Mathematics for Machine Learning

— Linear Algebra

Singular Value Decomposition & Matrix Approximation

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Fall 2025

Credits for the resource

- The slides are based on the textbooks:
 - Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.
 - Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.
 - Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.
- We could partially refer to the monograph: Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

Outline

- Singular Value Decomposition (SVD)
 - Construction of the SVD
 - Example

Matrix Approximation

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- Singular Value Decomposition (SVD)
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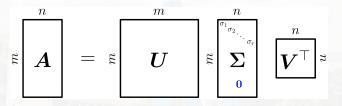
2 Matrix Approximation

Why Singular Value Decomposition?

- It can be applied to all matrices (not only to square matrices).
- It always exists.

Illustration

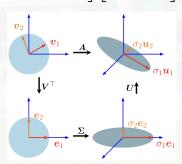
$$\mathbf{A} \in \mathbb{R}^{m \times n}$$
, rank $(\mathbf{A}) = r \leq \min(m, n)$:



- $U \in \mathbb{R}^{m \times m}$ with orthogonal columns vectors u_i , $i = 1, \dots, m$.
- $V \in \mathbb{R}^{n \times n}$ with orthogonal columns vectors \mathbf{v}_j , $j = 1, \dots, n$.
- $\Sigma \in \mathbb{R}^{m \times n}$ with $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0$ for $i \neq j$.
 - σ_i : singular values; $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r \geq 0$.
 - u_i: left-singular vectors;
 v_i: right-singular vectors;

Illustration & Example

$$\mathbf{A} = \begin{bmatrix} 1 & -0.8 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\top} \\
= \begin{bmatrix} -0.79 & 0 & -0.62 \\ 0.38 & -0.78 & -0.49 \\ -0.48 & -0.62 & 0.62 \end{bmatrix} \begin{bmatrix} 1.62 & 0 \\ 0 & 1.0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} -0.78 & 0.62 \\ -0.62 & -0.78 \end{bmatrix}$$



Exercise

Exercise

Prove that for an $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{A} \mathbf{A}^{\top}$ and $\mathbf{A}^{\top} \mathbf{A}$ have the same nonzero eigenvalues.

ML Math - Linear Algebra Singular Value Decomposition (SVD) Construction of the SVD

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2 Matrix Approximation

SVD & Eigendecomposition

Recall the eigendecomposition of a symmetric positive definite matrix

$$S = S^{\top} = PDP^{\top}$$
.

SVD & Eigendecomposition

Recall the eigendecomposition of a symmetric positive definite matrix

$$S = S^{\top} = PDP^{\top}.$$

with the corresponding SVD

$$S = U\Sigma V^{\top}$$

so
$$oldsymbol{U} = oldsymbol{P} = oldsymbol{V}$$
 , $oldsymbol{D} = oldsymbol{\Sigma}$.

The Overall Idea

- Computing the SVD of $\mathbf{A} \in \mathbb{R}^{m \times n} \Leftrightarrow$ Finding two sets of orthonormal bases $U = (\mathbf{u}_1, \dots, \mathbf{u}_m)$ and $V = (\mathbf{v}_1, \dots, \mathbf{v}_n)$ respectively.
- Images of Av_i 's form a set of orthogonal vectors.

The first step: Constructing the right-singular vectors

- **Recall:** Eigenvectors of a *symmetric* matrix form an orthonormal basis (the Spectral theorem).
- Also, we can always construct a symmetric, positive semidefinite matrix $\mathbf{A}^{\top} \mathbf{A} \in \mathbb{R}^{n \times n}$ from any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- Thus,

$$\mathbf{A}^{\top}\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{\top} = \mathbf{P} \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{bmatrix} \mathbf{P}^{\top},$$

where **P** is orthogonal and composed of orthonormal eigenbasis.

* $\lambda_i \geq 0$ are the eigenvalues of $\mathbf{A}^{\top} \mathbf{A}$.

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Assume the SVD of A exists.

