

中国科学院大学
2026

数值代数 Numerical Algebra

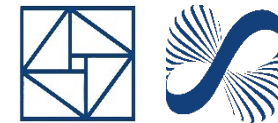
第二章、线性代数基础

Fundamentals of Linear Algebra

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第二章、线性代数基础

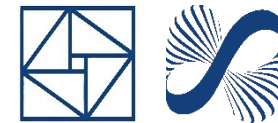
本章旨在回顾并扩展大学《线性代数》的核心理论，为后续讨论数值线性代数方法打下基础。主要内容包括常用矩阵类型、特征值与特征多项式、矩阵范数与距离度量、正交与投影变换，以及几类重要的矩阵分解如Schur分解与奇异值分解。与此同时，本章将简单介绍矩阵的扰动理论与稳定性分析，帮助学生理解数值稳定性与误差传播的基本数学理论。

基础知识与常用变换

Concepts, notations, and useful linear transformations

/2.1

Linear Spaces



A **linear space** consists of two components: a set of objects (vectors, denoted as $\mathcal{V}$) and a field of scalars (usually real numbers, denoted as F), equipped with **addition** and **scalar multiplication**.

- Axioms of **Addition** (加法)

- 1) Commutativity of vector addition 交换律

$$u + v = v + u, \quad \forall u, v \in \mathcal{V}$$

- 2) Associativity of vector addition 结合律

$$(u + v) + w = u + (v + w), \quad \forall u, v, w \in \mathcal{V}$$

- 3) Additive identity 零向量

$$\exists \mathbf{0} \in \mathcal{V} : \mathbf{0} + u = u, \quad \forall u \in \mathcal{V}$$

- 4) Existence of additive inverses 负向量

$$\forall u \in \mathcal{V}, \exists (-u) \in \mathcal{V} : u + (-u) = \mathbf{0}$$

- Axioms of **Scalar Multiplication** (标量乘法)

- 1) Distributivity axiom (scalar addition) 标量分配律

$$(a + b) \cdot u = a \cdot u + b \cdot u, \quad \forall u \in \mathcal{V}$$

- 2) Distributivity axiom (vector addition) 向量分配律

$$a \cdot (u + v) = a \cdot u + a \cdot v, \quad \forall u, v \in \mathcal{V}$$

- 3) Associativity axiom of scalar multiplication 结合律

$$a \cdot (b \cdot u) = (ab) \cdot u, \quad \forall u \in \mathcal{V}$$

- 4) Identity scalar axiom 乘法单位元

$$\exists 1 \in F : 1 \cdot u = u, \quad \forall u \in \mathcal{V}$$

Basis of A Linear Space



A **basis** B is a set of vectors $\{v_1, \dots, v_n\}$, $v_i \in \mathcal{V}$ ($i = 1, \dots, n$) that defines the entire structure of a vector space $\mathcal{V}$ through linear combinations.

- **Linearly independent**

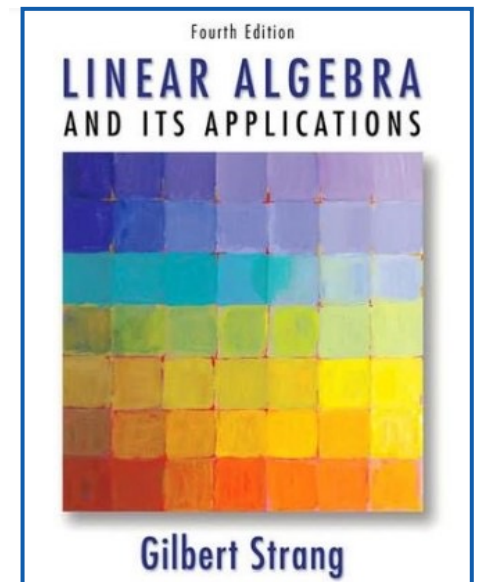
If $\sum_{i=1}^n c_i v_i = \mathbf{0}$, then $c_1 = \dots = c_n = 0$

- It spans the whole space

If $u \in \mathcal{V}$, $\exists a_1, \dots, a_n \in F : u = \sum_{i=1}^n a_i v_i$ **Unique representation**

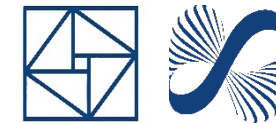
- **Dimension of $\mathcal{V}$** : the number of vectors in any basis for the linear space

- Invariance property: All bases of a vector space $\mathcal{V}$ contain the **same number** of vectors
- The dimension equals the maximum number of linearly independent vectors in $\mathcal{V}$



Gilbert Strang: "The miracle of linear algebra: Simple rules generate profound structure."

Linear Transformation and Matrix



A **linear transformation** between vector spaces $\mathcal{V}$ and $\mathcal{W}$ is a mapping $T : \mathcal{V} \rightarrow \mathcal{W}$ that satisfies:

- **Additivity:** $T(\mathbf{u} + \mathbf{v}) = T(\mathbf{u}) + T(\mathbf{v})$ for all $\mathbf{u}, \mathbf{v} \in \mathcal{V}$
- **Homogeneity:** $T(\alpha \cdot \mathbf{v}) = \alpha \cdot T(\mathbf{v})$ for all scalars $\alpha \in F$ and $\mathbf{v} \in \mathcal{V}$

Matrix Representation

Given a linear transformation $T : \mathbb{C}^n \rightarrow \mathbb{C}^m$ and bases B_1 for $\mathbb{C}^n$ and B_2 for $\mathbb{C}^m$. There exists a unique complex matrix $[T]_{B_2}^{B_1}$ such that

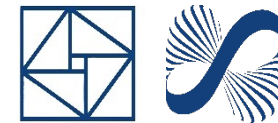
$$[T(\mathbf{v})]_{B_2} = [T]_{B_2}^{B_1} [\mathbf{v}]_{B_1}$$

Q: Why are we interested in matrix operations?

- Provide concrete algorithms for applying transformations
- Allow studying transformations via matrix algebra
- Applications in computer graphics, statistics, ML...

Composition $T \circ S$	Matrix multiplication $[T][S]$
Kernel of T	Null space of $[T]$
Image/Range of T	Column space of $[T]$

Subspaces and Direct Sum



- **Subspace**

A subset $\mathcal{S} \subseteq \mathcal{V}$ of a vector space $\mathcal{V}$ is a subspace if and only if $\mathcal{S}$ is a vector space under the same operations as those of $\mathcal{V}$.

- **Direct sum $\oplus$ of subspaces**

Let $\mathcal{S}_1, \mathcal{S}_2 \subseteq \mathcal{V}$ be two subspaces of $\mathcal{V}$. Then the following are equivalent:

(1) $\mathcal{S}_1 + \mathcal{S}_2 = \mathcal{S}_1 \oplus \mathcal{S}_2$

(2) $\mathbf{x}_1 \in \mathcal{S}_1, \mathbf{x}_2 \in \mathcal{S}_2 : \mathbf{x}_1 + \mathbf{x}_2 = \mathbf{0} \implies \mathbf{x}_1 = \mathbf{x}_2 = \mathbf{0}$

(3) $\mathcal{S}_1 \cap \mathcal{S}_2 = \{\mathbf{0}\}$

(4) $\dim(\mathcal{S}_1) + \dim(\mathcal{S}_2) = \dim(\mathcal{S}_1 + \mathcal{S}_2)$

- If $\mathcal{S}_1 \subseteq \mathcal{V}$ be a subspace, then there exists another subspace $\mathcal{S}_2 \subseteq \mathcal{V}$ such that $\mathcal{S}_1 \oplus \mathcal{S}_2 = \mathcal{V}$.

Fundamental Subspaces



- Subspace spanned by

$$\{\mathbf{v}_1, \dots, \mathbf{v}_m\}, \mathbf{v}_i \in \mathbb{R}^n \ (i = 1, \dots, m)$$

$$\text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_m\} := \left\{ \sum_{i=1}^m a_i \mathbf{v}_i : a_i \in \mathbb{R} \right\}$$

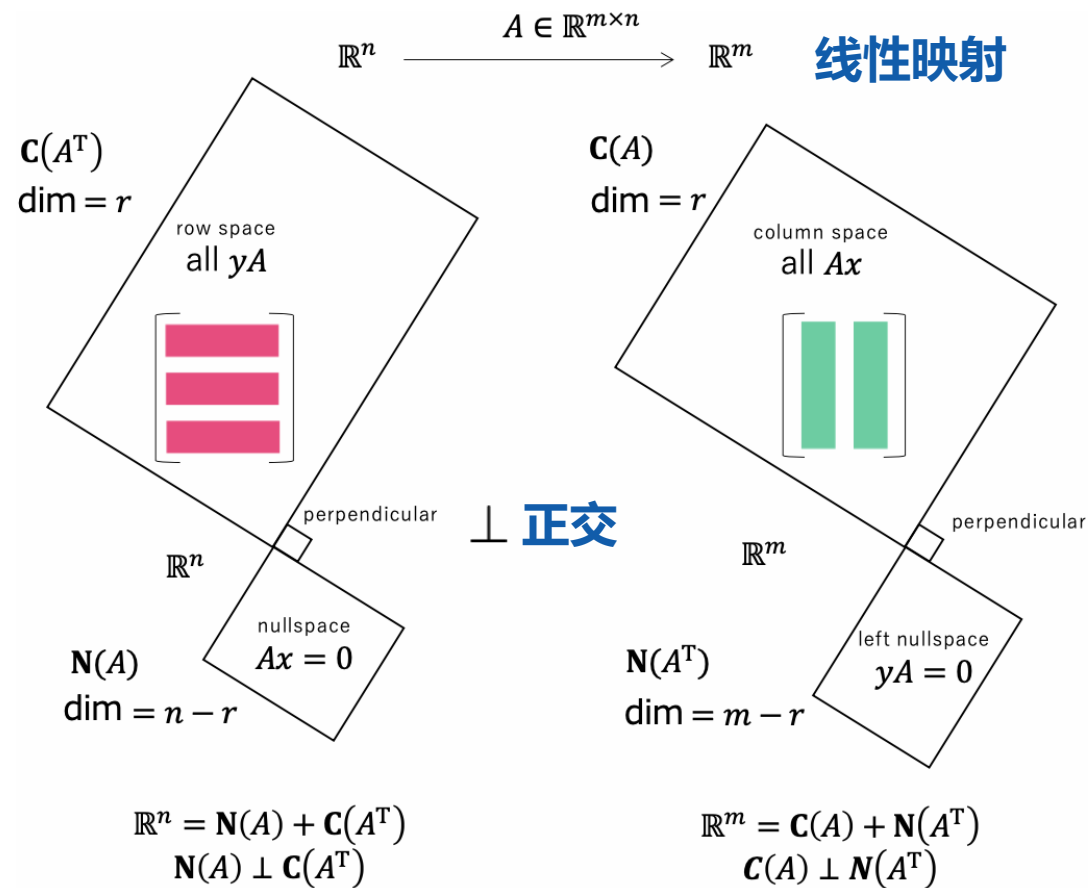
- Some special subspaces

$$\text{range}(A) \equiv \mathbf{C}(A)$$

$$:= \{\mathbf{y} \in \mathbb{R}^m : \mathbf{y} = A\mathbf{x}, \mathbf{x} \in \mathbb{R}^n\}$$

$$\text{null}(A) \equiv \mathbf{N}(A) := \{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \mathbf{0}\}$$

$$\text{rank}(A) \equiv r := \dim(\text{range}(A)) \quad \text{矩阵的秩}$$



Source: Kenji Hiranabe, <https://github.com/kenjihiranabe/The-Art-of-Linear-Algebra/>, 2022

Range and Null Spaces



- A and $A^T A$ have same **null space**

$$\text{null}(A) = \text{null}(A^T A)$$

We show one direction and the other direction is trivial: $A^T A \mathbf{x} = \mathbf{0}$, $\forall \mathbf{x} \in \text{null}(A^T A)$

$$\Rightarrow \|\mathbf{Ax}\|^2 = \mathbf{x}^T A^T A \mathbf{x} = 0 \implies \mathbf{Ax} = \mathbf{0} \implies \mathbf{x} \in \text{null}(A)$$

- A and AA^T have same **column space**

$$\text{range}(A) = \text{range}(AA^T)$$

$$\text{null}(A^T) = \text{null}(AA^T) \Rightarrow \text{range}(A) = \text{null}(A^T)^\perp = \text{range}(AA^T)$$

- **Remark:** These relations can also be shown elegantly using SVD, which makes the range and null structures transparent.

