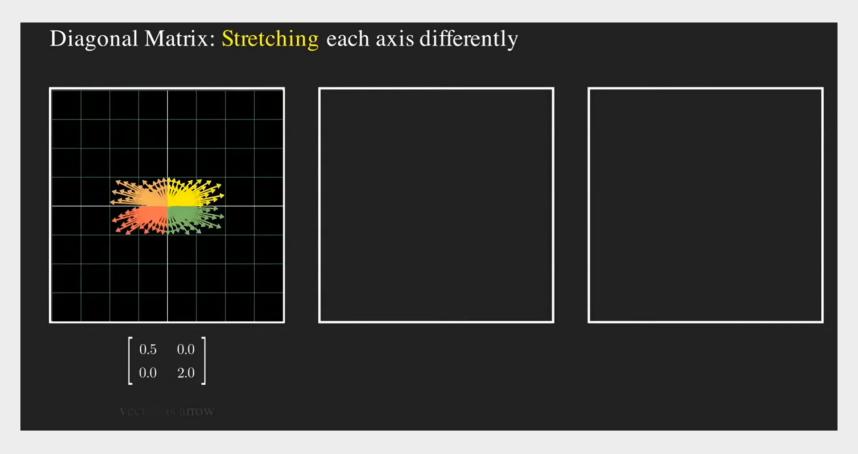


- If $m \neq n$ then A^*A , AA^* have different sizes, but they still have essentially the same eigenvalues—whichever one is larger just has some extra 0 eigenvalues.
- □ The same is actually true of AB and BA for any A and B.

□ Proof SVD in another view!!

Review



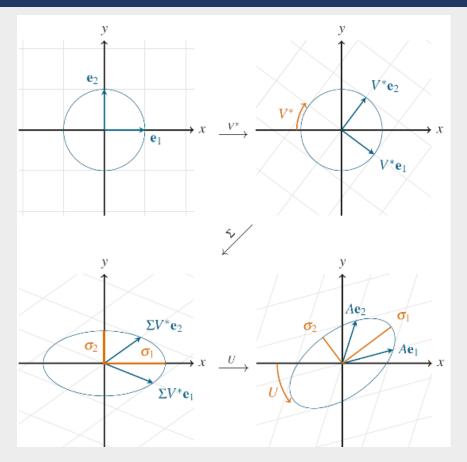


Geometric Interpretation and the Fundamental Subspaces



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

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



Determining the rank of a matrix



 \square Suppose A is a m x n rectangular matrix where m > n:

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

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

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

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

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

$$U = [u_1 \mid u_2 \mid ... \mid u_m]$$
 and $V = [v_1 \mid v_2 \mid ... \mid v_n]$

Then

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

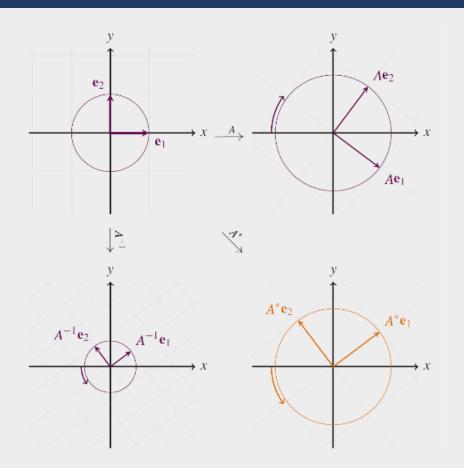
A Geometric Interpretation



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

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

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



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 $\mathrm{rank}(A) = r$. There exist orthonormal sets of vectors $\left\{u_j\right\}_{j=1}^r \subset \mathbb{F}^m$ and $\left\{v_j\right\}_{j=1}^r \subset \mathbb{F}^n$ such that

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

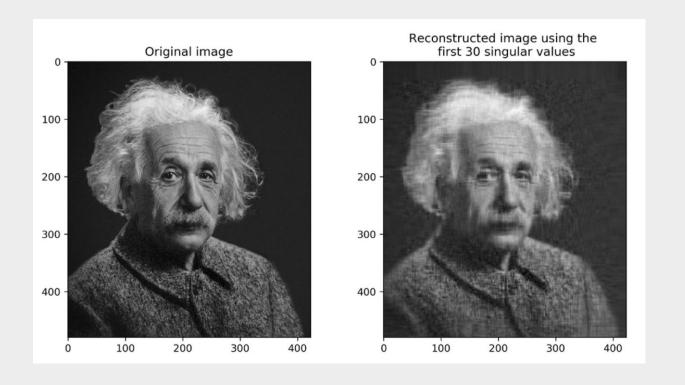
where $\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_r > 0$ are the non-zero singular values of A.