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

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where U, V are orthonormal matrices $(: U^T U = I)$. So,

$$m{A}^{ op}m{A} = m{V}m{\Sigma}^{ op}m{\Sigma}m{V}^{ op} = m{V} egin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_n^2 \end{bmatrix} m{V}^{ op}$$

• Hence, we identify $\mathbf{V}^{\top} = \mathbf{P}^{\top}$ (right-singular vectors) and $\sigma_i^2 = \lambda_i$.

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The second step: Constructing the left-singular vectors

- Similarly, we can always construct a symmetric, positive semidefinite matrix $\mathbf{A}\mathbf{A}^{\top} \in \mathbb{R}^{m \times m}$ from any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- Thus, by assuming the SVD of **A** exists, we have

$$\mathbf{A}\mathbf{A}^{\top} = (\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\top})(\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\top})^{\top} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\top}\mathbf{V}\boldsymbol{\Sigma}^{\top}\mathbf{U}^{\top}$$
$$= \mathbf{U}\begin{bmatrix} \sigma_{1}^{2} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_{m}^{2} \end{bmatrix} \mathbf{U}^{\top}$$

Note: AA^{\top} and $A^{\top}A$ have the same nonzero eigenvalues.

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Note: AA^{\top} and $A^{\top}A$ have the same nonzero eigenvalues.

 \Rightarrow The nonzero entries of Σ in the SVD for both steps must be the same.

Images of the v_i under A must be orthogonal.

$$(\mathbf{A}\mathbf{v}_i)^{\top}(\mathbf{A}\mathbf{v}_j) = \mathbf{v}_i^{\top}(\mathbf{A}^{\top}\mathbf{A})\mathbf{v}_j = \mathbf{v}_i^{\top}(\lambda_j\mathbf{v}_j) = \lambda_j\mathbf{v}_i^{\top}\mathbf{v}_j = 0.$$

(For $m \ge r$) We observe that $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is a basis of an r-dimensional subspace of \mathbb{R}^m .

Construction of the SVD

The last step: Link up all parts (1/2)

Images of the v_i under A must be orthogonal.

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(For $m \ge r$) We observe that $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is a basis of an r-dimensional subspace of \mathbb{R}^m .

Normalize the images of these right-singular vectors:

$$\mathbf{u}_i := \frac{\mathbf{A}\mathbf{v}_i}{\|\mathbf{A}\mathbf{v}_i\|} = \frac{\mathbf{A}\mathbf{v}_i}{\sqrt{(\mathbf{A}\mathbf{v}_i)^{\top}(\mathbf{A}\mathbf{v}_i)}} = \frac{1}{\sqrt{\lambda_i}}\mathbf{A}\mathbf{v}_i = \frac{1}{\sigma_i}\mathbf{A}\mathbf{v}_i.$$

• That is, $\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i$, for $i = 1, \dots, r$.

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- Concatenate the \mathbf{v}_i 's as the columns of \mathbf{V} ;
- Concatenate the \mathbf{u}_i 's as the columns of \mathbf{U} ;

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Thus,

$$A = AVV^{\top} = U\Sigma V^{\top}$$

Exercise

Why do we have $\mathbf{A} = \mathbf{AVV}^{\top}$?

•
$$\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i$$
 (from $\mathbf{A}^{\top} \mathbf{A} \mathbf{v}_i = \lambda_i \mathbf{u}_i \ \& \ \mathbf{u}_i := \mathbf{A} \mathbf{v}_i / \| \mathbf{A} \mathbf{v}_i \|$).

- $\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i$ (from $\mathbf{A}^{\top} \mathbf{A} \mathbf{v}_i = \lambda_i \mathbf{u}_i$ & $\mathbf{u}_i := \mathbf{A} \mathbf{v}_i / \|\mathbf{A} \mathbf{v}_i\|$). $\Rightarrow \mathbf{u}_i = \frac{1}{\sigma_i} \mathbf{A} \mathbf{v}_i$.
- $\bullet \ \mathbf{A}^{\top}\mathbf{u}_{i} = \frac{1}{\sigma_{i}}\mathbf{A}^{\top}\mathbf{A}\mathbf{v}_{i} = \frac{1}{\sigma_{i}}\lambda_{i}\mathbf{v}_{i} = \frac{\sigma_{i}\mathbf{v}_{i}}{\sigma_{i}}.$

