

# Numerical Linear Algebra

## for Computational Science and Information Engineering

### Essentials of Linear Algebra

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# Vector spaces

Section 2.1 in Darve & Wootters (2021)

## Vectors

- We are interested in vectors in vector spaces  $\mathbb{F}^n$  with real ( $\mathbb{F} := \mathbb{R}$ ) and complex ( $\mathbb{F} := \mathbb{C}$ ) scalar coefficients.

A vector  $\mathbf{x} \in \mathbb{F}^n$  is an  $n$ -tuple given by

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \text{ with scalar coefficients } x_1, x_2, \dots, x_n \in \mathbb{F}.$$

- The vector space  $\mathbb{F}^n$  is said to support addition, and scalar multiplication. That is, for every pair  $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$  and  $\alpha \in \mathbb{F}$ , we have

$$\mathbf{x} + \alpha \mathbf{y} = \begin{bmatrix} x_1 + \alpha y_1 \\ x_2 + \alpha y_2 \\ \vdots \\ x_n + \alpha y_n \end{bmatrix} \in \mathbb{F}^n.$$

# Vector spaces

- Vector spaces are fundamental structures of (numerical) linear algebra.

## Definition (Vector space)

A vector space  $\mathcal{V}$  over a scalar field  $\mathbb{F}$  is a non-empty set which supports addition and multiplication with the following axioms:

1. Associative addition:  $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z} \quad \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{V}$
2. Commutative addition:  $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$
3. Additive identity:  $\exists \mathbf{0} \in \mathcal{V}$  s.t.  $\mathbf{x} + \mathbf{0} = \mathbf{x} \quad \forall \mathbf{x} \in \mathcal{V}$
4. Additive inverse:  $\forall \mathbf{x} \in \mathcal{V}, \exists -\mathbf{x} \in \mathcal{V}$  s.t.  $\mathbf{x} + (-\mathbf{x}) = \mathbf{0}$
5. Field-multiplication compatibility:  $\alpha(\beta\mathbf{x}) = (\alpha\beta)\mathbf{x} \quad \forall \mathbf{x} \in \mathcal{V}, \alpha, \beta \in \mathbb{F}$
6. Field-multiplicative identity:  $\exists 1 \in \mathbb{F}$  s.t.  $1\mathbf{x} = \mathbf{x} \quad \forall \mathbf{x} \in \mathcal{V}$
7. Distributive field multiplication w.r.t. vector addition:  $\alpha(\mathbf{x} + \mathbf{y}) = \alpha\mathbf{x} + \alpha\mathbf{y} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}, \alpha \in \mathbb{F}$
8. Distributive field multiplication w.r.t. field addition:  $(\alpha + \beta)\mathbf{x} = \alpha\mathbf{x} + \beta\mathbf{x} \quad \forall \mathbf{x} \in \mathcal{V}, \alpha, \beta \in \mathbb{F}$

## Vector spaces, cont'd

- In practice, most axioms are trivially satisfied, and verifying whether  $\mathcal{V}$  is a vector space boils down to checking for **closure under addition** and **scalar multiplication**, i.e., whether

$$\mathbf{x} + \mathbf{y} \in \mathcal{V} \text{ and } \alpha \mathbf{x} \in \mathcal{V} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}, \alpha \in \mathbb{F}.$$

### Example and counter-examples

- $\mathbb{R}^n$  **is** a vector space over  $\mathbb{R}$ .
- $\mathcal{V} := \{\mathbf{x} \in \mathbb{R}^n \text{ s.t. } x_i > 0, i = 1, \dots, n\}$  **is not** a vector space.
- The set of floating-point numbers **does not** form a field, and cannot serve as the scalar field for a vector space.

### Disclaimer

- The elements of a vector space  $\mathcal{V}$  may not always be finite-dimensional vectors; they can also be **functions**, even when  $\mathcal{V}$  is **finite-dimensional**.
- In this course, we generally assume  $\mathcal{V} \subseteq \mathbb{F}^n$ , where the field  $\mathbb{F}$  is either  $\mathbb{R}$  or  $\mathbb{C}$ .
- Note that much of what we cover here also applies to function spaces, which can be useful when developing methods to solve PDEs, ODEs, when processing spatio-temporal data, ...