Rank of A Matrix



- The **rank** of a matrix is defined to be the maximum number of linearly independent column vectors (**column rank**), or equivalently, row vectors (**row rank**).

column rank = row rank

$$\forall A, B \in \mathbb{R}^{m \times n}$$

$$\left\{ \begin{array}{l} \text{rank}(A) \leq \min\{m, n\} \\ \text{rank}(A^T) = \text{rank}(A) \\ \text{rank}(A^T A) = \text{rank}(A A^T) = \text{rank}(A) \\ \text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B) \end{array} \right.$$

Properties:

$$\forall X \in \mathbb{R}^{m \times m}, Y \in \mathbb{R}^{n \times n} \text{ nonsingular}$$

$$\text{rank}(XA) = \text{rank}(AY) = \text{rank}(A)$$

If $\text{rank}(A) = r$, there exist nonsingular matrices X and Y , such that

$$A = X \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} Y, \quad X \in \mathbb{R}^{m \times m}, Y \in \mathbb{R}^{n \times n}$$

$$\text{rank}(A) = \text{rank}(B) \quad \longleftrightarrow$$

$$\exists \text{ nonsingular } X \in \mathbb{R}^{m \times m}, Y \in \mathbb{R}^{n \times n}$$

$$A = XBY$$

Eigenvalues and Eigenvectors



- **Eigenvalues** of a **square** matrix $A \in \mathbb{C}^{n \times n}$:

right eigenvector $A\mathbf{u} = \lambda\mathbf{u}, \mathbf{u} \neq \mathbf{0}$

left eigenvector $\mathbf{v}^H A = \lambda\mathbf{v}^H, \mathbf{v} \neq \mathbf{0}$

spectrum (set of eigenvalues) $\lambda(A)$

spectral radius $\rho(A) := \max \{|\lambda| : \lambda \in \lambda(A)\}$

- **Characteristic Polynomial:**

$$p(\lambda) := \det(\lambda I - A)$$

$$\lambda \in \lambda(A) \iff \det(\lambda I - A) = 0$$

$$\det(\lambda I - A) = \det(\lambda I - A^T) \Rightarrow \lambda(A) = \lambda(A^T)$$

- ▶ **Algebraic Multiplicity (代数重数或重数)**

$$p(\lambda) = \prod_{i=1}^r (\lambda - \lambda_i)^{n(\lambda_i)}, \quad \lambda_i \neq \lambda_j \ (i \neq j)$$

$$\sum_{i=1}^r n(\lambda_i) = n$$

- ▶ **Geometric Multiplicity (几何重数)**

$$m(\lambda_i) = n - \text{rank}(\lambda_i I - A)$$

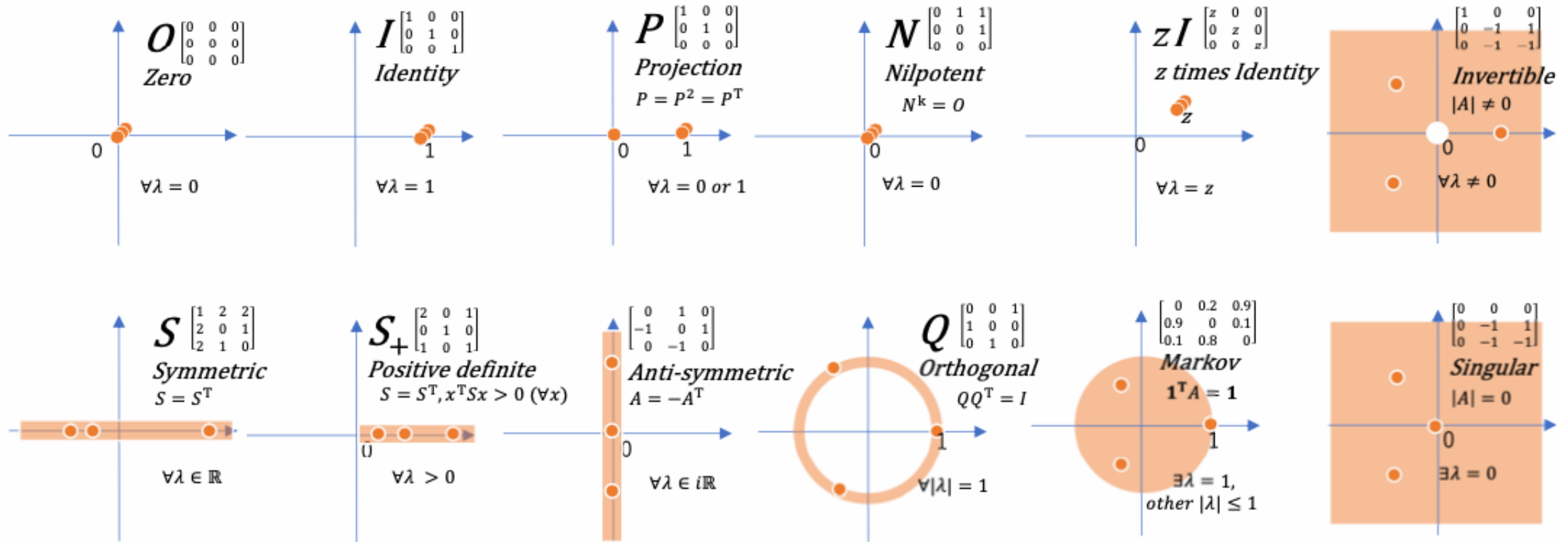
is the number of linearly independent eigenvectors of λ_i

$$1 \leq m(\lambda_i) \leq n(\lambda_i) \leq n$$

Eigenvalues of Some Matrices

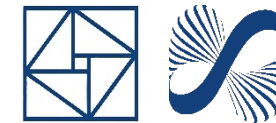


Eigenvalues of some frequently-used types of matrices



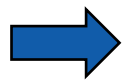
Source: Kenji Hiranabe, <https://github.com/kenjihiranabe/The-Art-of-Linear-Algebra/>, 2022

Geometric Meaning



- A symmetric example:

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



$$\left\{ \begin{array}{ll} \lambda_1 = 3, & \mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ \lambda_2 = 1, & \mathbf{v}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{array} \right.$$

$$\mathbf{u}_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

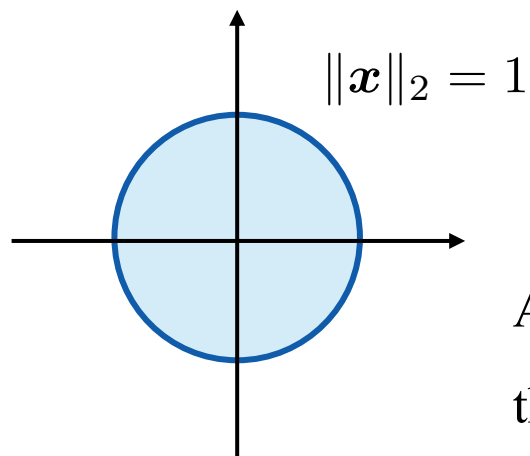
$$\mathbf{u}_2 = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$$

Normalized eigenvectors



Principle axes

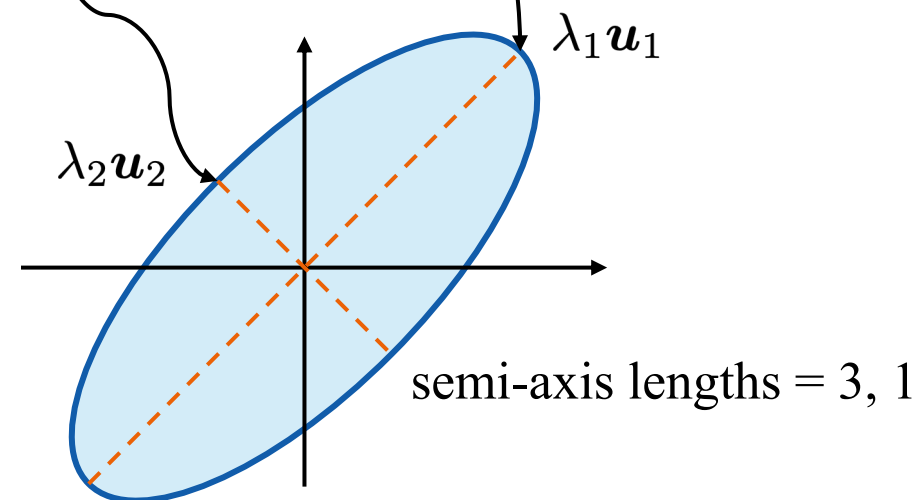
- Geometric interpretation:



$A\mathbf{x}$

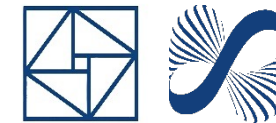


Along eigenvector directions,
the transformation is just a
pure scaling



Note: Only for real symmetric case

Geometric Meaning: Alternative Perspective



- Quadratic form

If A is SPD, $\|x\|_A^2 = x^T A x = 1$

Q: What is its shape?

$x = c_1 u_1 + c_2 u_2$ (not normalized)



$$x^T A x = c_1^2 \lambda_1 \|u_1\|_2^2 + c_2^2 \lambda_2 \|u_2\|_2^2$$

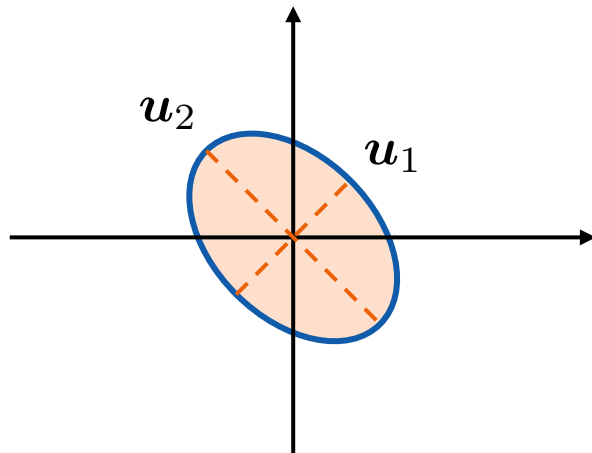
Let $\|u_i\|_A = 1$



$$1 = u_i^T A u_i = \lambda_i u_i^T u_i$$



$$\|u_i\|_2 = \frac{1}{\sqrt{\lambda_i}}$$



semi-axis lengths = $1/\sqrt{3}$, 1

$$\nabla(x^T A x - 1) = 2A x$$



$$n := A x$$

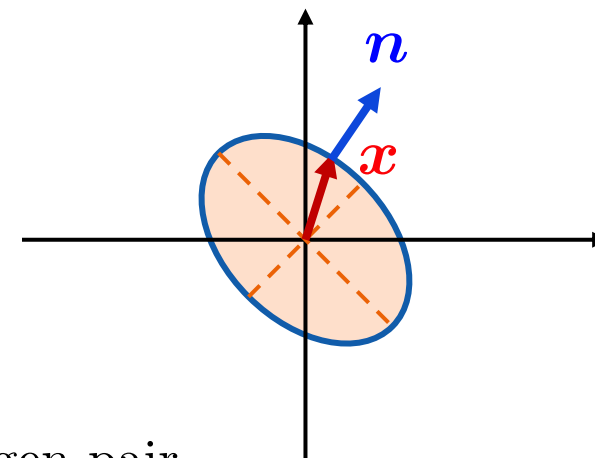
If $x = \alpha n$



$$A x = \alpha^{-1} x$$



(α^{-1}, x) is an eigen-pair



Eigenspace



- **Eigenspace:**

The eigenspace associated with λ is $\ker(A - \lambda I) = \{\mathbf{x} \in \mathbb{C}^n : A\mathbf{x} = \lambda\mathbf{x}\}$

This subspace is called an eigenspace. **特征子空间**

By definition, the dimension of the eigenspace of λ is its geometric multiplicity, $m(\lambda)$.

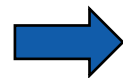
- **Invariant subspace:**

$\mathcal{S} \subseteq \mathbb{C}^n : \mathbf{x} \in \mathcal{S} \implies A\mathbf{x} \in \mathcal{S}$ e.g., an eigenspace and range of A are both invariant subspaces

$$AX = XB, \quad B \in \mathbb{C}^{k \times k}, \quad X \in \mathbb{C}^{n \times k} \quad \longrightarrow \quad \begin{cases} \text{range}(X) \text{ is invariant} \\ B\mathbf{y} = \lambda\mathbf{y} \implies A(X\mathbf{y}) = X(B\mathbf{y}) = \lambda(X\mathbf{y}) \end{cases}$$



Special Case



If X has full column rank, then $\lambda(B) \subseteq \lambda(A)$

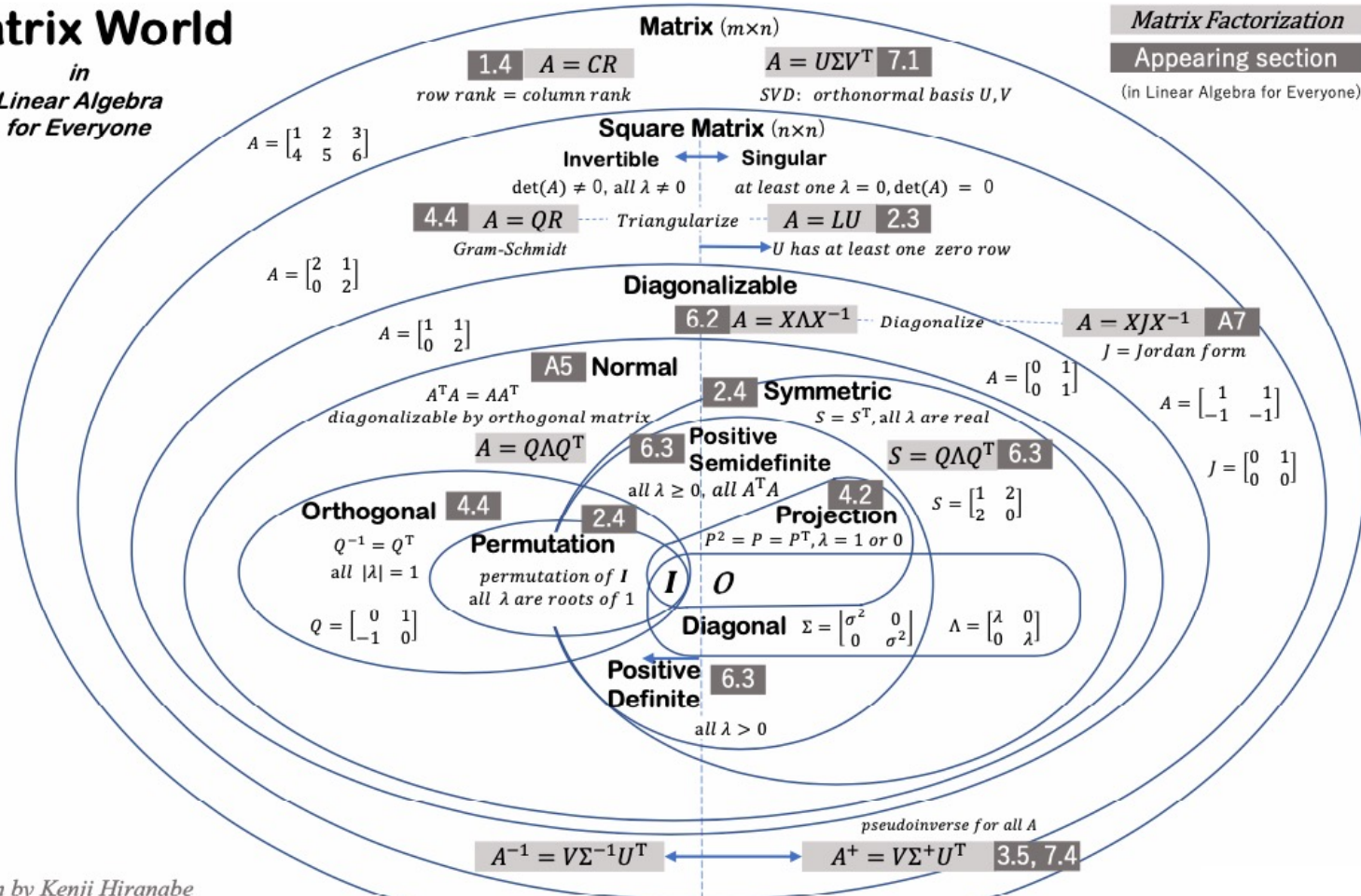
$$AX = XB, \quad B \in \mathbb{C}^{n \times n}, \quad X \in \mathbb{C}^{n \times n} \text{ nonsingular} \implies \lambda(A) = \lambda(B), \quad B = X^{-1}AX \quad \text{相似变换}$$