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- $\mathbf{A}^{\top}\mathbf{u}_{i} = \frac{1}{\sigma_{i}}\mathbf{A}^{\top}\mathbf{A}\mathbf{v}_{i} = \frac{1}{\sigma_{i}}\lambda_{i}\mathbf{v}_{i} = \sigma_{i}\mathbf{v}_{i}.$ Also, $\mathbf{A}\mathbf{A}^{\top}\mathbf{u}_{i} = \sigma_{i}\mathbf{A}\mathbf{v}_{i} = \sigma_{i}^{2}\mathbf{u}_{i} = \lambda_{i}\mathbf{u}_{i}.$

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- $\mathbf{A}^{\top}\mathbf{u}_{i} = \frac{1}{\sigma_{i}}\mathbf{A}^{\top}\mathbf{A}\mathbf{v}_{i} = \frac{1}{\sigma_{i}}\lambda_{i}\mathbf{v}_{i} = \sigma_{i}\mathbf{v}_{i}.$ Also, $\mathbf{A}\mathbf{A}^{\top}\mathbf{u}_{i} = \sigma_{i}\mathbf{A}\mathbf{v}_{i} = \sigma_{i}^{2}\mathbf{u}_{i} = \lambda_{i}\mathbf{u}_{i}.$
- Starting from the eigendecomposition of $\mathbf{A}\mathbf{A}^{\top}$ we can still get \mathbf{u}_{i} .

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Singular Value Decomposition (SVD)
Example

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Example

Find the singular value decomposition of

$$\mathbf{A} = \left[\begin{array}{rrr} 1 & 0 & 1 \\ -2 & 1 & 0 \end{array} \right]$$

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Note:

$$\mathbf{A}^{\top}\mathbf{A} = \begin{bmatrix} 1 & -2 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 5 & -2 & 1 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}.$$

SVD Example (step 1/2)

Goal: Find $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\top}$.

Perform eigendecomposition of $\mathbf{A}^{\top}\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{\top}$:

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Perform eigendecomposition of $\mathbf{A}^{\top}\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{\top}$:

$$\mathbf{A}^{\top}\mathbf{A} = \begin{bmatrix} \frac{5}{\sqrt{30}} & 0 & \frac{-1}{\sqrt{6}} \\ \frac{-2}{\sqrt{30}} & \frac{1}{\sqrt{5}} & \frac{-2}{\sqrt{6}} \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 6 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{5}{\sqrt{30}} & \frac{-2}{\sqrt{30}} & \frac{1}{\sqrt{30}} \\ 0 & \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{-1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix}$$

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So,

$$m{V} = m{P} = \left[egin{array}{cccc} rac{5}{\sqrt{30}} & 0 & rac{-1}{\sqrt{6}} \ rac{-2}{\sqrt{30}} & rac{1}{\sqrt{5}} & rac{-2}{\sqrt{6}} \ rac{1}{\sqrt{20}} & rac{2}{\sqrt{6}} & rac{1}{\sqrt{6}} \end{array}
ight], \; m{\Sigma} = \left[egin{array}{cccc} \sqrt{6} & 0 & 0 \ 0 & 1 & 0 \end{array}
ight]$$

where $\sigma^2 = 6$, $\sigma_2^2 = 1 \implies \sigma_1 = \sqrt{6}$, $\sigma_2 = 1$.

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Singular Value Decomposition (SVD)
Example

SVD Example (step 2/2)

Left-singular vectors:



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Example

SVD Example (step 2/2)