## Linear combinations

- ▶ A linear combination of vectors  $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{F}^n$  is prescribed by some scalars  $\alpha_1, \dots, \alpha_k \in \mathbb{F}$  and given by

$$\alpha_1 \mathbf{x}_1 + \cdots + \alpha_k \mathbf{x}_k \in \mathbb{F}^n.$$

- ▶ The span of  $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{F}^n$  is a subspace of  $\mathbb{F}^n$  which consists of all the linear combinations of  $\mathbf{x}_1, \dots, \mathbf{x}_n$ , i.e.,

$$\text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\} := \{\alpha_1 \mathbf{x}_1 + \cdots + \alpha_k \mathbf{x}_k \text{ s.t. } \alpha_1, \dots, \alpha_k \in \mathbb{F}\}$$

- ▶ The information that can be captured by linear combination depends on the **linear independence**, or lack thereof, of the spanning vectors.

### Definition (Linear independence)

$\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{F}^n$  are linearly independent if no  $\mathbf{x}_i$  can be written as a linear combination of the other vectors. Or, equivalently, if

$$\sum_{i=1}^k \alpha_i \mathbf{x}_i = 0 \implies \alpha_1, \dots, \alpha_k = 0.$$

## Bases, dimension and subspaces of vector spaces

- The elements of a vector space can all be represented using a basis.

### Definition (Basis & dimension of vector space)

- The vectors  $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathcal{V}$  form a basis of the vector space  $\mathcal{V}$ , if they are linearly independent, and  $\text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_k\} = \mathcal{V}$ .
- While  $\mathcal{V}$  admits infinitely many different bases, all of these consist of  $k$  linearly independent vectors. We call  $k$  the dimension of  $\mathcal{V}$ , and we write  $\dim(\mathcal{V}) = k$ .

For a basis  $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathcal{V}$  of  $\mathcal{V}$ , we define  $\mathbf{V} := [\mathbf{v}_1, \dots, \mathbf{v}_k]$ , so that for each  $\mathbf{x} \in \mathcal{V}$ , there is a unique  $\boldsymbol{\alpha} \in \mathbb{F}^k$  such that  $\mathbf{x} = \mathbf{V}\boldsymbol{\alpha} = \sum_{i=1}^k \alpha_i \mathbf{v}_i$ .

- In practice, linear subspaces, i.e., lower-dimensional vector spaces within vector spaces, are often used in place of high-dimensional vector spaces.

### Definition (Linear subspace)

A linear subspace  $\mathcal{S} \subset \mathcal{V}$  of a vector space  $\mathcal{V}$  is a non-empty subset which is **closed under addition and scalar multiplication**, i.e.,

$$\mathbf{x} + \mathbf{y} \in \mathcal{S} \text{ and } \alpha \mathbf{x} \in \mathcal{S} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{S}, \alpha \in \mathbb{F}.$$

# Inner products and norms

Section 2.2 in Darve & Wootters (2021)

## Vector inner products

- The abstract definition of length of a vector, angles and orthogonality between vectors, which are important notions in numerical linear algebra, is made possible with the use of inner products.

### Definition (Inner product)

An inner product  $(\cdot, \cdot)$  on a vector space  $\mathcal{V}$  over  $\mathbb{F}$  is a mapping  $\mathcal{V} \times \mathcal{V} \rightarrow \mathbb{F}$  s.t.

1.  $(\cdot, \cdot)$  is linear w.r.t. to its first argument:

$$(\alpha \mathbf{x}_1 + \beta \mathbf{x}_2, \mathbf{y}) = \alpha (\mathbf{x}_1, \mathbf{y}) + \beta (\mathbf{x}_2, \mathbf{y}) \quad \forall \mathbf{x}_1, \mathbf{x}_2, \mathbf{y} \in \mathcal{V}, \alpha, \beta \in \mathbb{F}$$

2.  $(\cdot, \cdot)$  is Hermitian:  $(\mathbf{y}, \mathbf{x}) = \overline{(\mathbf{x}, \mathbf{y})} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$

3.  $(\cdot, \cdot)$  is positive-definite:  $(\mathbf{x}, \mathbf{x}) \geq 0 \quad \forall \mathbf{x} \in \mathcal{V}$  and  $(\mathbf{x}, \mathbf{x}) = 0 \iff \mathbf{x} = \mathbf{0}$

$\bar{\alpha} := \Re\{\alpha\} - i\Im\{\alpha\}$  is the complex conjugate of  $\alpha \in \mathbb{F}$ .