Commonly Used Matrices



Matrix World

in
Linear Algebra
for Everyone



Drawn by Kenji Hiranabe
with the help of Prof. Gilbert Strang
(v1.5, Mar.2nd, 2023)

- Square matrix
- Invertible matrix
- Singular matrix
- Diagonalizable matrix
- Normal matrix
- Orthogonal matrix
- Symmetric matrix
- Positive semidefinite matrix
- Positive definite matrix
- Projection matrix
- Permutation matrix
- Diagonal matrix


$$R_\theta := \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \quad \longrightarrow \quad \begin{cases} x' = x \cos(\theta) - y \sin(\theta) \\ y' = x \sin(\theta) + y \cos(\theta) \end{cases}$$

- **Orthogonality:** Rotation matrices are orthogonal, $R^T R = R R^T = I$.
- **Determinant:** The determinant of a rotation matrix is 1.
- **Distance Preservation:** Rotation is an isometry -- distances are preserved.
- **Inverse:** The inverse of a rotation matrix is its transpose, i.e., $R^{-1} = R^T$.
- **Inverse rotation:** Corresponds to rotation with angle $-\theta$.
- **Composition:** Combining rotations adds their angles, namely $R_\alpha R_\beta = R_{\alpha+\beta}$.



Example 2: Pauli Matrices



- **Pauli Matrices** [Wolfgang Pauli, 1927] describe how a spin- $1/2$ quantum state changes under basic rotations and how its spin is measured along the three spatial axes.

$$\sigma_z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \sigma_x := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

It is easy to see that $\sigma_j^H = \sigma_j$, $\sigma_j^2 = I$, $j = x, y, z$.

Z-Direction States	X-Direction States	Y-Direction States
Up state ($ \uparrow\rangle$): $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	Right state ($ \rightarrow\rangle$): $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$	Forward state ($ \nearrow\rangle$): $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$
Down state ($ \downarrow\rangle$): $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	Left state ($ \leftarrow\rangle$): $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$	Backward state ($ \nwarrow\rangle$): $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$

$$|\rightarrow\rangle := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \longrightarrow \quad \sigma_z |\rightarrow\rangle = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \times \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$\sigma_z |\rightarrow\rangle = |\leftarrow\rangle$ shows that $|\rightarrow\rangle$ is not an eigenstate of σ_z ; it does not describe the electron state after measurement.

A z-measurement yields $|\pm z\rangle$ with probability $1/2$ each.

Symmetric Positive Definiteness



Positive-definiteness: $A \in \mathbb{R}^{n \times n}$ is SPD i.e. $\mathbf{x}^T A \mathbf{x} > 0, \forall \mathbf{x} \neq \mathbf{0}$ and $A^T = A$

- An SPD matrix is real, nonsingular, and symmetric
- If A is SPD, then we have $X \in \mathbb{R}^{n \times k}, \text{rank}(X) = k \implies B = X^T A X \in \mathbb{R}^{k \times k}$ is SPD
- **Sylvester's Criterion**: If A is real and symmetric, then A is positive-definite if and only if
all its leading principal minors are positive, i.e. $D_k := \det(A_k) > 0$

On the other hand, A is **negative-definite** if and only if the signs of its leading principal minors **alternate**, starting with **negative**:

$$D_1 < 0, \quad D_2 > 0, \quad D_3 < 0, \quad D_4 > 0, \quad \dots$$

- If A is SPD, then $A_k := A(1:k, 1:k) \in \mathbb{R}^{k \times k}$ is also SPD; all diagonal entries of A are positive.

Gershgorin Circle Theorem



Theorem 2.1 (Gershgorin Circle, 1931)

If $A \in \mathbb{C}^{n \times n}$, then we have

$$\lambda(A) \subset \bigcup_{i=1}^n G_i(A), \quad G_i(A) := \left\{ z \in \mathbb{C} : |z - a_{ii}| \leq \sum_{j \neq i} |a_{ij}| \right\} \quad \text{盖氏圆盘}$$

Moreover, if m of these disks form a connected region G that is disjoint from the other disks, then G contains m eigenvalues (counting algebraic multiplicity).

Remarks:

- For a strictly diagonally dominant matrix A , no Gershgorin disk can contain the origin. Therefore, in this case, zero cannot be an eigenvalue, which proves that A is invertible.
- The theorem can also be applied to the columns of A to get an alternate set of disks.
- **Q: Are eigenvalues “stable” under small perturbations of the matrix entries?**

Sherman–Morrison–Woodbury Formula



- It is easy to check the **resolvent identity**: $B^{-1} = A^{-1} - B^{-1}(B - A)A^{-1}$
- Sherman–Morrison–Woodbury (SMW) formula ([Sherman, Morrison 1950](#); [Woodbury 1950](#))

$A \in \mathbb{R}^{n \times n}$ is non-singular

$U, V \in \mathbb{R}^{n \times r}$, $I + V^T A^{-1} U$ is non-singular

$$\Rightarrow (A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1}$$

- **Rank-1 update** using the SMW formula

$$(A + \mathbf{u}\mathbf{v}^T)^{-1} = A^{-1} - A^{-1}\mathbf{u}\mathbf{v}^T A^{-1} / (1 + \mathbf{v}^T A^{-1}\mathbf{u})$$

The SMW formula provides a way to compute the inverse after a low-rank update; it is widely used in several algorithms, like quasi-Newton methods.

Cayley–Hamilton Theorem



Theorem 2.2 (Cayley–Hamilton, 1878)

Let the characteristic polynomial of $A \in \mathbb{C}^{n \times n}$ be denoted as

$$p(\lambda) := \det(\lambda I - A)$$

Then we have

$$p(A) = 0$$

If $A \in \mathbb{C}^{n \times n}$ is invertible, there exists a polynomial $q_{n-1}(\lambda) \in \mathcal{P}_{n-1}$, such that

$$A^{-1} = q_{n-1}(A)$$

Remark:

If $p(A) = A^n + c_{n-1}A^{n-1} + \cdots + c_1A + c_0I = 0$, provided $c_0 \neq 0$ (A is invertible). Then

$$A^{-1} = -\frac{1}{c_0}(A^{n-1} + c_{n-1}A^{n-2} + \cdots + c_1I)$$

距离与范数

Distances and norms

/2.2



- **Norm of a vector space**

$$f(\mathbf{x}) \geq 0, \quad \mathbf{x} \in \mathbb{R}^n$$

$$f(\mathbf{x}) = 0, \quad \text{iff } \mathbf{x} = \mathbf{0}$$

$$f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$$

$$f(\alpha \mathbf{x}) = |\alpha| f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n, \alpha \in \mathbb{R}$$

- Examples of vector norms (p -norm)

$$\|\mathbf{x}\|_p := (|x_1|^p + \cdots + |x_n|^p)^{\frac{1}{p}}, \quad p \geq 1$$

$$\|\mathbf{x}\|_1 = |x_1| + \cdots + |x_n|$$

$$\|\mathbf{x}\|_2 = (\mathbf{x}^T \mathbf{x})^{\frac{1}{2}}$$

$$\|\mathbf{x}\|_\infty = \max_i |x_i|$$

In finite-dimensional vector spaces, all norms are equivalent; for example:

$$\|\mathbf{x}\|_2 \leq \|\mathbf{x}\|_1 \leq \sqrt{n} \|\mathbf{x}\|_2, \quad \|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_1 \leq n \|\mathbf{x}\|_\infty, \quad \forall \mathbf{x} \in \mathbb{R}^n$$

- **Hölder inequality** (generalization of the well-known **Cauchy–Schwarz inequality**)

$$|\mathbf{x}^T \mathbf{y}| \leq \|\mathbf{x}\|_p \|\mathbf{y}\|_q, \quad \frac{1}{p} + \frac{1}{q} = 1$$

Matrix Norms



- p -Norm for matrices: For a real matrix $A \in \mathbb{R}^{m \times n}$

$$\|A\|_p := \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p}$$

$$\|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^m |a_{ij}|, \quad \|A\|_\infty = \max_{1 \leq i \leq m} \sum_{j=1}^n |a_{ij}|, \quad \|A\|_2 = \sqrt{\lambda_{\max}(A^H A)}$$

- Frobenius norm for matrices

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

- Consistent norms

$$\|AB\|_p \leq \|A\|_p \|B\|_p, \quad A \in \mathbb{R}^{m \times n}, \quad B \in \mathbb{R}^{n \times k}$$

Remark: Note that there are **3 norms** in this inequality (p -norms in different spaces)!

Spectral Radius



- **Spectral radius** of $A \in \mathbb{C}^{n \times n}$

$$\rho(A) := \max \{ |\lambda| : \lambda \in \lambda(A) \}$$

The spectral radius possesses profound implications beyond pure mathematics, finding crucial utility in a wide array of scientific and engineering fields. Its significance stems from its role in governing the asymptotic behavior—specifically the **stability and convergence**—of linear dynamical systems.

$$(1) \quad \rho(A) \leq \|A\|, \quad \forall \|\cdot\|$$

$$(2) \quad \forall \varepsilon > 0, \exists \|\cdot\|, \text{ s.t. } \|A\| \leq \rho(A) + \varepsilon$$

$$(3) \quad \lim_{k \rightarrow \infty} A^k = 0 \iff \rho(A) < 1$$

$$(4) \quad \sum_{k=0}^{\infty} A^k \text{ converges} \iff \rho(A) < 1$$

$$(5) \quad \sum_{k=0}^{\infty} A^k = (I - A)^{-1}, \text{ if it converges}$$

$$(6) \quad \lim_{k \rightarrow \infty} \|A^k\|^{1/k} = \rho(A)$$

Non-negative Matrices



- Non-negative / positive (real) matrices

$$A = [a_{ij}] \in \mathbb{R}^{m \times n}, \quad a_{ij} \geq 0 \iff A \geq 0 \quad \text{non-negative}$$

$$A = [a_{ij}] \in \mathbb{R}^{m \times n}, \quad a_{ij} > 0 \iff A > 0 \quad \text{positive}$$

Ordering

$$A, B \in \mathbb{R}^{m \times n}$$

$$A - B \geq 0 \iff A \geq B$$

- A positive (non-negative) matrix is a matrix in which every entry is greater than (or equal to) zero.
- **Applications:** Non-negative matrices are crucial in many areas because they naturally model quantities that cannot be negative, such as probability matrices (Markov chains), adjacency matrices of graphs, models of goods and production, Google's PageRank matrix.
- **Monotonicity of spectral radius:**

$$A \in \mathbb{C}^{n \times n}, \quad B \in \mathbb{R}^{n \times n} : |A| \leq B \implies \rho(A) \leq \rho(B)$$

Irreducible Matrices



- **Reducible matrix:**

$A \in \mathbb{R}^{n \times n}$ ($n \geq 2$), $\exists$ permutation P , s.t.

$$PAP^T = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}$$

Otherwise, A is called **irreducible**.

Theorem 2.3

$A \in \mathbb{R}^{n \times n}$ is non-negative ($n \geq 2$). Then

A is irreducible $\iff (I + A)^{n-1} > 0$

- A reducible matrix is a square matrix that can be transformed into a block upper triangular form by applying the same permutation to its rows and columns. In other words, it represents a linear system that can be broken down into **smaller subsystems with a one-way block dependency**.

- It is handy in computation:
$$\begin{cases} \lambda(A) = \lambda(A_{11}) \cup \lambda(A_{22}) \\ A_{22} \mathbf{y}_2 = \mathbf{b}_2, \quad A_{11} \mathbf{y}_1 = \mathbf{b}_1 - A_{12} \mathbf{y}_2 \end{cases}$$

Perron–Frobenius Theorem



Theorem 2.4 (Perron–Frobenius Theorem, 1912)

If $A \in \mathbb{R}^{n \times n}$ ($n \geq 2$) is **non-negative** and **irreducible**, then

$\rho(A) > 0$ is a **simple** eigenvalue, and $\exists \mathbf{x} > 0$, s.t. $A\mathbf{x} = \rho(A)\mathbf{x}$.

Remarks:

- Perron (1907) analyzed positive matrices and Frobenius (1912) considered more general cases.
- The **dominant eigenvalue** $\lambda_1 = \rho(A)$ of a graph's adjacency matrix A (代数) provides information about the graph's connectivity and the number of walks between nodes (几何):
 - $(A^k)_{ij}$ gives the **number of walks of length** k from node i to j ;
 - If A is **primitive** and $\mathbf{u}, \mathbf{v}$ are **normalized** Perron vectors we have the asymptotic relation: $A^k \sim (\mathbf{v}\mathbf{u}^T) \lambda_1^k$;
 - The number of walks of length k from node i to node j grows exponentially at a rate determined by λ_1 .