Left-singular vectors:

$$\mathbf{u}_1 = \frac{1}{\sigma_1} \mathbf{A} \mathbf{v}_1 = \frac{1}{\sqrt{6}} \left[\begin{array}{ccc} 1 & 0 & 1 \\ -2 & 1 & 0 \end{array} \right] \left[\begin{array}{c} 5/\sqrt{30} \\ -2/\sqrt{30} \\ 1/\sqrt{30} \end{array} \right] = \left[\begin{array}{c} 1/\sqrt{5} \\ -2/\sqrt{5} \end{array} \right],$$

$$\mathbf{u}_2 = \frac{1}{\sigma_2} \mathbf{A} \mathbf{v}_2 = \frac{1}{1} \left[\begin{array}{cc} 1 & 0 & 1 \\ -2 & 1 & 0 \end{array} \right] \left[\begin{array}{c} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{array} \right] = \left[\begin{array}{c} 2/\sqrt{5} \\ 1/\sqrt{5} \end{array} \right].$$

Then, we derive
$$\boldsymbol{U} = [\mathbf{u}_1, \mathbf{u}_2] = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}$$
.

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Matrix Approximation

Motivation

- Represent a matrix A as a sum of simpler low-rank matrices A_i .
- Cheaper than computing the full SVD.
- Rank-1 matrix $\mathbf{A}_i \in \mathbb{R}^{m \times n}$:

$$\mathbf{A}_i = \mathbf{u}_i \mathbf{v}_i^{\top}$$
. (outer product)

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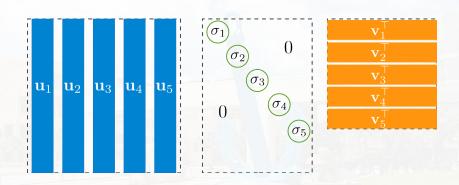
$$\mathbf{A}_i = \mathbf{u}_i \mathbf{v}_i^{\top}$$
. (outer product)

In fact, we can derive

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_{i} \mathbf{u}_{i} \mathbf{v}_{i}^{\top} = \sum_{i=1}^{r} \sigma_{i} \mathbf{A}_{i}.$$

• Outer-product matrices A_i weighted by the *i*th singular value σ_i .

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• σ_i is multiplied with \mathbf{u}_i and \mathbf{v}_i^{\top} .

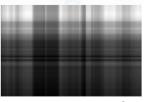
Rank-k Approximation

Up to an intermediate value k < r (assume that σ_i 's are sorted in decreasing order),

$$\hat{\mathbf{A}}(k) := \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^{\top} = \sum_{i=1}^k \sigma_i \mathbf{A}_i$$

Illustrating example







(a) Original image A.

(b) Rank-1 approximation $\widehat{A}(1)$.(c) Rank-2 approximation $\widehat{A}(2)$.







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(d) Rank-3 approximation $\widehat{A}(3)$.(e) Rank-4 approximation $\widehat{A}(4)$.(f) Rank-5 approximation $\widehat{A}(5)$.

Measure the difference b/w \boldsymbol{A} and $\hat{\boldsymbol{A}}$

Spectral Norm

For $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, the spectral norm of $\mathbf{A} \in \mathbb{R}^{m \times n}$ is

$$\|\boldsymbol{A}\|_2 = \max_{\mathbf{x}} \frac{\|\boldsymbol{A}\mathbf{x}\|_2}{\|\mathbf{x}\|_2}$$

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• Think about why we need to divide the norm $\|\mathbf{x}\|_2$.

Theorem & Exercise

Theorem (4.24)

The spectral norm of \boldsymbol{A} is its largest singular value σ_1 .

Eckart-Young Theorem

Theorem [Eckart & Young 1936]

Consider $\mathbf{A} \in \mathbb{R}^{m \times n}$ of rank r and let $\mathbf{B} \in \mathbb{R}^{m \times n}$ be a matrix of rank k.

Then for any $k \leq r$ with $\hat{\mathbf{A}}(k) = \sum_{i=1}^k \sigma_1 \mathbf{u}_i \mathbf{v}_i^{\top}$, it holds that

$$\hat{\mathbf{A}}(k) = \underset{\mathsf{rank}(\mathbf{B})=k}{\mathsf{arg min}} \|\mathbf{A} - \mathbf{B}\|_2,$$

$$\|\mathbf{A} - \hat{\mathbf{A}}(k)\|_2 = \sigma_{k+1}.$$

Physical meaning:

- We can view the rank-k approximation as a projection of the matrix
 A onto a lower-dimensional space of rank-at-most-k matrices.
- The approximation error: the next singular value (i.e., σ_{k+1})!