- In particular, **dot products**, which are often used on  $\mathcal{V} \subseteq \mathbb{F}^n$ , are given by:

- $(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^n x_i y_i \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V} \subseteq \mathbb{R}^n,$
- $(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y} = \mathbf{x}^H \mathbf{y} = \sum_{i=1}^n \bar{x}_i y_i \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V} \subseteq \mathbb{C}^n.$

$\mathbf{x}^H := \bar{\mathbf{x}}^T$  denotes the conjugate transpose of  $\mathbf{x} \in \mathbb{F}^n$ .

## Properties of inner products

- By the **Hermitian property**, every inner product  $(\cdot, \cdot)$  on a vector space  $\mathcal{V}$  is such that, for all  $\mathbf{x} \in \mathcal{V}$ ,  $(\mathbf{x}, \mathbf{x})$  is **real**, even if  $\mathcal{V}$  is defined over  $\mathbb{C}$ .

### Theorem (Cauchy-Schwarz inequality)

Inner products  $(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{F}$  are s.t.  $|(\mathbf{x}, \mathbf{y})|^2 \leq (\mathbf{x}, \mathbf{x})(\mathbf{y}, \mathbf{y}) \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$ .

#### Proof.

Let  $f(\mathbf{x}, \mathbf{y}, \alpha) := (\mathbf{x} - \alpha\mathbf{y}, \mathbf{x} - \alpha\mathbf{y})$  for  $\mathbf{x}, \mathbf{y} \in \mathcal{V} \setminus \{\mathbf{0}\}$ ,  $\alpha \in \mathbb{F}$ .

By linearity of 1st argument and Hermitian property, we have

$$\begin{aligned} f(\mathbf{x}, \mathbf{y}, \alpha) &= (\mathbf{x}, \mathbf{x} - \alpha\mathbf{y}) - \alpha(\mathbf{y}, \mathbf{x} - \alpha\mathbf{y}) = \overline{(\mathbf{x} - \alpha\mathbf{y}, \mathbf{x})} - \alpha \overline{(\mathbf{x} - \alpha\mathbf{y}, \mathbf{y})} \\ &= (\mathbf{x}, \mathbf{x}) - \overline{\alpha} \cdot (\mathbf{x}, \mathbf{y}) - \alpha \cdot (\mathbf{y}, \mathbf{x}) + |\alpha|^2 \cdot (\mathbf{y}, \mathbf{y}) \end{aligned}$$

By positive-definiteness, we have  $f(\mathbf{x}, \mathbf{y}, \alpha) \geq 0$  so that

$$(\mathbf{x}, \mathbf{x}) + |\alpha|^2 \cdot (\mathbf{y}, \mathbf{y}) \geq \overline{\alpha} \cdot (\mathbf{x}, \mathbf{y}) + \alpha \cdot (\mathbf{y}, \mathbf{x})$$

Then, if we let  $\alpha := (\mathbf{x}, \mathbf{y}) / (\mathbf{y}, \mathbf{y})$ , we get

$$(\mathbf{x}, \mathbf{x}) + \frac{|(\mathbf{x}, \mathbf{y})|^2}{(\mathbf{y}, \mathbf{y})} \geq \frac{|(\mathbf{x}, \mathbf{y})|^2}{(\mathbf{y}, \mathbf{y})} + \frac{|(\mathbf{x}, \mathbf{y})|^2}{(\mathbf{y}, \mathbf{y})} \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V} \setminus \{\mathbf{0}\}, \text{ then } \times \text{ by } (\mathbf{y}, \mathbf{y}). \quad \square$$

# Vector norms

- ▶ Vector norms are abstract measures of length in vector spaces.

## Definition (Vector norm)

A vector norm  $\|\cdot\|$  on a vector space  $\mathcal{V}$  over  $\mathbb{F}$  is any real-valued function s.t.