Google Matrix and PageRank



- Revisit Chapter 1: M is a column-stochastic matrix (column sums are 1)
- With probability d , follow a hyperlink; with probability $1 - d$, jump uniformly to any page:

Google matrix $G := dM + \frac{1-d}{n} \mathbf{1}\mathbf{1}^\top, \quad 0 < d < 1$

- It is easy to see that the Google matrix is also column-stochastic

$$\mathbf{1}^\top G = \mathbf{1}^\top \quad \text{and} \quad \|G\|_1 = 1 \quad \Rightarrow \quad \rho(G) = 1$$

- Furthermore, the Google matrix is also positive (hence irreducible)

$$G \geq \frac{1-d}{n} > 0$$

- The Perron–Frobenius theorem guarantees a unique positive normalized vector $\mathbf{r}$ satisfying

$$G\mathbf{r} = \mathbf{r}, \quad \mathbf{1}^\top \mathbf{r} = 1$$

Orthogonality



- **Orthogonal** matrix

$$Q := [\mathbf{q}_1, \dots, \mathbf{q}_n] \in \mathbb{R}^{n \times n}, \quad Q^T Q = I$$

The columns of Q form an orthonormal basis of $\mathbb{R}^n$

$$\|Q\mathbf{x}\|_2^2 = \mathbf{x}^T Q^T Q \mathbf{x} = \|\mathbf{x}\|_2^2$$

- Unitary matrix (酉矩阵)

$$Q := [\mathbf{q}_1, \dots, \mathbf{q}_n] \in \mathbb{C}^{n \times n}, \quad Q^H Q = I$$

- If Q and Z are orthogonal / unitary, then

$$\|QAZ\|_2 = \|A\|_2$$

$$\|QAZ\|_F = \|A\|_F$$

unitary-invariant norms

Projections



- **Projection Transform:**

A projection $P: \mathcal{V} \rightarrow \mathcal{V}$ is a linear idempotent transform from a vector space onto a subspace.

- **Idempotence:** Once a vector has been projected, projecting it again does nothing, i.e. $P^2 = P$

➡ $P^k = P, \quad k \in \mathbb{N}_+$ 幂等算子

- Any vector $\mathbf{x} \in \mathcal{V}$ can be decomposed as

$$\mathbf{x} = P\mathbf{x} + (I - P)\mathbf{x}$$

where $I - P$ is also an projection and

$$\text{null}(P) = \text{range}(I - P)$$

- It's easy to see that the matrix P^T is also a projection.

- The eigenvalues of a projection matrix P are **either 0 or 1!** (Exercise)

Orthogonal Projections



Orthogonal Projection

Subspace $\mathcal{S} \subseteq \mathbb{R}^n$ and

$$P \in \mathbb{R}^{n \times n}, \text{range}(P) = \mathcal{S},$$

$$P^2 = P, P^T = P$$

P is an orthogonal projection to $\mathcal{S}$

- Let P be a projection matrix. If $P^T = P$, then it is an **orthogonal projection**; otherwise, it is called an **oblique projection**.
- Orthogonal projection in **complex** vector spaces follows the same geometric principle as in real spaces.

Some Properties:

① $\mathbf{x} - P\mathbf{x} \in \mathcal{S}^\perp, \forall \mathbf{x} \in \mathbb{R}^n$

② $P\mathbf{x} = \mathbf{x}, \forall \mathbf{x} \in \mathcal{S}$

③ $\mathbf{v} - P_1\mathbf{v} \in \mathcal{S}^\perp, \mathbf{v} - P_2\mathbf{v} \in \mathcal{S}^\perp,$
 $\implies (P_1 - P_2)\mathbf{v} \in \mathcal{S}^\perp$

Moreover, $P_1\mathbf{v} - P_2\mathbf{v} \in \mathcal{S},$
 $\implies (P_1 - P_2)\mathbf{v} = \mathbf{0}$

④ Orthogonal projection onto $\text{range}(A)$:

$$P_{\text{range}(A)} = A(A^H A)^{-1} A^H$$

if A has **full column rank**.

Matrix Form of Projection



- Suppose that we have two k -dimensional subspaces:

$$\mathcal{S}_1, \mathcal{S}_2 \subseteq \mathbb{R}^n = \mathcal{S}_1 \oplus \mathcal{S}_2^\perp$$

Then there exists a unique projection P onto $\mathcal{S}_1$ along the direction orthogonal to $\mathcal{S}_2$, and

$$P = V(W^T V)^{-1} W^T \quad \text{oblique projection onto } \mathcal{S}_1 \text{ along } \mathcal{S}_2^\perp$$

$$\text{range}(P) = \mathcal{S}_1, \quad \text{null}(P) = \mathcal{S}_2^\perp$$

where columns of V and W form orthonormal bases of $\mathcal{S}_1$ and $\mathcal{S}_2$, respectively.

- **Examples:**

① $\mathcal{S}_1 = \mathcal{S}_2 = \mathbb{R}^n, \mathcal{S}_2^\perp = \{\mathbf{0}\} \implies P = I$

② $\mathcal{S}_1 = \mathcal{S}_2 = \{\mathbf{0}\}, \mathcal{S}_2^\perp = \mathbb{R}^n \implies P = 0$

③ More common usage:

$$\mathcal{S}_1 = \mathcal{S}_2 \subset \mathbb{R}^n$$

Derivation of Orthogonal Projection Matrix



- Let $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ be an orthonormal basis of $\mathcal{S} \subseteq \mathbb{R}^n$

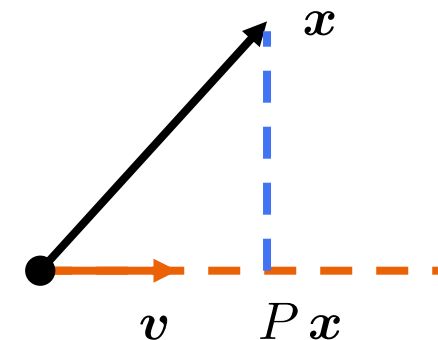
$\Rightarrow V := [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \dots \quad \mathbf{v}_k] \in \mathbb{R}^{n \times k} \Rightarrow V^T V = I_k$ **orthonormal**

- Deriving the matrix form (**Exercise**)

$$\forall \mathbf{x} \in \mathbb{R}^n : \frac{\mathbf{v}^T \mathbf{x}}{\mathbf{v}^T \mathbf{v}} \mathbf{v} \text{ is the projection to } \text{span}\{\mathbf{v}\}$$

$\Rightarrow P \mathbf{x} = \sum_{i=1}^k (\mathbf{v}_i^T \mathbf{x}) \mathbf{v}_i = V V^T \mathbf{x}$

$\Rightarrow P = V V^T$



It is easy to check that: $P^2 = P, \quad P^T = P \Rightarrow$ orthogonal projection

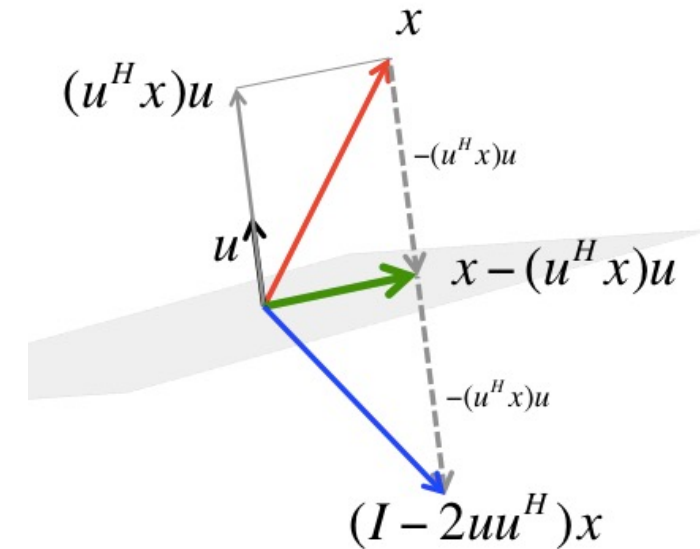
Householder Transformation



- **Householder matrix** or transformation

$$H = I - 2\mathbf{u}\mathbf{u}^T, \quad \mathbf{u} \in \mathbb{R}^n, \quad \|\mathbf{u}\|_2 = 1$$

- ▶ H is **symmetric** and **orthogonal**
- ▶ -1 is an eigenvalue of H and $\mathbf{u}$ is its eigenvector; 1 is another eigenvalue, apparently
- ▶ $\det(H) = -1$
- ▶ $H(\mathbf{y} + a\mathbf{u}) = \mathbf{y} - a\mathbf{u}, \quad \forall \mathbf{y} \perp \text{span}\{\mathbf{u}\}, a \in \mathbb{R}$



Theorem 2.5

$$\forall \mathbf{0} \neq \mathbf{x} \in \mathbb{R}^n, \exists \mathbf{u} \in \mathbb{R}^n, \text{ s.t. } H\mathbf{x} = a\mathbf{e}_1$$

$$\text{where } a = \pm\|\mathbf{x}\|_2, \quad \mathbf{u} = \frac{\mathbf{x} - a\mathbf{e}_1}{\|\mathbf{x} - a\mathbf{e}_1\|_2}$$

- The Householder transformation reflects a vector $\mathbf{x}$ such that only the **first entry** is nonzero.
- The vector $\mathbf{u}$ is called a Householder vector.
- Choose a such that the denominator is nonzero.

Givens Transformation



- **Givens matrix** or transformation

$$G(\Phi) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$$

$c = \cos(\Phi)$, $s = \sin(\Phi)$, and $\Phi \in \mathbb{R}$

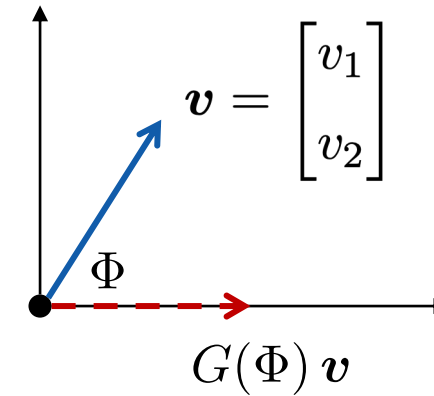
- It represents a **plane rotation**:

$$G(\Phi) \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} cx_1 + sx_2 \\ -sx_1 + cx_2 \end{bmatrix}$$

- Consider a complex plane:

$$G(\Phi) \quad \longrightarrow \quad u = \cos(\Phi) - \mathbf{i} \sin \Phi = e^{-\mathbf{i}\Phi}$$

$$u(x_1 + \mathbf{i}x_2) = (cx_1 + sx_2) + \mathbf{i}(-sx_1 + cx_2)$$



- ▶ Givens matrix is **orthogonal**
- ▶ Rotate a complex number by an angle of Φ clockwise (Passive, CW rotation)
- ▶ Numerical libraries (LAPACK) use this convention

奇异值分解

Singular value decomposition

/2.3

Schur Decomposition



Theorem 2.6 (Schur Decomposition Theorem, 1909)

Let $A \in \mathbb{C}^{n \times n}$ be a complex matrix. There exists a unitary matrix U such that

$$U^H A U = T$$

where T is an **upper triangular matrix**. Moreover, the diagonal entries of T are the eigenvalues of the matrix A .

Real Schur decomposition avoids introducing the imaginary unit $\mathbf{i}$. This is a significant advantage in numerical computation. By employing an orthogonal matrix and a block upper triangular matrix T with 1×1 or 2×2 blocks, it keeps all computations within real numbers:

$$\forall A \in \mathbb{R}^{n \times n} : \quad \exists Q \in \mathbb{R}^{n \times n} \text{ is orthogonal, s.t. } Q^T A Q = T$$

Proof of Schur Decomposition



- 1 If $n = 1$, the result is trivial; we then prove the theorem by induction.
- 2 Suppose we have an eigenpair: $A\mathbf{x} = \lambda\mathbf{x}$, $\mathbf{0} \neq \mathbf{x} \in \mathbb{C}^n$

There exist a Hermitian and unitary matrix H and a **nonzero** constant p , such that $H\mathbf{x} = p\mathbf{e}_1$

$$\text{Hence, we have } H A H \mathbf{e}_1 = H A \mathbf{x} / p = \lambda \mathbf{e}_1 \quad \Rightarrow \quad H A H = \begin{bmatrix} \lambda & * \\ \mathbf{0} & A_1 \end{bmatrix}$$

- 3 $A_1 \in \mathbb{C}^{(n-1) \times (n-1)}$, $\lambda(A_1) \subseteq \lambda(A)$ $\Rightarrow \exists U_1$ is unitary and $U_1^H A_1 U_1 = T_1$

$U := H \text{diag}(1, U_1)$ is unitary and satisfies the theorem.

Remarks on Schur Decomposition



- A triangular matrix is the **simplest** form of a complex matrix under **unitary similarity transformation**.
- Unlike diagonalization, which only applies to a class of matrices (namely, diagonalizable matrices), **any matrix** can be unitarily triangularized by the Schur decomposition.
- For a normal matrix: $A^H A = A A^H \iff U^H A U = \text{diag}(\lambda_1, \dots, \lambda_n), \lambda_i \in \mathbb{C} (i = 1 : n)$
- For a Hermitian matrix: $A^H = A \iff U^H A U = \text{diag}(\lambda_1, \dots, \lambda_n), \lambda_i \in \mathbb{R} (i = 1 : n)$
- The transformation by a unitary matrix **preserves important geometric properties** like lengths and angles, making the process numerically stable.
- The Schur decomposition is not unique; for example, the diagonal entries of T (i.e., the eigenvalues) can appear in any order.