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Note that

$$\mathbf{A} - \hat{\mathbf{A}}(k) = \sum_{i=k+1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\top}.$$

By Theorem 4.24, we have $\|\mathbf{A} - \hat{\mathbf{A}}(k)\|_2 = \sigma_{k+1}$ (spectral norm).

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But why $\hat{\mathbf{A}}$ is the best approximation in some sense?

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But why $\hat{\mathbf{A}}$ is the best approximation in some sense?

Assume that r > k and there is another **B** with rank(**B**) $\leq k$, such that

$$\|\mathbf{A} - \mathbf{B}\|_2 < \|\mathbf{A} - \hat{\mathbf{A}}(k)\|_2.$$

Note that $\dim(\operatorname{null}(\boldsymbol{B})) \geq n - k$.

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$$x \in Z, Bx = 0.$$

$$\Rightarrow \|\mathbf{A}\mathbf{x}\|_{2} = \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_{2} \le \|\mathbf{A} - \mathbf{B}\|_{2}\|\mathbf{x}\|_{2}$$

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$$\Rightarrow \|\mathbf{A}\mathbf{x}\|_{2} = \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_{2} \le \|\mathbf{A} - \mathbf{B}\|_{2}\|\mathbf{x}\|_{2} < \sigma_{k+1}\|\mathbf{x}\|_{2}. \quad \cdots (\dagger)$$

Note that $\dim(\operatorname{null}(\boldsymbol{B})) \geq n - k$.

There exists an $\geq (n-k)$ -dimensional null space $Z \subseteq \mathbb{R}^n$ such that

$$x \in Z, Bx = 0.$$

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However, there exists a (k+1)-dimensional subspace Y spanned by $\mathbf{v}_1, \dots, \mathbf{v}_{k+1}$.

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$$\Rightarrow \|\mathbf{A}\mathbf{x}\|_{2} = \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_{2} \leq \|\mathbf{A} - \mathbf{B}\|_{2}\|\mathbf{x}\|_{2} < \frac{\sigma_{k+1}}{2}\|\mathbf{x}\|_{2}, \quad \cdots (\dagger)$$

However, there exists a (k+1)-dimensional subspace Y spanned by $\mathbf{v}_1, \dots, \mathbf{v}_{k+1}$.

Note that for $\mathbf{x} \in Y$, $\|\mathbf{A}\mathbf{x}\|_2 \ge \sigma_{k+1}\|\mathbf{x}\|_2$. \cdots (‡) (Exercise!)

Note that $\dim(\operatorname{null}(\boldsymbol{B})) \geq n - k$.

There exists an $\geq (n-k)$ -dimensional null space $Z \subseteq \mathbb{R}^n$ such that

$$x \in Z, Bx = 0.$$

$$\Rightarrow \|\mathbf{A}\mathbf{x}\|_{2} = \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_{2} \leq \|\mathbf{A} - \mathbf{B}\|_{2}\|\mathbf{x}\|_{2} < \frac{\sigma_{k+1}}{2}\|\mathbf{x}\|_{2}, \quad \cdots (\dagger)$$

However, there exists a (k+1)-dimensional subspace Y spanned by $\mathbf{v}_1, \dots, \mathbf{v}_{k+1}$.

Note that for
$$\mathbf{x} \in Y$$
, $\|\mathbf{A}\mathbf{x}\|_2 \ge \sigma_{k+1}\|\mathbf{x}\|_2$. \cdots (‡) (Exercise!)