1.  $\|\cdot\|$  is positive-definite:  $\|\mathbf{x}\| \geq 0 \quad \forall \mathbf{x} \in \mathcal{V}$  and  $\|\mathbf{x}\| = 0 \iff \mathbf{x} = \mathbf{0}$
2.  $\|\cdot\|$  is homogeneous:  $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\| \quad \forall \mathbf{x} \in \mathcal{V}, \alpha \in \mathbb{F}$
3.  $\|\cdot\|$  satisfies the triangular inequality:  $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$

- ▶ Popular vector norms on vector spaces  $\mathcal{V} \subseteq \mathbb{F}^n$  are

- 1-norm:  $\|\mathbf{x}\|_1 := \sum_{i=1}^n |x_i| \quad \forall \mathbf{x} \in \mathcal{V}$ .
- 2-norm:  $\|\mathbf{x}\|_2 := \left( \sum_{i=1}^n |x_i|^2 \right)^{1/2} \quad \forall \mathbf{x} \in \mathcal{V}$ .
  - The 2-norm is induced by the dot product, i.e.,  $\|\mathbf{x}\|_2 = (\mathbf{x} \cdot \mathbf{x})^{1/2}$ .
  - Every inner product  $(\cdot, \cdot)$  on  $\mathcal{V}$  induces a norm  $\|\mathbf{x}\| := (\mathbf{x}, \mathbf{x})^{1/2} \quad \forall \mathbf{x} \in \mathcal{V}$ .
- $p$ -norm:  $\|\mathbf{x}\|_p := \left( \sum_{i=1}^n |x_i|^p \right)^{1/p} \quad \forall \mathbf{x} \in \mathcal{V}$ .
- $\infty$ -norm:  $\|\mathbf{x}\|_\infty := \max_{1 \leq i \leq n} |x_i| \quad \forall \mathbf{x} \in \mathcal{V}$ .

## Equivalence of vector norms

- ▶ A sequence of vectors  $\{\mathbf{x}_k\}_{k \in \mathbb{N}} \subset \mathcal{V}$  converges to a vector  $\mathbf{x} \in \mathcal{V}$  under the norm  $\|\cdot\|$  defined on  $\mathcal{V}$  if, for any real value  $\epsilon > 0$ , there exists  $K$  s.t.  $\|\mathbf{x}_k - \mathbf{x}\| < \epsilon$  for all  $k \geq K$ .
- ▶ Two vector norms  $\|\cdot\|$  and  $\|\cdot\|'$  are equivalent if convergence under one norm implies convergence under the other.

The equivalence of vector norms is usually revealed by making use of the following theorem:

### Theorem (Equivalent vector norms)

Two vector norms  $\|\cdot\|$  and  $\|\cdot\|'$  on a vector space  $\mathcal{V}$  are equivalent iff there exist real constants  $C_1, C_2 > 0$  s.t.  $C_1\|\mathbf{x}\| \leq \|\mathbf{x}\|' \leq C_2\|\mathbf{x}\| \forall \mathbf{x} \in \mathcal{V}$ .

- ▶ In finite-dimensional vector spaces  $\mathcal{V} \subseteq \mathbb{F}^n$ , all norms are equivalent.  
In particular, we have:

- $\|\mathbf{x}\|_2 \leq \|\mathbf{x}\|_1 \leq \sqrt{n} \|\mathbf{x}\|_2 \quad \forall \mathbf{x} \in \mathcal{V}$ ,
- $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2 \leq \sqrt{n} \|\mathbf{x}\|_\infty \quad \forall \mathbf{x} \in \mathcal{V}$ ,
- $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_1 \leq n \|\mathbf{x}\|_\infty \quad \forall \mathbf{x} \in \mathcal{V}$ .

## Orthogonality and orthonormality

- ▶ For any inner product  $(\cdot, \cdot)$  defined on a vector space  $\mathcal{V}$  over  $\mathbb{R}$ , the notion of angle between two vectors  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  is introduced through the relation

$$(\mathbf{x}, \mathbf{y}) = \|\mathbf{x}\| \|\mathbf{y}\| \cos(\angle(\mathbf{x}, \mathbf{y})) \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$$

where  $\|\cdot\|$  is the induced norm  $\|\mathbf{x}\| = (\mathbf{x}, \mathbf{x})^{1/2} \quad \forall \mathbf{x} \in \mathcal{V}$ .