Singular Value Decomposition



Theorem 2.7 (Singular Value Decomposition Theorem, 1870s)

$$A \in \mathbb{C}^{m \times n}, p := \min\{m, n\} \quad \longrightarrow \quad \begin{aligned} &\exists \text{ unitary matrices } U \in \mathbb{C}^{m \times m}, V \in \mathbb{C}^{n \times n}, \\ &\text{s.t. } A = U \Sigma V^H, \Sigma = \text{diag}(\sigma_1, \dots, \sigma_p) \in \mathbb{R}^{m \times n}, \\ &\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0 \end{aligned}$$

- Full/Regular SVD:

$$\forall A \in \mathbb{C}^{m \times n} : \quad A = U \Sigma V^H, \quad U \in \mathbb{C}^{m \times m}, V \in \mathbb{C}^{n \times n}, \Sigma = \text{diag}(\sigma_1, \dots, \sigma_p) \in \mathbb{R}^{m \times n} \\ p := \min\{m, n\}$$

SVD can be applied to **real** matrices via **orthogonal** transformations

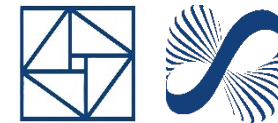
$$A = U \Sigma V^T \quad \longrightarrow \quad \begin{cases} A V = U \Sigma & A^T U = V \Sigma^T \\ A \mathbf{v}_i = \sigma_i \mathbf{u}_i & A^T \mathbf{u}_i = \sigma_i \mathbf{v}_i \end{cases}$$

σ_i singular value

$\mathbf{u}_i$ left singular vector

$\mathbf{v}_i$ right singular vector

Proof of Singular Value Decomposition



1 $\exists \mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m, \|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = 1, \text{ s.t. } A\mathbf{x} = \sigma\mathbf{y}, \sigma := \|A\|_2$

2 $\exists V_2 \in \mathbb{R}^{n \times (n-1)}, U_2 \in \mathbb{R}^{m \times (m-1)}, \text{ s.t. } V := [\mathbf{x} \ V_2], U := [\mathbf{y} \ U_2]$ Orthogonal extension

$$U^T A V = \begin{bmatrix} \sigma & \mathbf{w}^T \\ \mathbf{0} & B \end{bmatrix} =: A_1$$

3 Due to the fact $A_1^T \mathbf{e}_1 = \begin{bmatrix} \sigma \\ \mathbf{w} \end{bmatrix}$ and $\|\mathbf{e}_1\|_2 = 1, \|A_1^T \mathbf{e}_1\|_2^2 = \sigma^2 + \mathbf{w}^T \mathbf{w}$

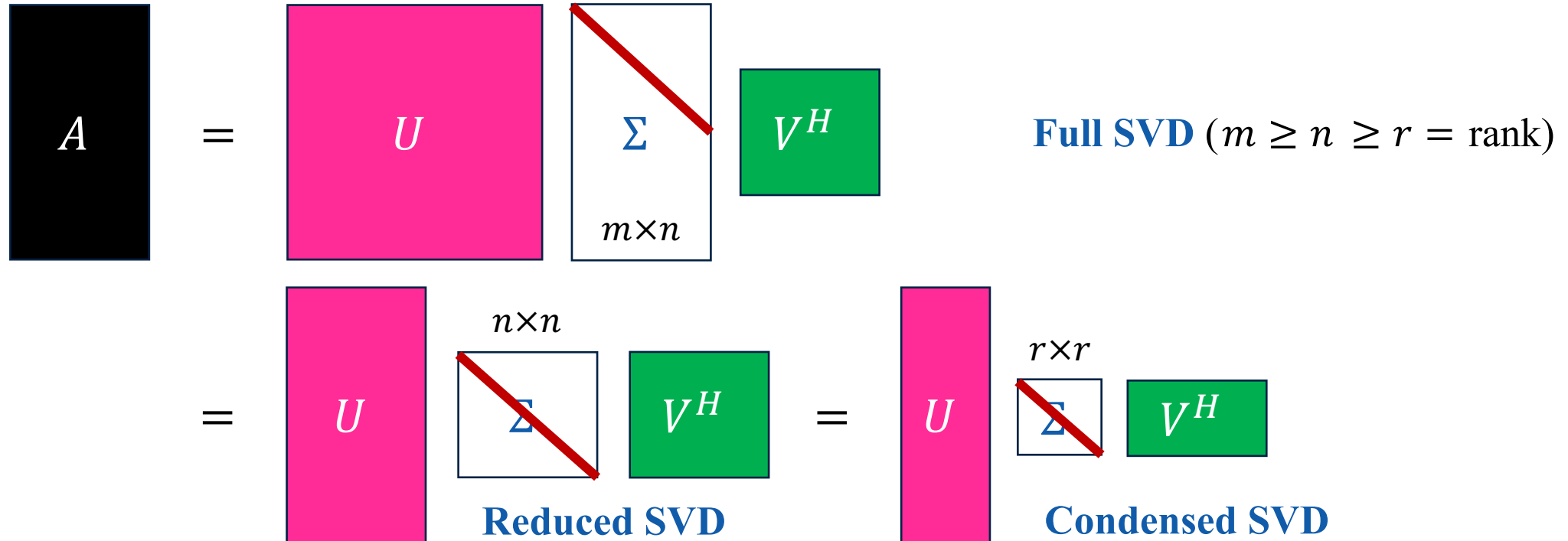
$$\sigma^2 = \|A\|_2^2 = \|A_1\|_2^2 \geq \sigma^2 + \mathbf{w}^T \mathbf{w} \implies \mathbf{w} = \mathbf{0} \quad \Rightarrow \quad U^T A V = \begin{bmatrix} \sigma & \mathbf{0}^T \\ \mathbf{0} & B \end{bmatrix}$$

4 Hence, we can show the SVD theorem by induction.

Reduced and Condensed SVD



$$\forall A \in \mathbb{C}^{m \times n} : A = U \Sigma V^H, U \in \mathbb{C}^{m \times n}, V \in \mathbb{C}^{n \times n}, \Sigma = \text{diag}(\sigma_1, \dots, \sigma_n) \in \mathbb{R}^{n \times n}$$



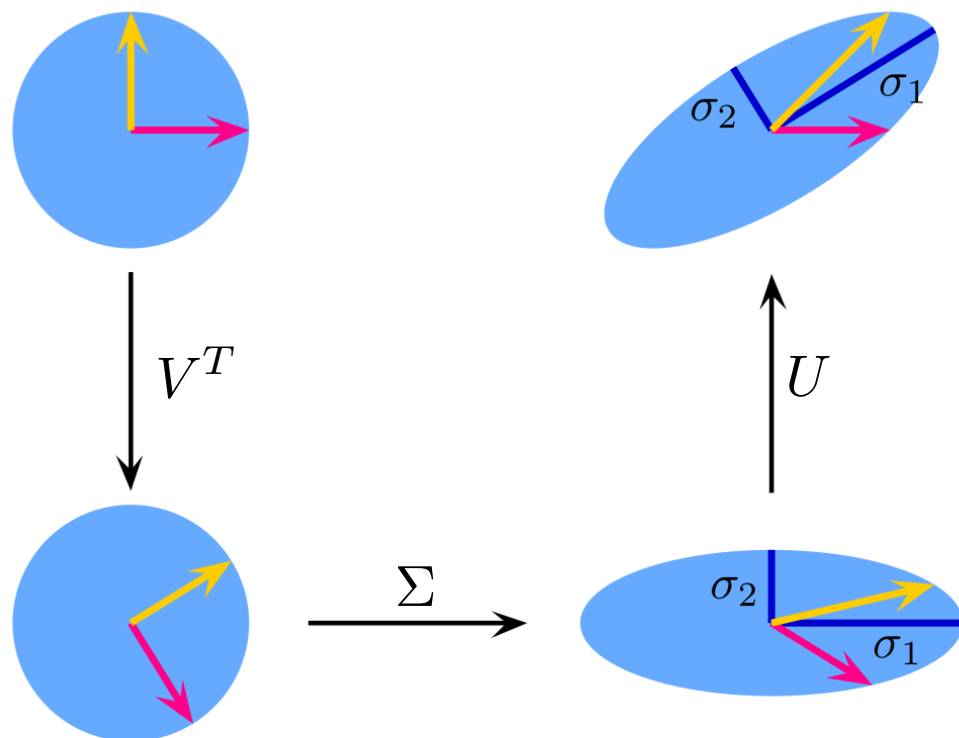
- The reduced (thin) and condensed SVDs are ways to remove the redundant parts from the full SVD, **without losing mathematical information.**

Geometric Meaning of SVD



Singular values: Semi-axis lengths of the ellipsoid $\{A\mathbf{x} : \|\mathbf{x}\|_2 = 1\}$ 椭球的半轴长

$A = U \Sigma V^T$ $\Rightarrow$ Any linear transformation = **Rotate** $\rightarrow$ **Scale** $\rightarrow$ **Rotate**

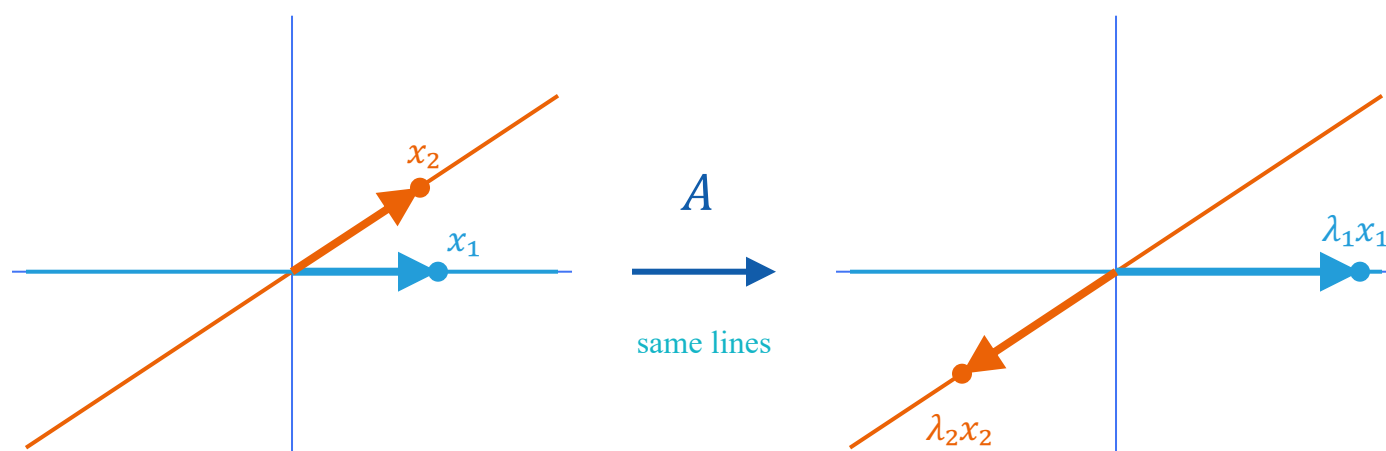
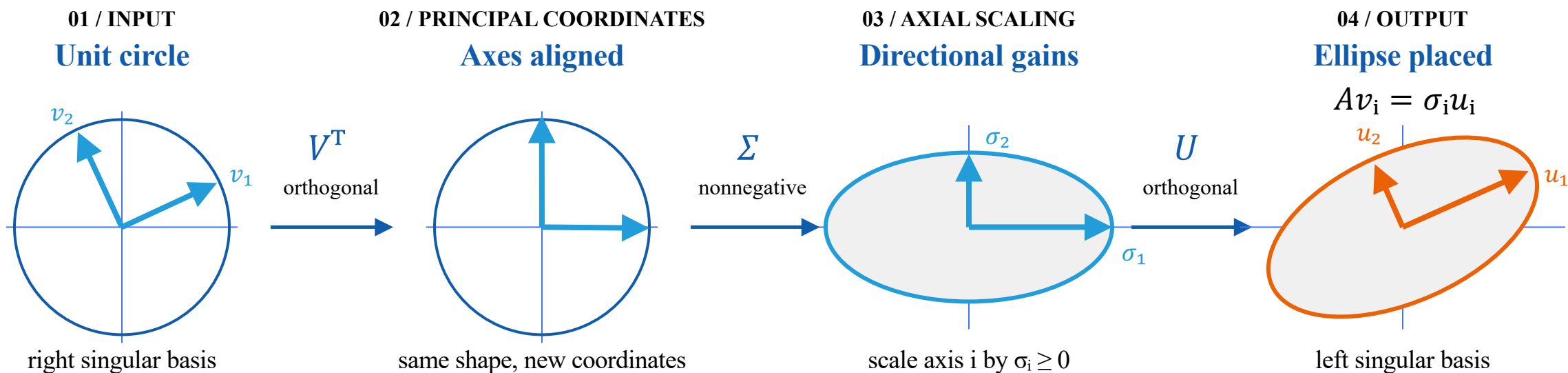


Any linear transformation $A: \mathbb{R}^n \rightarrow \mathbb{R}^m$ can be decomposed into three simple steps:

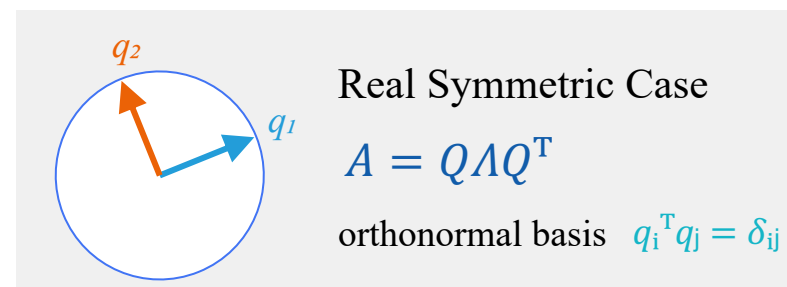
1. **Rotation/Reflection** V^T : Rotate in $\mathbb{R}^n$
2. **Scaling** (Σ): Stretch/compress along axes
3. **Rotation/Reflection** U : Rotate in $\mathbb{R}^m$

SVD = “**Swiss Army Knife**” of NLA!

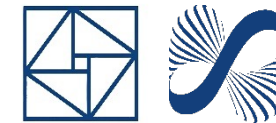
Geometric Meaning of SVD and EVD



$A = X\Lambda X^{-1}$ requires a complete eigenbasis; X might not be orthogonal



Comparison of SVD and EVD



LENS	SVD	EVD
MATRIX CLASS	Every real $m \times n$ matrix	Square matrix
DIRECTIONS	Domain $v_i \rightarrow$ codomain u_i	Eigenvectors x_i
SCALARS	$\sigma_i \geq 0$: geometric gains	λ_i may be positive, negative, or complex
ORTHOGONALITY	Both bases are orthonormal	Not guaranteed; real symmetric A is special
GEOMETRY	Unit ball $\rightarrow$ ellipsoid	Action along invariant lines or modes

BRIDGE

via $A^T A$

$$A^T A = V \Sigma^2 V^T, \quad \sigma_i^2 = \lambda_i(A^T A)$$

SVD measures geometric gain; EVD identifies invariant modes.

