

Mathematics for Machine Learning

— Linear Algebra

Singular Value Decomposition & Matrix Approximation

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

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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.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

Outline

- 1 Singular Value Decomposition (SVD)
 - Construction of the SVD
 - Example
- 2 Matrix Approximation

Outline

1 Singular Value Decomposition (SVD)

- Construction of the SVD
- Example

2 Matrix Approximation

Why Singular Value Decomposition?

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

Illustration

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

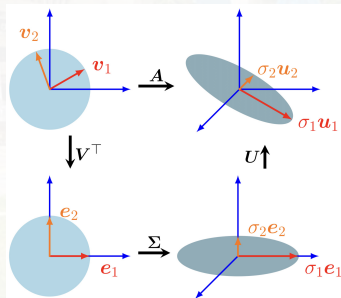
$$\begin{matrix} n \\ \boxed{\mathbf{A}} \\ m \end{matrix} = \begin{matrix} m \\ \boxed{\mathbf{U}} \\ m \end{matrix} \begin{matrix} n \\ \boxed{\Sigma} \\ m \end{matrix} \begin{matrix} n \\ \boxed{\mathbf{V}^T} \\ n \end{matrix}$$

Matrix Σ contains singular values $\sigma_1, \sigma_2, \dots, \sigma_r$ on the diagonal and a zero block below.

- $\mathbf{U} \in \mathbb{R}^{m \times m}$ with orthogonal columns vectors \mathbf{u}_i , $i = 1, \dots, m$.
- $\mathbf{V} \in \mathbb{R}^{n \times n}$ 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**; $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r \geq 0$.
 - \mathbf{u}_i : **left-singular vectors**;
 - \mathbf{v}_j : **right-singular vectors**;

Illustration & Example

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



Exercise

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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.

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SVD & Eigendecomposition

- Recall the eigendecomposition of a symmetric positive definite matrix

$$\mathbf{S} = \mathbf{S}^{\top} = \mathbf{P}\mathbf{D}\mathbf{P}^{\top}.$$

SVD & Eigendecomposition

- Recall the eigendecomposition of a symmetric positive definite matrix

$$\mathbf{S} = \mathbf{S}^T = \mathbf{P}\mathbf{D}\mathbf{P}^T.$$

with the corresponding SVD

$$\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

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

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 $\mathbf{A}\mathbf{v}_i$'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 \mathbf{P} is orthogonal and composed of orthonormal eigenbasis.

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

The first step (2/2)

- Assume the SVD of \mathbf{A} exists.

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

where \mathbf{U} , \mathbf{V} are orthonormal matrices

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where \mathbf{U}, \mathbf{V} are orthonormal matrices ($\because \mathbf{U}^\top \mathbf{U} = \mathbf{I}$). So,

$$\mathbf{A}^\top \mathbf{A} = \mathbf{V} \mathbf{\Sigma}^\top \mathbf{\Sigma} \mathbf{V}^\top = \mathbf{V} \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_n^2 \end{bmatrix} \mathbf{V}^\top$$

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

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 \mathbf{A} exists, we have

$$\begin{aligned}\mathbf{A}\mathbf{A}^\top &= (\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top)(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top)^\top = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\mathbf{V}\mathbf{\Sigma}^\top\mathbf{U}^\top \\ &= \mathbf{U} \begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_m^2 \end{bmatrix} \mathbf{U}^\top\end{aligned}$$

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

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⇒ The nonzero entries of $\mathbf{\Sigma}$ in the SVD for both steps must be the same.

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

Images of the \mathbf{v}_i under \mathbf{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 $m \geq r$) We observe that $\{\mathbf{A}\mathbf{v}_1, \dots, \mathbf{A}\mathbf{v}_r\}$ is a basis of an r -dimensional subspace of \mathbb{R}^m .

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- Normalize the images of these right-singular vectors:

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

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

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

- Concatenate the \mathbf{v}_i 's as the columns of \mathbf{V} ;
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$$\mathbf{A}\mathbf{V} = \mathbf{U}\mathbf{\Sigma} \in \mathbb{R}^{m \times n}.$$

Thus,

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

Exercise

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

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Example

Find the singular value decomposition of

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{bmatrix}$$

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Note:

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

SVD Example (step 1/2)

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

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

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

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

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So,

$$\mathbf{V} = \mathbf{P} = \begin{bmatrix} \frac{5}{\sqrt{30}} & 0 & \frac{-1}{\sqrt{6}} \\ \frac{-2}{\sqrt{30}} & \frac{1}{\sqrt{5}} & \frac{-2}{\sqrt{6}} \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{6}} \end{bmatrix}, \quad \mathbf{\Sigma} = \begin{bmatrix} \sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

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

SVD Example (step 2/2)

Left-singular vectors:

SVD Example (step 2/2)