Consequently, non-zero vectors  $\mathbf{x}, \mathbf{y} \in \mathcal{V}$  form a right angle, which is  $\cos(\angle(\mathbf{x}, \mathbf{y})) = 0$ , iff  $(\mathbf{x}, \mathbf{y}) = 0$ . More generally,

### Definition (Orthogonality & orthonormality)

- A set of vectors  $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathcal{V}$  in a vector space  $\mathcal{V}$  equipped with an inner product  $(\cdot, \cdot)$  over a scalar field  $\mathbb{F}$  is orthogonal if

$$i \neq j \implies (\mathbf{x}_i, \mathbf{x}_j) = 0 \quad \text{for } i, j = 1, \dots, k.$$

- If  $(\mathbf{x}_i, \mathbf{x}_j) = \delta_{ij}$  for  $i, j = 1, \dots, k$ , then the vectors  $\mathbf{x}_1, \dots, \mathbf{x}_k$  are orthonormal.

## Orthogonality and orthonormality, cont'd

- The notion of orthogonal subspaces is useful for the definition and analysis of numerical methods in linear algebra.

### Definition (Orthogonal subspace & orthogonal complement)

- Let  $\mathcal{S}$  and  $\mathcal{T}$  be linear subspaces of the vector space  $\mathcal{V}$  equipped with an inner product  $(\cdot, \cdot)$ . Then, we say that  $\mathcal{S}$  is orthogonal to  $\mathcal{T}$ , i.e.,  $\mathcal{S} \perp \mathcal{T}$ , iff  $(\mathbf{x}, \mathbf{y}) = 0 \forall \mathbf{x}, \mathbf{y} \in \mathcal{S} \times \mathcal{T}$ .
- The orthogonal complement of  $\mathcal{S}$ , denoted by  $\mathcal{S}^\perp$ , consists of all the vectors in  $\mathcal{V}$  which are orthogonal to  $\mathcal{S}$ , i.e.,

$$\mathcal{S}^\perp := \{\mathbf{x} \in \mathcal{V} \text{ s.t. } (\mathbf{x}, \mathbf{y}) = 0 \forall \mathbf{y} \in \mathcal{S}\}.$$

### Theorem (Orthogonal decomposition of vector spaces)

If  $\mathcal{S}$  is a linear subspace of a vector space  $\mathcal{V} \subseteq \mathbb{F}^n$ , then every  $\mathbf{x} \in \mathcal{V}$  admits a **unique decomposition**  $\mathbf{x} = \mathbf{y} + \mathbf{z}$  where  $\mathbf{y} \in \mathcal{S}$  and  $\mathbf{z} \in \mathcal{S}^\perp$ :

$$\mathcal{V} = \mathcal{S} \oplus \mathcal{S}^\perp \text{ and } \dim(\mathcal{V}) = \dim(\mathcal{S}) + \dim(\mathcal{S}^\perp).$$

We say that  $\mathcal{V}$  is decomposed by the **direct sum** of  $\mathcal{V}$  and  $\mathcal{V}^\perp$ .

# Linear transformations and matrices

Section 2.3 in Darve & Wootters (2021)

## From linear transformations between vector spaces to matrices

- Linear transformations (a.k.a. linear maps) are essential operations which are used over and over again in (numerical) linear algebra.

### Definition (Linear transformation)

A linear transformation  $T$  from a vector space  $\mathcal{V}$  to another vector space  $\mathcal{W}$ , both defined over a field  $\mathbb{F}$ , i.e.,  $T : \mathbf{x} \in \mathcal{V} \mapsto T(\mathbf{x}) \in \mathcal{W}$ , is such that

$$T(\mathbf{x} + \alpha\mathbf{y}) = T(\mathbf{x}) + \alpha T(\mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}, \alpha \in \mathbb{F}.$$

- Irrespective of whether a linear map operates between function or discrete vector spaces, practical problem-solving often benefits from expressing the action of such maps in a discrete, matrix form.

### Proposition (Matrix representation)

The action of a linear transformation  $T : \mathcal{V} \rightarrow \mathcal{W}$  between **finite-dimensional** vector spaces defined over a same field  $\mathbb{F}$ , can be recast into a matrix-vector product with a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  where  $n := \dim(\mathcal{V})$  and  $m := \dim(\mathcal{W})$ .

Remark: A **function space** can be a finite dimensional vector space.

# Review of matrix arithmetic

The components of  $\mathbf{A}, \mathbf{B} \in \mathbb{F}^{m \times n}$  and  $\mathbf{C} \in \mathbb{F}^{n \times p}$  are denoted by  $a_{ij}$ ,  $b_{ij}$  and  $c_{ij}$ .