SVD and Matrix Similarity

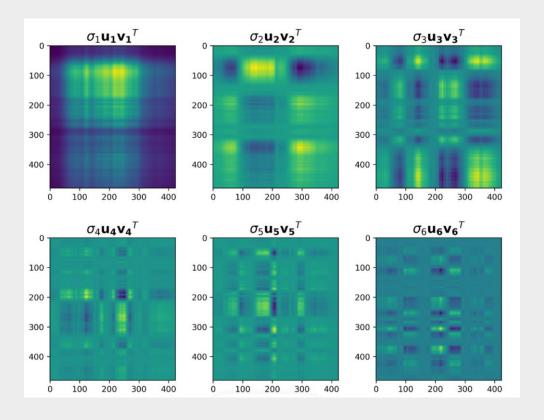


- \square Suppose you want to find best rank-k approximation to **A**
 - Answer: set all but the largest k singular values to zero
- fill Can form compact representation by eliminating columns of f U and f V corresponding to zeroed Σ_i

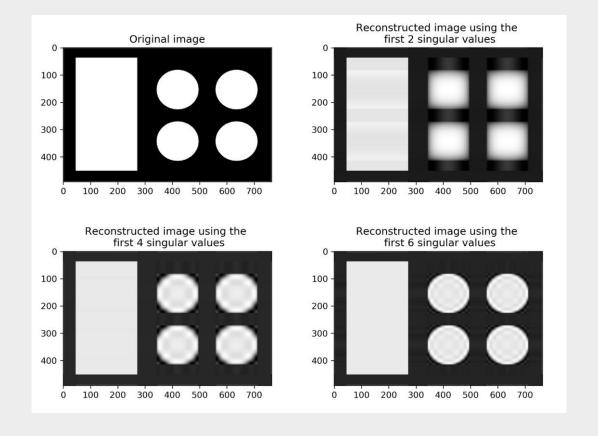




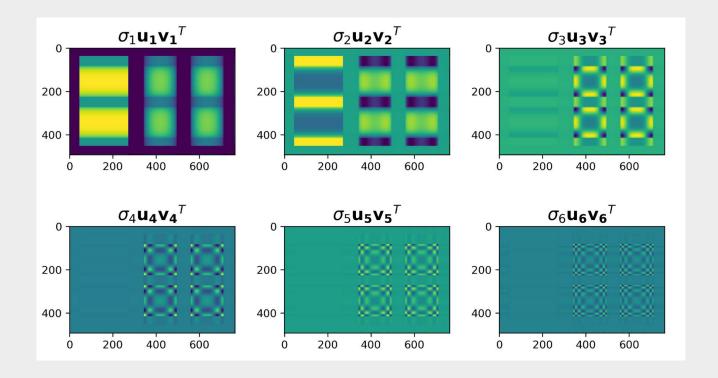












Image



Low Rank Approximation of Image



SVD and Inverses



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

- \Box This fails when some Σ_i are 0
 - o It's supposed to fail singular matrix
- \square Pseudoinverse: if $\Sigma_i = 0$, set $\frac{1}{\Sigma_i}$ to 0 (!)
 - o "Closest" matrix to inverse
 - Defined for all (even non-square, singular, etc.) matrices
 - \circ 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:

$$(\Sigma^{+})_{i} = \begin{cases} \frac{1}{\sigma_{i}}, & if \ \sigma_{i} \neq 0 \\ 0, & if \ \sigma_{i} = 0 \end{cases}$$

□ Pseudo Inverse of a matrix A:

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

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

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

- o If A is 'tall' (m > n) and has full rank $A^+ = (A^TA)^{-1}A^T \qquad \qquad \text{(it gives the least-squares solution } x_{lsq} = A^+b)$
- o If A is 'short' (n > m) and has full rank $A^+ = A^T (AA^T)^{-1} \qquad \qquad \text{(it gives the least-norm solution } x_{l-n} \\ = A^+b)$
- \circ In general, $x_{pinv} = A^+b$ is the minimum-norm, least-square solution.

SVD and Matrix Similarity



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

$$||A||_F = \sum_i \sum_j a_{ij}^2$$

□ Frobenius norm can be computed from SVD

$$||A||_{\mathcal{F}} = \sum_{i} \sum_{i}^{2}$$

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