Symmetric Case:

$$\sigma_i = |\lambda_i|$$

If A is SPD: $U = V = Q, \Sigma = \Lambda$

Comments on SVD and EVD



- A matrix and its Schur decomposition have the same singular values, i.e.

$$\sigma(A) = \sigma(Q^H A Q) = \sigma(\text{diag}(\lambda_i) + N)$$

- For a **normal** matrix, $N = 0$, and its singular values are equal to $|\lambda_i|$.
- Relation between singular values and λ_i :

$$\sigma_{\min}(A) \leq \min_i |\lambda_i| \leq \max_i |\lambda_i| \leq \sigma_{\max}(A)$$

- Sometimes, eigenvalues are not as useful as singular values: $\max_{i,j} \frac{|\lambda_i|}{|\lambda_j|} \leq \kappa_2(A)$
- For each singular triplet, $A\mathbf{v}_i = \sigma_i \mathbf{u}_i$: the right singular vector $\mathbf{v}_i$ is an input direction, the left singular vector $\mathbf{u}_i$ is the corresponding output direction, and σ_i (non-negative and real) is the basis-independent amplification factor.

SVD and Norms



- From regular (full) SVD, we have:

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

- For a complex matrix, $\sigma(A) = \sqrt{\lambda(A^H A)}$
- In symmetric case, $\sigma(A) = |\lambda(A)|$

- SVD and standard matrix norms:

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_p = 0 \quad \Rightarrow \quad \text{rank}(A) = r$$

$$\|A\|_F^2 = \sum_{i=1}^p \sigma_i^2$$

$$\|A\|_2 = \sigma_1$$

$$\min_{\mathbf{x} \neq 0} \frac{\|A\mathbf{x}\|_2}{\|\mathbf{x}\|_2} = \sigma_n \quad (m \geq n)$$

- SVD and the nuclear norm (convex and continuous):

$$\|A\|_* := \sum_{i=1}^r \sigma_i \quad \text{Widely used in machine learning to promote low-rank structure}$$

Low-Rank Approximation



- **Low-rank approximation (LRA)**

Simplifying a matrix by representing it with **fewer fundamental components**. The following theorem gives the best possible low-rank approximation for the chosen rank k ; we can precisely calculate the approximation error:

Theorem 2.8 (Eckart–Young–Mirsky Theorem, 1936, 1960)

$$A \in \mathbb{C}^{m \times n}, \quad A = U \Sigma V^H$$

$$\text{For any } 0 \leq k \leq r := \text{rank}(A) \quad \Rightarrow \quad A_k := U_k \Sigma_k V_k^H = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^H$$

Then we have

$$\min_{\text{rank}(B) \leq k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}, \quad \min_{\text{rank}(B) \leq k} \|A - B\|_F = \|A - A_k\|_F = \sqrt{\sum_{i=k+1}^r \sigma_i^2}$$

SVD and Numerical Rank



- Numerical rank

$$r_\varepsilon \equiv \text{rank}(A, \varepsilon) := \min_{\|A-B\|_2 \leq \varepsilon} \text{rank}(B)$$

- Numerical rank and SVD

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{r_\varepsilon} > \varepsilon \geq \sigma_{r_\varepsilon+1} \geq \cdots \geq \sigma_p$$

$$r_\varepsilon(A) = \#\{i : \sigma_i > \varepsilon\}$$

- Applications in **Digital Signal Processing (DSP)**: Singular values less than a tolerance ε are usually discarded as noise.

- Q: How to choose ε ?

$$\varepsilon = \max(m, n) u \sigma_1$$

Eye-ball Norm: Plot the singular values and identify the “**kink**” in the curve, after which the singular values become negligible.

SVD for Invertible Matrices



- From regular (full) SVD of an invertible (square) matrix, we have:

$$\begin{array}{c} \text{A} \\ \text{rank}(A) = r = m = n \end{array} = \begin{array}{c} \text{U} \\ \text{rank}(U) = r = m = n \end{array} \begin{array}{c} \Sigma \\ \text{rank}(\Sigma) = r = m = n \end{array} \begin{array}{c} \text{V}^H \\ \text{rank}(V^H) = r = m = n \end{array} \quad \text{Full SVD}$$

- SVD and inverse:

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

- SVD and determinant:

$$|\det(A)| = \prod_{i=1}^n \sigma_i(A)$$

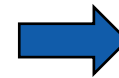
SVD and Moore–Penrose Pseudoinverse



- **Generalized Inverse:**

Suppose that $A \in \mathbb{R}^{m \times n}$. $X \in \mathbb{R}^{n \times m}$ satisfies that

$$\begin{array}{ll} AXA = A & (AX)^T = AX \\ XAX = X & (XA)^T = XA \end{array}$$

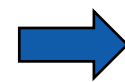


X is called the Moore–Penrose pseudoinverse, denoted by $A^\dagger$.

- **M–P Pseudoinverse and SVD**

$$A = U \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} V^T, \quad U \in \mathbb{R}^{m \times m}, \quad V \in \mathbb{R}^{n \times n}, \quad \Sigma_r = \text{diag}(\sigma_1, \dots, \sigma_r), \quad \sigma_1 \geq \dots \geq \sigma_r > 0$$

$m \times n$



$$A^\dagger = V \begin{bmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{bmatrix} U^T$$

$n \times m$

M–P Pseudoinverse

SVD and Fundamental Subspaces



- Rank of a matrix:

$$\text{rank}(A) = \text{rank}(A^T) = \text{rank}(AA^T) = \text{rank}(A^T A) = r$$

- From condensed SVD, we have:

$$A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T \iff \begin{bmatrix} \text{ } \end{bmatrix} = \begin{bmatrix} | & | & | \\ \text{1} & \text{2} & \text{3} \\ | & | & | \end{bmatrix} \begin{bmatrix} \bullet & & \\ & \bullet & \\ & & \end{bmatrix} \begin{bmatrix} \text{1} \\ \text{2} \end{bmatrix} = \bullet \begin{bmatrix} \text{1} \\ \text{1} \\ \text{ } \end{bmatrix} + \bullet \begin{bmatrix} \text{2} \\ \text{2} \\ \text{ } \end{bmatrix}$$

$$\text{range}(A) = \text{range}(AA^T) = \text{range}(U_r) = \text{span}\{\mathbf{u}_1, \dots, \mathbf{u}_r\}$$

$$\text{range}(A^T) = \text{range}(A^T A) = \text{range}(V_r) = \text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_r\}$$

$$\text{null}(A) = \text{span}\{\mathbf{v}_{r+1}, \dots, \mathbf{v}_n\} \qquad \text{null}(A^T) = \text{span}\{\mathbf{u}_{r+1}, \dots, \mathbf{u}_m\}$$

Source: Kenji Hiranabe, <https://github.com/kenjihiranabe/The-Art-of-Linear-Algebra/>, 2022

SVD and Orthogonal Projections



- Reminder: If the columns of V form an orthonormal basis of the subspace $\mathcal{S} \subseteq \mathbb{R}^n$, then

$P = V V^T$ is the unique orthogonal projection onto $\mathcal{S}$

- According to full SVD: $A = U \Sigma V^T \in \mathbb{R}^{m \times n}$, $r := \text{rank}(A)$

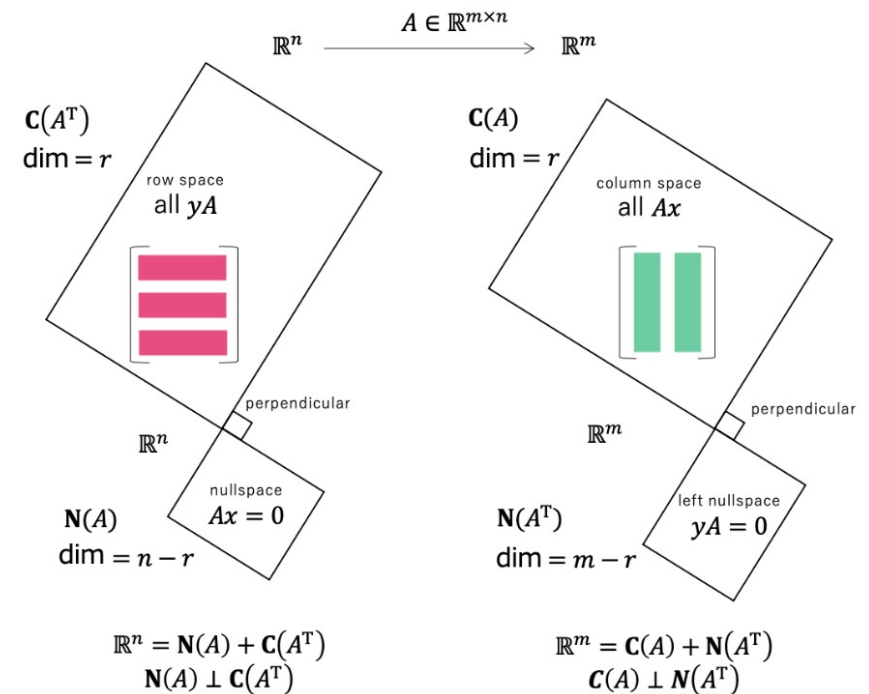
Partitioning
$$\begin{cases} U = [U_r & \tilde{U}_r], & U_r \in \mathbb{R}^{m \times r} \\ V = [V_r & \tilde{V}_r], & V_r \in \mathbb{R}^{n \times r} \end{cases}$$

$U_r U_r^T$: orthogonal projection to $\text{range}(A)$

$\tilde{V}_r \tilde{V}_r^T$: orthogonal projection to $\text{null}(A)$

$V_r V_r^T$: orthogonal projection to $\text{range}(A^T) = \text{null}(A)^\perp$

$\tilde{U}_r \tilde{U}_r^T$: orthogonal projection to $\text{null}(A^T) = \text{range}(A)^\perp$



Projection to Column Space



- Inclusions of column spaces

$$\text{range}(A^\dagger A) = \text{range}((A^\dagger A)^H) = \text{range}(A^H (A^\dagger)^H) \subseteq \text{range}(A^H)$$

$$\text{range}(A^\dagger) = \text{range}(A^\dagger A A^\dagger) \subseteq \text{range}(A^\dagger A) \subseteq \text{range}(A^H)$$

- The other direction is also true. Hence

$$\text{range}(A^\dagger) \equiv \text{range}(A^H) \qquad \text{range}(A^\dagger A) \equiv \text{range}(A^H)$$

- By the definition of orthogonal projection (Hermitian, idempotent, and range preservation):

$$P_{\text{range}(A)} = A A^\dagger$$

$$P_{\text{range}(A^H)} = A^\dagger A$$

- If A has full column rank, then

$$A^\dagger = (A^H A)^{-1} A^H \quad \Rightarrow \quad P_{\text{range}(A)} = A (A^H A)^{-1} A^H$$

Distance Between Subspaces



- Measuring distance b/w two subspaces:

$$\mathcal{S}_1, \mathcal{S}_2 \subseteq \mathbb{R}^n, \dim(\mathcal{S}_1) = \dim(\mathcal{S}_2)$$

$$\text{dist}(\mathcal{S}_1, \mathcal{S}_2) := \|P_1 - P_2\|_2$$

P_i is an orthogonal projection onto $\mathcal{S}_i$

- Example (A special case):**

Partition two orthogonal matrices

$$W = [W_1 \quad W_2] \in \mathbb{R}^{n \times n}, \quad W_1 \in \mathbb{R}^{n \times k}$$

$$Z = [Z_1 \quad Z_2] \in \mathbb{R}^{n \times n}, \quad Z_1 \in \mathbb{R}^{n \times k}$$



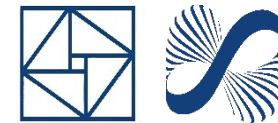
$$\mathcal{S}_1 := \text{range}(W_1), \quad \mathcal{S}_2 := \text{range}(Z_1)$$

Remark: Geometrically, we can relate the distance between two subspaces with the **Largest Principal Angle**, i.e.

$$\|P_1 - P_2\|_2 = \sin(\theta_{\max})$$

$$\begin{aligned} \text{dist}(\mathcal{S}_1, \mathcal{S}_2) &= \|W_1 W_1^T - Z_1 Z_1^T\|_2 \\ &= \|W^T (W_1 W_1^T - Z_1 Z_1^T) Z\|_2 \\ &= \left\| \begin{bmatrix} 0 & W_1^T Z_2 \\ -W_2^T Z_1 & 0 \end{bmatrix} \right\|_2 \\ \text{Exercise } ? &= \max\{\|W_1^T Z_2\|_2, \|W_2^T Z_1\|_2\} \end{aligned}$$

Distance Between Subspaces, Continued



- We notice the following matrix is also orthogonal

$$W^T Z = \begin{bmatrix} W_1^T Z_1 & W_1^T Z_2 \\ W_2^T Z_1 & W_2^T Z_2 \end{bmatrix} =: \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} =: Q$$

$$\forall \mathbf{x} \in \mathbb{R}^k, \|\mathbf{x}\|_2 = 1 : Q \begin{bmatrix} \mathbf{x} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} Q_{11}\mathbf{x} \\ Q_{21}\mathbf{x} \end{bmatrix} \quad \Rightarrow \quad \|Q_{11}\mathbf{x}\|_2^2 + \|Q_{21}\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2 = 1$$

$$\Rightarrow \|Q_{21}\|_2^2 = \max_{\|\mathbf{x}\|_2=1} \|Q_{21}\mathbf{x}\|_2^2 = 1 - \min_{\|\mathbf{x}\|_2=1} \|Q_{11}\mathbf{x}\|_2^2 = 1 - \sigma_{\min}(Q_{11})^2$$

$$\Rightarrow \|Q_{12}\|_2^2 = 1 - \sigma_{\min}(Q_{11})^2 = \|Q_{21}\|_2^2$$

- Partition two orthogonal matrices W and Z , the distance between k -dimensional subspaces:

$$\text{dist}(\mathcal{S}_1, \mathcal{S}_2) = \|W_1^T Z_2\|_2 = \|Z_1^T W_2\|_2$$

Cos-Sin Decomposition



Let $Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \in \mathbb{R}^{n \times n}$ be an orthogonal matrix.