The vector  $\mathbf{x} \in \mathbb{F}^n$  has components  $x_i$  and  $\alpha \in \mathbb{F}$ .

## Basic Operations:

- Addition:  $(\mathbf{A} + \mathbf{B})_{ij} = a_{ij} + b_{ij}$
- Scalar mult.:  $(\alpha \mathbf{A})_{ij} = \alpha a_{ij}$
- Matrix mult.:  $(\mathbf{AC})_{ij} = \sum_k a_{ik} c_{kj}$
- Matrix-vector:  $(\mathbf{Ax})_i = \sum_j a_{ij} x_j$

## Transposition and Conjugation:

- $(\mathbf{A}^T)_{ij} = a_{ji}$ ,  $(\mathbf{A}^H)_{ij} = \overline{a_{ji}}$
- $(\mathbf{A} + \mathbf{B})^H = \mathbf{A}^H + \mathbf{B}^H$
- $(\mathbf{AC})^H = \mathbf{C}^H \mathbf{A}^H$
- $(\mathbf{A}^H)^H = \mathbf{A}$

## Inverse ( $m = n$ , $\mathbf{A}, \mathbf{B} \in \mathrm{GL}(n, \mathbb{F})$ ):

- $\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$
- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
- $(\mathbf{A}^H)^{-1} = (\mathbf{A}^{-1})^H$

## Trace:

- $\mathrm{tr}(\mathbf{A}) = \sum_i a_{ii}$
- $\mathrm{tr}(\mathbf{A} + \mathbf{B}) = \mathrm{tr}(\mathbf{A}) + \mathrm{tr}(\mathbf{B})$
- $\mathrm{tr}(\mathbf{AC}) = \mathrm{tr}(\mathbf{CA})$
- $\mathrm{tr}(\mathbf{A}^H) = \overline{\mathrm{tr}(\mathbf{A})}$

## Determinant ( $m = n$ ):

- $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$
- $\det(\mathbf{A}^H) = \overline{\det(\mathbf{A})}$
- $\det(\mathbf{A}^{-1}) = (\det(\mathbf{A}))^{-1}$  ( $\mathbf{A} \in \mathrm{GL}(n, \mathbb{F})$ )
- $\det(\alpha \mathbf{A}) = \alpha^n \det(\mathbf{A})$

## Other Identities:

- $\mathrm{tr}(\mathbf{A}^H \mathbf{A}) = \|\mathbf{A}\|_F^2 = \sum_{i,j} |a_{ij}|^2$

## Other Identities ( $m = n$ ):

- $\mathrm{tr}(\mathbf{A}) = \sum_i \lambda_i$  ( $\lambda_i$  are eigenvalues)
- $\det(\mathbf{A}) = \prod_i \lambda_i$

## Fundamental subspaces associated with a matrix

- For every matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$ , four linear subspaces of  $\mathbb{F}^n$  and  $\mathbb{F}^m$  are defined, whose characterization provides insight into the structure of linear systems, revealing key properties like solvability and the geometry of solutions.

### Definition (Range of $\mathbf{A}$ )

The range (or column space) of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is a linear subspace of  $\mathbb{F}^m$  given by

$$\text{range}(\mathbf{A}) := \{\mathbf{Ax} \text{ s.t. } \mathbf{x} \in \mathbb{F}^n\}.$$

### Definition (Null space of $\mathbf{A}$ )

The null space (or kernel) of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is a linear subspace of  $\mathbb{F}^n$  given by

$$\text{null}(\mathbf{A}) := \{\mathbf{x} \in \mathbb{F}^n \text{ s.t. } \mathbf{Ax} = \mathbf{0}\}.$$

### Definition (Row space of $\mathbf{A}$ )

The row space of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is a linear subspace of  $\mathbb{F}^n$  given by

$$\text{range}(\mathbf{A}^H) := \{\mathbf{A}^H \mathbf{y} \text{ s.t. } \mathbf{y} \in \mathbb{F}^m\}.$$

## Fundamental subspaces associated with a matrix, cont'd

### Definition (Left null space of $\mathbf{A}$ )

The left null space of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is a linear subspace of  $\mathbb{F}^m$  given by

$$\text{null}(\mathbf{A}^H) := \{\mathbf{y} \in \mathbb{F}^m \text{ s.t. } \mathbf{A}^H \mathbf{y} = \mathbf{0}\}.$$