But by the Dimension Theorem (rank-nullity theorem), there must be $x \in Y \cap Z$. ($\Rightarrow \Leftarrow$)

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Sketch of the Proof of (\ddagger)

- For any $\mathbf{x} \in Y = \text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$, write $\mathbf{x} = \sum_{i=1}^{k+1} \alpha_i \mathbf{v}_i$.
- \mathbf{v}_i 's and \mathbf{u}_i 's are orthonormal \Rightarrow

$$\|\mathbf{x}\|_2^2 = \sum_{i=1}^{k+1} \alpha_i^2, \qquad \mathbf{A}\mathbf{x} = \sum_{i=1}^{k+1} \alpha_i \mathbf{A} \mathbf{v}_i = \sum_{i=1}^{k+1} \alpha_i \sigma_i \mathbf{u}_i.$$

Hence,

$$\|\mathbf{A}\mathbf{x}\|_{2}^{2} = \left\| \sum_{i=1}^{k+1} \alpha_{i} \sigma_{i} \mathbf{u}_{i} \right\|_{2}^{2} = \sum_{i=1}^{k+1} \sigma_{i}^{2} \alpha_{i}^{2} \ge \sigma_{k+1}^{2} \sum_{i=1}^{k+1} \alpha_{i}^{2} = \sigma_{k+1}^{2} \|\mathbf{x}\|_{2}^{2}.$$

Proof of Theorem 4.24

$$\|\mathbf{A}\|_2 = \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \sup_{\mathbf{x} \neq \mathbf{0}} \|\mathbf{A}\frac{\mathbf{x}}{\|\mathbf{x}\|_2}\|_2 = \sup_{\|\mathbf{x}\|_2 = 1} \|\mathbf{A}\mathbf{x}\|_2.$$

- Let $\mathbf{B} := \mathbf{A}^{\top} \mathbf{A} \in \mathbb{R}^{n \times n}$.
- Then \boldsymbol{B} is symmetric positive semidefinite and admits the eigen-decomposition $\boldsymbol{A}^{\top}\boldsymbol{A} = \boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{\top}$, for $\boldsymbol{P} = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ containing orthonormal column vectors, and $\boldsymbol{D} = \operatorname{diag}(\lambda_1, \dots, \lambda_n), \ \lambda_i \geq 0$.

Proof of Theorem 4.24 (Upper Bound)

Write
$$\mathbf{x} = \sum_{i=1}^{n} a_i \mathbf{v}_i$$
. Then

$$\|\mathbf{A}\mathbf{x}\|_{2}^{2} = \mathbf{x}^{\top}\mathbf{A}^{\top}\mathbf{A}\mathbf{x} = \left(\sum_{i=1}^{n} a_{i}\mathbf{v}_{i}\right)^{\top}\left(\sum_{i=1}^{n} a_{i}\lambda_{i}\mathbf{v}_{i}\right) = \sum_{i=1}^{n} a_{i}^{2}\lambda_{i}$$

$$\leq \left(\max_{1\leq i\leq n} \lambda_{i}\right)\sum_{i=1}^{n} a_{i}^{2} = \left(\max_{i} \lambda_{i}\right)\|\mathbf{x}\|_{2}^{2}.$$

Hence,

$$\|\mathbf{A}\mathbf{x}\|_2 \leq \sqrt{\max_i \lambda_i} \, \|\mathbf{x}\|_2 \quad \Rightarrow \quad \|\mathbf{A}\|_2 \leq \sqrt{\max_i \lambda_i} \,.$$

Proof of Theorem 4.24 (Lower Bound and Final)

• Let \mathbf{v}_k be an eigenvector of $\mathbf{A}^{\top}\mathbf{A}$ with $\lambda_k = \max_i \lambda_i$ and $\|\mathbf{v}_k\|_2 = 1$. Then

$$\|\mathbf{A}\mathbf{v}_k\|_2^2 = \mathbf{v}_k^{\top}\mathbf{A}^{\top}\mathbf{A}\mathbf{v}_k = \lambda_k.$$

• Therefore $\|\mathbf{A}\|_2 \ge \|\mathbf{A}\mathbf{v}_k\|_2 \ge \sqrt{\lambda_k} = \sqrt{\max_i \lambda_i}$. Combining with the upper bound gives

$$\|\mathbf{A}\|_2 = \sqrt{\lambda_{\max}(\mathbf{A}^{\top}\mathbf{A})} = \sigma_{\max}(\mathbf{A}) = \max_i \sigma_i,$$

where σ_i are the singular values of **A** and $\lambda_i = \sigma_i^2$.

Discussions