There exist orthogonal matrices:

$$\left. \begin{aligned} U &= \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \in \mathbb{R}^{n \times n} \\ V &= \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix} \in \mathbb{R}^{n \times n} \end{aligned} \right\} \Rightarrow U^T Q V = \begin{bmatrix} I & 0 & 0 & 0 & 0 & 0 \\ 0 & C & 0 & 0 & S & 0 \\ 0 & 0 & 0 & 0 & 0 & I \\ \hline 0 & 0 & 0 & I & 0 & 0 \\ 0 & -S & 0 & 0 & C & 0 \\ 0 & 0 & I & 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$C := \text{diag}(c_1, \dots, c_p), \quad S := \text{diag}(s_1, \dots, s_p), \quad 0 < c_i, s_i < 1, \quad c_i^2 + s_i^2 = 1 \quad (i = 1, \dots, p)$$

Cos-Sin Decomposition for Unitary Matrices



Theorem 2.9 (Cos-sin Decomposition for Unitary Matrices)

For a unitary matrix $Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \in \mathbb{C}^{n \times n}$, $Q_{11} \in \mathbb{C}^{k \times k}$, $Q_{22} \in \mathbb{C}^{j \times j}$ ($k \leq j$)

there exist unitary matrices $U = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \in \mathbb{C}^{n \times n}$, $V = \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix} \in \mathbb{C}^{n \times n}$

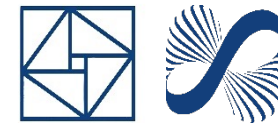
such that

$$U^H Q V = \begin{bmatrix} C & S & 0 \\ -S & C & 0 \\ 0 & 0 & I_{j-k} \end{bmatrix}$$

where

$$\begin{aligned} C &:= \text{diag}(c_1, \dots, c_k), & c_i &= \cos(\theta_i) \\ S &:= \text{diag}(s_1, \dots, s_k), & s_i &= \sin(\theta_i) \end{aligned} \quad \left(0 \leq \theta_1 \leq \dots \leq \theta_k \leq \frac{\pi}{2}\right)$$

Thin Cos-Sin Decomposition



Theorem 2.10 (Cos-sin decomposition for tall-skinny matrices)

Let Q be a matrix with orthonormal columns

$$Q = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}, \quad Q_1 \in \mathbb{R}^{m_1 \times n}, \quad Q_2 \in \mathbb{R}^{m_2 \times n} \quad (m_1 \geq n, m_2 \geq n)$$

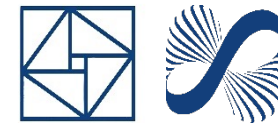
There exist orthogonal matrices $U_1 \in \mathbb{R}^{m_1 \times m_1}$, $U_2 \in \mathbb{R}^{m_2 \times m_2}$, $V_1 \in \mathbb{R}^{n \times n}$, such that

$$\begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix}^T \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V_1 = \begin{bmatrix} C \\ S \end{bmatrix}$$

where

$$C := \text{diag}(\cos(\theta_1), \dots, \cos(\theta_n)) \quad S := \text{diag}(\sin(\theta_1), \dots, \sin(\theta_n)) \quad 0 \leq \theta_1 \leq \dots \leq \theta_n \leq \frac{\pi}{2}$$

Proof of Cos-Sin Decomposition



1 $\|Q_1\|_2 \leq \|Q\|_2 = 1, \quad \sigma(Q) \subset [0, 1] \quad \Rightarrow \quad U_1^T Q_1 V_1 = C = \text{diag}(c_1, \dots, c_n)$

$$1 = c_1 = \dots = c_t > c_{t+1} \geq \dots \geq c_n \geq 0 \quad \Rightarrow \quad C = \begin{bmatrix} I_t & 0 \\ 0 & \Sigma \end{bmatrix}$$

2 $Q_2 V_1 = [W_1 \quad W_2], \quad W_1 \in \mathbb{R}^{m_2 \times t}, \quad W_2 \in \mathbb{R}^{m_2 \times (n-t)}$

$$\Rightarrow \begin{bmatrix} U_1 & 0 \\ 0 & I_{m_2} \end{bmatrix}^T \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V_1 = \begin{bmatrix} I_t & 0 \\ 0 & \Sigma \\ W_1 & W_2 \end{bmatrix} = \begin{bmatrix} I_t & 0 \\ 0 & \Sigma \\ 0 & W_2 \end{bmatrix}$$

orthonormal columns

$$\Rightarrow W_2^T W_2 = I_{n-t} - \Sigma^T \Sigma = \text{diag}(1 - c_{t+1}^2, \dots, 1 - c_n^2) =: \text{diag}(s_{t+1}^2, \dots, s_n^2)$$

3 Orthogonal matrix $U_2 = [* \quad W_2 \text{diag}(s_{t+1}^{-1}, \dots, s_n^{-1})]$ s.t. $U_2^T Q_2 V_1 = \text{diag}(s_1, \dots, s_n) =: S$

Example: Information Geometry



Parameter Space Compression Underlies Emergent Theories and Predictive Models

BENJAMIN B. MACHTA, RICKY CHACHRA, MARK K. TRANSTRUM, AND JAMES P. SETHNA [Authors Info & Affiliations](#)

SCIENCE • 1 Nov 2013 • Vol 342, Issue 6158 • pp. 604-607 • DOI:10.1126/science.1238723

↓ 3,975 227



CHECK ACCESS

Key question: Why do macroscopic predictions often depend on only a few parameter combinations, despite a large number of microscopic parameters?

- Let $\theta \in \mathbb{R}^n$ denote the model parameters and $f(\theta)$ the predicted observables. Define:
 - $J = \partial f / \partial \theta$: **sensitivity matrix**, describing how parameters affect predictions;
 - C : **covariance matrix** of Gaussian observation noise, assumed parameter-independent;
 - $F = J^T C^{-1} J$: **Fisher information matrix**, quantifying the distinguishability of parameter perturbations.

- Applying SVD to the noise-weighted sensitivity matrix gives

$$C^{-1/2} J = U \Sigma V^T, \quad F = V \Sigma^2 V^T.$$

- For fixed parameter scaling, the singular values quantify distinguishability along parameter directions; the leading right singular vectors span a local effective parameter subspace.

Example: From Text to Latent Semantics



- **Latent Semantic Analysis** tries to discover hidden semantic structures in texts. It transforms words and documents into **vectors** in a latent space where semantic similarity can be measured.
- A mathematical framework to transform unstructured text into structured mathematical objects:
 - EVD and SVD tools can be used in this case;
 - Numerical algebra enables us to discover hidden patterns and relationships not visible in the raw text data;
 - This ability to capture semantic relationships, not just surface-level word matching, is what makes SVD and other numerical algebra techniques powerful for text analysis.
- Applications: **潜在语义分析**
 - Latent Semantic Indexing: Fixes vocabulary mismatch by searching in semantic space (not in word space).
 - Document Classification: Classifies more accurately by providing more meaningful features.
 - Plagiarism Detection: Catches plagiarism by detecting semantic similarity rather than text copying.

Data Analysis Step 1: Preprocessing



Sample Documents:

```
Document 1: "Numerical algebra is important for solving linear systems."  
Document 2: "Machine learning uses numerical algebra and optimization."  
Document 3: "Basketball games require teamwork and strategy."  
Document 4: "Football matches need strategy and coordination."  
Document 5: "Deep learning and numerical algebra are used in AI."
```

1. Convert to lowercase, **tokenize**, and **remove punctuation and the stop words**

```
Document 1: ["numerical", "algebra", "important", "solving", "linear", "systems"]  
Document 2: ["machine", "learning", "uses", "numerical", "algebra", "optimization"]  
Document 3: ["basketball", "games", "require", "teamwork", "strategy"]  
Document 4: ["football", "matches", "need", "strategy", "coordination"]  
Document 5: ["deep", "learning", "numerical", "algebra", "used", "ai"]
```

Data Analysis Step 1: Preprocessing



2. Create a sorted vocabulary (22 words)

```
["ai", "algebra", "basketball", "coordination", "deep", "football", "games",  
"important", "learning", "linear", "machine", "matches", "need", "numerical",  
"optimization", "require", "solving", "strategy", "systems", "teamwork",  
"used", "uses"]
```

3. Document-term matrix 5×22 (raw term frequencies)

```
Document 1: [0,1,0,0,0,0,0,1,0,1,0,0,0,1,0,0,1,0,1,0,0,0]  
Document 2: [0,1,0,0,0,0,0,0,1,0,1,0,0,1,1,0,0,0,0,0,0,1]  
Document 3: [0,0,1,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,1,0,1,0]  
Document 4: [0,0,0,1,0,1,0,0,0,0,0,1,1,0,0,0,0,1,0,0,0,0]  
Document 5: [1,1,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,1,0]
```

Sparse

Data Analysis Step 2: Computing Weights



TF-IDF Weights:

$$\text{TF-IDF} = \text{Term Frequency (TF)} \times \text{Inverse Document Frequency (IDF)}$$

1. Calculate term frequency $\text{TF}(t, d) = f(t, d) / (\text{total words in document } d)$

Doc1: 6 words $\rightarrow \text{TF} = 1/6 \approx 0.17$

Doc2: 6 words $\rightarrow \text{TF} = 1/6 \approx 0.17$

Doc3: 5 words $\rightarrow \text{TF} = 1/5 = 0.20$

Doc4: 5 words $\rightarrow \text{TF} = 1/5 = 0.20$

Doc5: 6 words $\rightarrow \text{TF} = 1/6 \approx 0.17$

Term Frequency: How often a word appears in a single document? The more a word appears in a document, the more important it is to that document

Data Analysis Step 2: Computing Weights



2. Calculate $IDF(t) = \ln(\text{Number of documents} / \text{Number of documents containing the term } t) + 1$

avoid zero IDF

ai: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

algebra: $\ln(5/3) + 1 = 0.51 + 1 = 1.51$

basketball: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

coordination: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

deep: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

football: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

games: $\ln(5/1) + 1 = 1.61 + 1 = 2.61$

...

Inverse Document Frequency: How unique or rare a word is across all documents? Words that appear in many documents are less informative than words that appear in few documents

Data Analysis Step 2: Computing Weights



3. Multiply normalized term frequencies by the corresponding IDF values. Intermediate values are rounded for display only; all computations use full precision.

For Document 1:

numerical: $0.17 \times 1.51 = 0.25$

algebra: $0.17 \times 1.51 = 0.25$

important: $0.17 \times 2.61 = 0.43$

solving: $0.17 \times 2.61 = 0.43$

linear: $0.17 \times 2.61 = 0.43$

systems: $0.17 \times 2.61 = 0.43$

For Document 2:

...

...

Data Analysis Step 2: Computing Weights



4. Calculate TF-IDF matrix: Approximate TF-IDF matrix (rounded for display only)

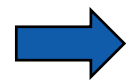
Document 1: [0.00, 0.25, 0.00, 0.00, 0.00, 0.00, 0.00, 0.43, 0.00, 0.43, 0.00, 0.00, 0.00, 0.25, 0.00, 0.00, 0.43, 0.00, 0.43, 0.00, 0.00, 0.00]

Document 2: [0.00, 0.25, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.32, 0.00, 0.43, 0.00, 0.00, 0.25, 0.43, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.43]

Document 3: [0.00, 0.00, 0.52, 0.00, 0.00, 0.00, 0.52, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.52, 0.00, 0.38, 0.00, 0.52, 0.00, 0.00]

Document 4: [0.00, 0.00, 0.00, 0.52, 0.00, 0.52, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.52, 0.52, 0.00, 0.00, 0.00, 0.38, 0.00, 0.00, 0.00, 0.00]

Document 5: [0.43, 0.25, 0.00, 0.00, 0.43, 0.00, 0.00, 0.00, 0.32, 0.00, 0.00, 0.00, 0.00, 0.25, 0.00, 0.00, 0.00, 0.00, 0.00, 0.43, 0.00]



TF-IDF matrix A (5×22)

Applying SVD to TF-IDF Matrix



1. Find singular values of the TF-IDF matrix

$$\sigma_1 = 1.176$$

$$\sigma_2 = 1.071$$

$$\sigma_3 = 1.044$$

$$\sigma_4 = 0.873$$

$$\sigma_5 = 0.753$$

Select the first three singular values. They retain 73.15% of the squared Frobenius norm, compared with 51.13% for two components. Because σ_2 and σ_3 are nearly equal, truncating after σ_2 would separate two almost equally important modes. The gap after σ_3 is the largest among the leading singular values, although there is no sharp cutoff.

2. Take first 3 columns of U and multiply by corresponding singular values

Document 1: (0.000, 0.602, 0.000)

Document 2: (0.000, 0.626, 0.000)

Document 3: (0.832, 0.000, 0.738)

Document 4: (0.832, 0.000, -0.738)

Document 5: (0.000, 0.626, 0.000)

Dimensionality Reduction to 3D Space



3. Take first 3 rows of V^T and multiply by corresponding singular values

ai	(0.000, 0.254, 0.000)
machine	(0.000, 0.254, 0.000)
learning	(0.000, 0.373, 0.000)
linear	(0.000, 0.245, 0.000)
algebra	(0.000, 0.436, 0.000)
numerical	(0.000, 0.436, 0.000)
basketball	(0.369, 0.000, 0.369)
football	(0.369, 0.000, -0.369)
games	(0.369, 0.000, 0.369)

The 1st coordinate identifies the sports subspace, while the 3rd coordinate separates basketball/games-related terms from football/matches-related terms. The 2nd coordinate represents the numerical-algebra/AI terms.