### Definition / Theorem (Rank of $\mathbf{A}$ )

- The **column rank** of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is the dimension of the column space of  $\mathbf{A}$ , i.e.,  $\dim(\text{range}(\mathbf{A}))$ .
- The **row rank** of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is the dimension of the row space of  $\mathbf{A}$ , i.e.,  $\dim(\text{range}(\mathbf{A}^H))$ .
- The column rank and row ranks of  $\mathbf{A} \in \mathbb{F}^{m \times n}$  are always equal. This common value is the **rank** of  $\mathbf{A}$ , and is denoted by  $\text{rank}(\mathbf{A})$ , with  $\text{rank}(\mathbf{A}) \leq \min(m, n)$ .

### Definition (Full rank)

- A matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is **full-column-rank** if  $\dim(\text{range}(\mathbf{A})) = n$ .
- A matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is **full-row-rank** if  $\dim(\text{range}(\mathbf{A}^H)) = m$ .
- A matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is **full-rank** if  $\text{rank}(\mathbf{A}) = \min(m, n)$ .

## Equivalence of column and row ranks

- The equivalence between the row rank and the column rank of a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  can be shown as follows.

### Proof.

- Let  $\mathbf{A}$  have row rank  $r$ , and  $\mathbf{r}_1, \dots, \mathbf{r}_r \in \mathbb{F}^n$  be a basis of  $\text{range}(\mathbf{A}^H)$ .
- Then, the vectors  $\mathbf{A}\mathbf{r}_1, \dots, \mathbf{A}\mathbf{r}_r$  are linearly independent:
  - Consider  $\alpha_1, \dots, \alpha_r \in \mathbb{F}$  such that  $\alpha_1\mathbf{A}\mathbf{r}_1 + \dots + \alpha_r\mathbf{A}\mathbf{r}_r = \mathbf{0}$ .
  - Then,  $\mathbf{x} := \alpha_1\mathbf{r}_1 + \dots + \alpha_r\mathbf{r}_r \in \text{range}(\mathbf{A}^H)$  is such that  $\mathbf{Ax} = \mathbf{0}$ .
  - For all  $\mathbf{y} \in \mathbb{F}^m$ , we then have  $\mathbf{y}^H \mathbf{Ax} = \mathbf{x}^H \mathbf{A}^H \mathbf{y} = \mathbf{0}$ , which implies  $\mathbf{x} \perp \text{range}(\mathbf{A}^H)$ .
  - $\mathbf{x} \in \text{range}(\mathbf{A}^H)$  and  $\mathbf{x} \perp \text{range}(\mathbf{A}^H)$  imply  $\mathbf{x} = \mathbf{0}$ .  $\square$
- Then, since  $\mathbf{A}\mathbf{r}_i \in \text{range}(\mathbf{A})$  for  $i = 1, \dots, r$ , we have  $c := \dim(\text{range}(\mathbf{A})) \geq r$ .
- Let  $\mathbf{c}_1, \dots, \mathbf{c}_c \in \mathbb{F}^m$  be a basis of  $\text{range}(\mathbf{A})$ .
- Similarly, we can show that the vectors  $\mathbf{A}^H \mathbf{c}_1, \dots, \mathbf{A}^H \mathbf{c}_c$  are linearly independent.
- Since  $\mathbf{A}^H \mathbf{c}_i \in \text{range}(\mathbf{A}^H)$  for  $i = 1, \dots, c$ , we have  $r = \dim(\text{range}(\mathbf{A}^H)) \geq c$ .
- From  $c \geq r$  and  $r \geq c$ , we have  $r = c$ .  $\square$

## Characterization of linear systems

- ▶ A key goal of numerical linear algebra is to develop and analyze methods to find an unknown vector  $\mathbf{x} \in \mathbb{F}^n$  such that  $\mathbf{Ax} = \mathbf{b}$  where  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is a matrix and  $\mathbf{b} \in \mathbb{F}^m$  is a given right-hand side.
- ▶ Each such matrix equation corresponds to a system of  $m$  linear equations with  $n$  scalar unknowns  $x_1, \dots, x_n \in \mathbb{F}$ , of the form

$$\begin{cases} a_{11}x_1 + \cdots + a_{1n}x_n = b_1 \\ \vdots \quad \vdots \quad \vdots \quad \vdots \\ a_{m1}x_1 + \cdots + a_{mn}x_n = b_m \end{cases}$$