Left-singular vectors:

$$\mathbf{u}_1 = \frac{1}{\sigma_1} \mathbf{A} \mathbf{v}_1 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{bmatrix} \begin{bmatrix} 5/\sqrt{30} \\ -2/\sqrt{30} \\ 1/\sqrt{30} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{5} \\ -2/\sqrt{5} \end{bmatrix},$$

$$\mathbf{u}_2 = \frac{1}{\sigma_2} \mathbf{A} \mathbf{v}_2 = \frac{1}{1} \begin{bmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix} = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}.$$

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

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Motivation

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

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

Motivation

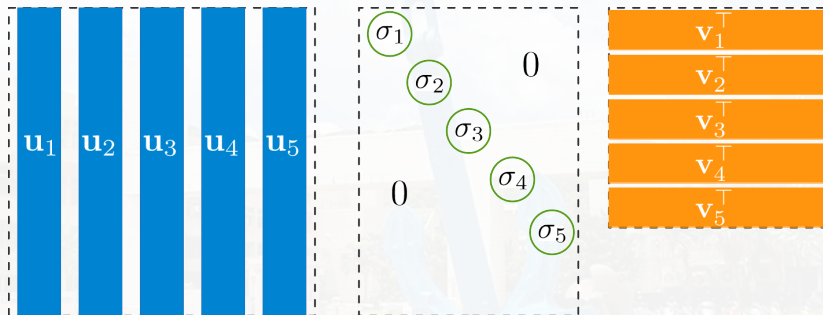
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- In fact, we can derive

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

- Outer-product matrices \mathbf{A}_i weighted by the i th singular value σ_i .



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

Rank- k Approximation

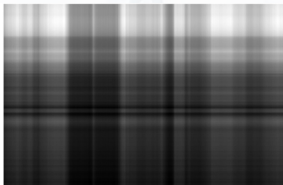
Up to an intermediate value $k < r$ (assume that σ_i 's are sorted in decreasing order),

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

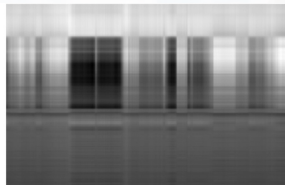
Illustrating example



(a) Original image A .



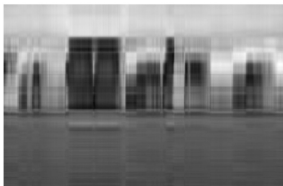
(b) Rank-1 approximation $\hat{A}(1)$.



(c) Rank-2 approximation $\hat{A}(2)$.



(d) Rank-3 approximation $\hat{A}(3)$.



(e) Rank-4 approximation $\hat{A}(4)$.



(f) Rank-5 approximation $\hat{A}(5)$.

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

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

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

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

$$\hat{\mathbf{A}}(k) = \arg \min_{\text{rank}(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_2,$$

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

Physical meaning:

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

Sketch of the Proof (1/2)

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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Assume that $r > k$ and there is another \mathbf{B} with $\text{rank}(\mathbf{B}) \leq k$, such that

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

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

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$$\Rightarrow \|\mathbf{A}\mathbf{x}\|_2 = \|(\mathbf{A} - \mathbf{B})\mathbf{x}\|_2 \leq \|\mathbf{A} - \mathbf{B}\|_2 \|\mathbf{x}\|_2 < \sigma_{k+1} \|\mathbf{x}\|_2. \quad \cdots (\dagger)$$

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

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

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

Sketch of the Proof of (\dagger)

- 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

$$\|\mathbf{x}\|_2^2 = \sum_{i=1}^{k+1} \alpha_i^2, \quad \mathbf{Ax} = \sum_{i=1}^{k+1} \alpha_i \mathbf{Av}_i = \sum_{i=1}^{k+1} \alpha_i \sigma_i \mathbf{u}_i.$$

- Hence,

$$\|\mathbf{Ax}\|_2^2 = \left\| \sum_{i=1}^{k+1} \alpha_i \sigma_i \mathbf{u}_i \right\|_2^2 = \sum_{i=1}^{k+1} \sigma_i^2 \alpha_i^2 \geq \sigma_{k+1}^2 \sum_{i=1}^{k+1} \alpha_i^2 = \sigma_{k+1}^2 \|\mathbf{x}\|_2^2.$$

Proof of Theorem 4.24

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

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

Proof of Theorem 4.24 (Upper Bound)

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

$$\begin{aligned}\|\mathbf{Ax}\|_2^2 &= \mathbf{x}^\top \mathbf{A}^\top \mathbf{Ax} = \left(\sum_{i=1}^n a_i \mathbf{v}_i \right)^\top \left(\sum_{i=1}^n a_i \lambda_i \mathbf{v}_i \right) = \sum_{i=1}^n a_i^2 \lambda_i \\ &\leq \left(\max_{1 \leq i \leq n} \lambda_i \right) \sum_{i=1}^n a_i^2 = \left(\max_i \lambda_i \right) \|\mathbf{x}\|_2^2.\end{aligned}$$

Hence,

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

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 $\|\mathbf{A}\|_2 \geq \|\mathbf{A}\mathbf{v}_k\|_2 \geq \sqrt{\lambda_k} = \sqrt{\max_i \lambda_i}$. 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 \mathbf{A} and $\lambda_i = \sigma_i^2$.

Discussions