Document Similarity Calculation



- Cosine similarity formula: $\cos\theta = (\mathbf{u} \cdot \mathbf{v}) / (\|\mathbf{u}\| \times \|\mathbf{v}\|)$

Similarity Matrix (in the TF-IDF Space)

	D1	D2	D3	D4	D5
D1	1.00	0.15	0.00	0.00	0.15
D2	0.15	1.00	0.00	0.00	0.29
D3	0.00	0.00	1.00	0.12	0.00
D4	0.00	0.00	0.12	1.00	0.00
D5	0.15	0.29	0.00	0.00	1.00

Similarity Matrix (in the Rank-3 SVD Space)

	D1	D2	D3	D4	D5
D1	1.00	1.00	0.00	0.00	1.00
D2	1.00	1.00	0.00	0.00	1.00
D3	0.00	0.00	1.00	0.12	0.00
D4	0.00	0.00	0.12	1.00	0.00
D5	1.00	1.00	0.00	0.00	1.00

- Document 1, 2, and 5 are similar: discuss numerical algebra and AI related topics
- Document 3 and 4 are related: both discuss sports
- Sports documents and numerical algebra documents have low similarity (dissimilar)

矩阵的扰动分析

Perturbation analysis on matrices

/2.4

Condition of A Linear System



- Estimating sensitivity of solving linear systems:

$$A \in \mathbb{R}^{n \times n} \text{ non-singular, } \mathbf{b} \in \mathbb{R}^n, F \in \mathbb{R}^{n \times n}, \mathbf{f} \in \mathbb{R}^n$$

$$\Rightarrow (A + \varepsilon F)\mathbf{x}(\varepsilon) = \mathbf{b} + \varepsilon \mathbf{f}, \quad \mathbf{x}(0) = \mathbf{x}_*$$

$$\Rightarrow \dot{\mathbf{x}}(0) = A^{-1}(\mathbf{f} - F\mathbf{x}_*) \quad \Rightarrow \mathbf{x}(\varepsilon) = \mathbf{x}_* + \varepsilon \dot{\mathbf{x}}(0) + O(\varepsilon^2)$$

- Condition number:

$$\underbrace{\frac{\|\mathbf{x}(\varepsilon) - \mathbf{x}_*\|}{\|\mathbf{x}_*\|}}_{\text{Relative Error}} \leq |\varepsilon| \|A^{-1}\| \left(\frac{\|\mathbf{f}\|}{\|\mathbf{x}_*\|} + \|F\| \right) + O(\varepsilon^2) \leq \kappa(A) |\varepsilon| \underbrace{\left(\frac{\|F\|}{\|A\|} + \frac{\|\mathbf{f}\|}{\|\mathbf{b}\|} \right)}_{\text{Relative Perturbation}} + O(\varepsilon^2)$$

Relative Error

Relative Perturbation

$$\kappa(A) := \|A\| \|A^{-1}\|$$

Examples of Ill-Conditioned Systems



- Reminder: Eigenvalues are not as useful as singular values: $\max_{i,j} \frac{|\lambda_i|}{|\lambda_j|} \leq \kappa_2(A)$
- Typical examples of ill-conditioned matrices: **(Exercise)**

$$A = \begin{bmatrix} 1 & 2 & & 0 \\ & 1 & \ddots & \\ & & \ddots & 2 \\ 0 & & & 1 \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$\kappa_2(A) = O(n^2)$$

Eigenvalues are all 1, but A is non-normal

$$H = \begin{bmatrix} 1 & \frac{1}{2} & \cdots & \frac{1}{n} \\ \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{n} & \frac{1}{n+1} & \cdots & \frac{1}{2n-1} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$\kappa_2(H) = O\left(\frac{(1 + \sqrt{2})^{4n}}{\sqrt{n}}\right)$$

Well-known ill-conditioned system

Inverse of Perturbed Matrix



Theorem 2.11

$$F \in \mathbb{R}^{n \times n}, \|F\|_p < 1 \quad \Rightarrow \quad (I - F)^{-1} = \sum_{k=0}^{\infty} F^k \quad \text{and} \quad \|(I - F)^{-1}\|_p \leq \frac{1}{1 - \|F\|_p}$$

$$I - F \text{ singular} \quad \Rightarrow \quad \exists \mathbf{x} \neq \mathbf{0}, \text{ s.t. } (I - F)\mathbf{x} = \mathbf{0} \quad \Rightarrow \quad \|\mathbf{x}\|_p = \|F\mathbf{x}\|_p \quad \Rightarrow \quad \|F\|_p \geq 1$$

$$\sum_{k=0}^N F^k (I - F) = I - F^{N+1} \quad \text{and} \quad \|F^{N+1}\|_p \leq \|F\|_p^{N+1} \rightarrow 0 \quad \Rightarrow \quad (I - F)^{-1} = \sum_{k=0}^{\infty} F^k$$

Application (Inverse of Perturbed Matrix):

$$A \text{ is nonsingular and } \gamma := \|A^{-1}E\|_p < 1 \quad \Rightarrow \quad \begin{aligned} &A + E \text{ is nonsingular and} \\ &\|(A + E)^{-1} - A^{-1}\|_p \leq \|E\|_p \|A^{-1}\|_p^2 / (1 - \gamma) \end{aligned}$$

Sensitivity of Matrix Inversion



- Q: For a nonsingular matrix, how to check sensitivity of inversion?
- According to Theorem 2.8, closeness of A to the rank-deficient matrices can be defined as:

$$A_k := \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^T \quad (k < r = \text{rank}(A)) \quad \Rightarrow \quad \min_{\text{rank}(B)=k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$$

The minimal singular value of a matrix is its distance to the rank-deficient matrices in 2-norm.

- For a nonsingular square matrix, **SVD** gives

$$A = U \Sigma V^T = \sum_{i=1}^n \sigma_i \mathbf{u}_i \mathbf{v}_i^T \quad \Rightarrow \quad A^{-1} \mathbf{b} = (U \Sigma V^T)^{-1} \mathbf{b} = \sum_{i=1}^n \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i$$

Roughly speaking, if $\sigma_n > 0$ is small, the solution is sensitive to perturbations of data.

Bauer–Fike Theorem



Theorem 2.12 (Bauer–Fike Theorem, 1960)

$A \in \mathbb{C}^{n \times n}$ is diagonalizable, i.e. $A = X^{-1}\Lambda X$, Λ diagonal, X nonsingular.

For $B \in \mathbb{C}^{n \times n}$, $\mu \in \lambda(B)$, $\exists \lambda \in \lambda(A)$, s.t. $|\lambda - \mu| \leq \|X\|_2 \|X^{-1}\|_2 \|A - B\|_2$.

Sketch of Proof:

$Bx = \mu x$, $0 \neq x \in \mathbb{C}^n$ being an eigen-pair

Assume that $\mu \notin \lambda(A) \Rightarrow \mu I - A$ is nonsingular

$$(B - A)x = \mu x - Ax = (\mu I - A)x$$

$$A \text{ diagonalizable} \Rightarrow x = (\mu I - A)^{-1}(B - A)x = X^{-1}(\mu I - \Lambda)^{-1}X(B - A)x$$

$$\Rightarrow 1 \leq \|X\|_2 \|X^{-1}\|_2 \|A - B\|_2 \left(\min_{\lambda \in \lambda(A)} |\lambda - \mu| \right)^{-1}$$

The sensitivity of eigenvalues is determined by the condition number of the eigenvector matrix, $\kappa_2(X)$

Eigenvalues of A Normal Matrix



- **Normal matrix:**

$$A \in \mathbb{C}^{n \times n}, \quad A^H A = A A^H$$

A is normal if and only if it is unitarily diagonalizable, i.e. $A = U \Lambda U^H$ (**Spectral Theorem**)

Theorem 2.13 (Krylov–Bogoljubov–Weinstein Theorem)

$A \in \mathbb{C}^{n \times n}$ is a normal matrix. $\forall \mathbf{x} \in \mathbb{C}^n, \|\mathbf{x}\|_2 = 1, \mu(\mathbf{x}) := \mathbf{x}^H A \mathbf{x}$

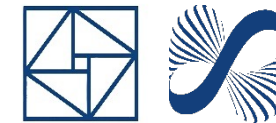
$$\min_{\lambda \in \lambda(A)} |\lambda - \mu(\mathbf{x})| \leq \|(A - \mu(\mathbf{x})I)\mathbf{x}\|_2$$

Remark: Each of the following disks contains at least one eigenvalue of A

$$\tilde{D}_i(A) := \left\{ z \in \mathbb{C} : |z - a_{ii}| \leq \left(\sum_{j \neq i} |a_{ij}|^2 \right)^{\frac{1}{2}} \right\}, \quad i = 1, \dots, n$$

This result can be shown by choosing $\mathbf{x} = \mathbf{e}_i$ in Theorem 2.13.

Hoffman–Wielandt Theorem



Theorem 2.14 (Hoffman–Wielandt Theorem, 1953)

$A, B \in \mathbb{C}^{n \times n}$ are normal matrices. $\lambda(A) = \{\lambda_1, \dots, \lambda_n\}$, $\lambda(B) = \{\mu_1, \dots, \mu_n\}$

$$\exists \text{ permutation } \pi, \text{ s.t. } \sum_{i=1}^n |\lambda_i - \mu_{\pi(i)}|^2 \leq \|A - B\|_F^2$$

- It shows **stable collective behavior** of the eigenvalues of normal matrices under perturbations
- We have the following corollaries:

If A and B are Hermitian, $\lambda_1 \geq \dots \geq \lambda_n$, $\mu_1 \geq \dots \geq \mu_n$ $\Rightarrow \sum_{i=1}^n (\lambda_i - \mu_i)^2 \leq \|A - B\|_F^2$

$\sigma_1 \geq \dots \geq \sigma_n \geq 0$, $\tau_1 \geq \dots \geq \tau_n \geq 0$ are singular values of $A, B \in \mathbb{C}^{m \times n}$ ($m \geq n$)

$$\Rightarrow \sum_{i=1}^n (\sigma_i - \tau_i)^2 \leq \|A - B\|_F^2$$

Courant–Fischer Theorem



Theorem 2.15 (Min-Max Theorem, 1920s)

$A \in \mathbb{C}^{n \times n}$ is a Hermitian matrix, and $\lambda_1 \geq \cdots \geq \lambda_n$. Then

$$\lambda_k = \max_{\dim(\mathcal{S})=k} \min_{\mathbf{0} \neq \mathbf{x} \in \mathcal{S}} \frac{\mathbf{x}^H A \mathbf{x}}{\mathbf{x}^H \mathbf{x}} = \min_{\dim(\mathcal{T})=n-k+1} \max_{\mathbf{0} \neq \mathbf{x} \in \mathcal{T}} \frac{\mathbf{x}^H A \mathbf{x}}{\mathbf{x}^H \mathbf{x}}$$

- ▶ $\lambda_1 = \max_{\mathbf{0} \neq \mathbf{x} \in \mathbb{C}^n} \frac{\mathbf{x}^H A \mathbf{x}}{\mathbf{x}^H \mathbf{x}}$: the largest eigenvalue (**Rayleigh–Ritz theorem**; see Chapter 8)
- ▶ $\lambda_n = \min_{\mathbf{0} \neq \mathbf{x} \in \mathbb{C}^n} \frac{\mathbf{x}^H A \mathbf{x}}{\mathbf{x}^H \mathbf{x}}$: the smallest eigenvalue (minimum value of the **Rayleigh quotient**)

The min-max theorem provides a variational characterization of the eigenvalues of a **Hermitian** matrix. It is powerful for estimating eigenvalues without computing them directly.

Proof of Courant–Fischer Theorem



- 1 $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ are the orthonormal eigenvectors corresponding to $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$

$$\mathcal{S}_k := \text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \quad \Rightarrow \quad \dim(\mathcal{S}_k) = k$$

$$\forall \mathbf{x} = \sum_{i=1}^k c_i \mathbf{v}_i \in \mathcal{S}_k, \quad \mathbf{x} \neq \mathbf{0} \quad \Rightarrow \quad R_A(\mathbf{x}) := \frac{\mathbf{x}^H A \mathbf{x}}{\mathbf{x}^H \mathbf{x}} = \frac{\sum_{i=1}^k |c_i|^2 \lambda_i}{\sum_{i=1}^k |c_i|^2} \geq \lambda_k$$

$$\Rightarrow \quad \max_{\dim(\mathcal{S})=k} \min_{\mathbf{x} \in \mathcal{S}} R_A(\mathbf{x}) \geq \lambda_k$$

arbitrary
 $\dim(\mathcal{S}) = k$

- 2 $\mathcal{T}_k := \text{span}\{\mathbf{v}_k, \mathbf{v}_{k+1}, \dots, \mathbf{v}_n\} \quad \Rightarrow \quad \dim(\mathcal{T}_k) = n - k + 1 \quad \Rightarrow \quad \mathcal{S} \cap \mathcal{T}_k \neq \{\mathbf{0}\}$

$$\mathbf{0} \neq \mathbf{y} \in \mathcal{S} \cap \mathcal{T}_k : \mathbf{y} = \sum_{i=k}^n d_i \mathbf{v}_i \quad \Rightarrow \quad R_A(\mathbf{y}) = \frac{\sum_{i=k}^n |d_i|^2 \lambda_i}{\sum_{i=k}^n |d_i|^2} \leq \lambda_k$$

- 3 Combining (1) and (2) shows the first equality; and, the other equality can be proved similarly.

Weyl Theorem



- Separation of eigenvalues

$A \in \mathbb{C}^{n \times n}$ is Hermitian, and $\lambda_1 \geq \cdots \geq \lambda_n$

$\mu_1 \geq \cdots \geq \mu_{n-1}$ are eigenvalues of $C = U^H A U$, $U \in \mathbb{C}^{n \times (n-1)}$ and $U^H U = I_{n-1}$

$$\Rightarrow \lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \lambda_n$$

Theorem 2.16 (Weyl's Inequality)

If A and B are Hermitian and their respective eigenvalues are $\lambda_1 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \cdots \geq \mu_n$, then

$$\lambda_i + \lambda_{\min}(B - A) \leq \mu_i \leq \lambda_i + \lambda_{\max}(B - A), \quad i = 1, \dots, n$$

and

$$|\mu_i - \lambda_i| \leq \|B - A\|_2, \quad i = 1, \dots, n$$

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数值代数
Numerical Algebra

THANKS

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