- ▶ A linear system is either:
  - **over-determined**: the number  $m$  of equations is larger than the number  $n$  of unknowns, i.e.,  $m > n$ .  $\mathbf{A}$  is a "tall"/"skinny" matrix.
  - **under-determined**: the number  $m$  of equations is smaller than the number  $n$  of unknowns, i.e.,  $m < n$ .  $\mathbf{A}$  is a "short"/"fat" matrix.
  - **square**: the number of equations  $m$  is equal to the number  $n$  of unknowns, i.e.,  $m = n$ .  $\mathbf{A}$  is a square matrix.

## Characterization of linear systems, cont'd

- ▶ A linear system is characterized by either of 3 situations:
  - The system admits **no solution**.
  - The system has a **unique solution**.
  - The system admits **infinitely many solutions**.
- ▶ A proper characterization can be made using two notions:
  1. **Consistency:** A linear system is consistent if  $\mathbf{b} \in \text{range}(\mathbf{A})$ , which means there exists at least one vector  $\mathbf{x} \in \mathbb{F}^n$  such that  $\mathbf{Ax} = \mathbf{b}$ .  
An equivalent statement of consistency is  $\text{rank}([\mathbf{A}, \mathbf{b}]) = \text{rank}(\mathbf{A})$ , which implies that  $\mathbf{b}$  can be formed by linear combination of the columns of  $\mathbf{A}$ .
  2. **Full column rank:** A **consistent** linear system has a **unique solution** iff the column rank of  $\mathbf{A}$  equals the number of unknowns, i.e.,  $\dim(\text{range}(\mathbf{A})) = n$ .  
On the other hand, if  $\dim(\text{range}(\mathbf{A})) < n$ , and the linear system is consistent, then there exist infinitely many vectors  $\mathbf{x} \in \mathbb{F}^m$  such that  $\mathbf{Ax} = \mathbf{b}$ .
- ▶ In conclusion:
  - A linear system has **solution(s)** iff it is **consistent**.
  - A linear system has a **unique solution** iff it is **consistent** and it has **full column rank**.
  - An **under-determined** linear system **cannot have a unique solution**.

## Invertible and singular matrices

- ▶ The **identity matrix**, which we denote by  $\mathbf{I}_n \in \mathbb{R}^{n \times n}$ , is the matrix with ones on the diagonal, and zeros everywhere else.
- ▶ A **square matrix**  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is **invertible** if there exists a matrix  $\mathbf{B} \in \mathbb{F}^{n \times n}$  such that

$$\mathbf{BA} = \mathbf{AB} = \mathbf{I}_n.$$

If such a matrix exists, it is unique, denoted by  $\mathbf{A}^{-1}$ , and referred to as the **inverse of  $\mathbf{A}$** .

- ▶ A matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  has an inverse  $\mathbf{A}^{-1} \in \mathbb{F}^{n \times n}$  iff
  - $\mathbf{Ax} = \mathbf{b}$  has a unique solution  $\mathbf{x} \in \mathbb{F}^n$  for every  $\mathbf{b} \in \mathbb{F}^n$ .
  - $\mathbf{A}$  is full-rank, i.e.,  $\text{rank}(\mathbf{A}) = n$ .
  - The columns of  $\mathbf{A}$  form a basis of  $\mathbb{F}^n$ , i.e.,  $\text{range}(\mathbf{A}) = \mathbb{F}^n$ .
  - The null space of  $\mathbf{A}$  is trivial, i.e.,  $\text{null}(\mathbf{A}) = \{\mathbf{0}\}$ .
  - 0 is neither an eigenvalue nor a singular value of  $\mathbf{A}$ .
  - $\det(\mathbf{A}) \neq 0$ .
- ▶ The set of invertible matrices is the general linear group of degree  $n$  over  $\mathbb{F}$ , denoted by  $\text{GL}(n, \mathbb{F})$ .

## Moore-Penrose inverse

- The **pseudo-inverse** (or **Moore-Penrose inverse**) of a matrix generalizes the concept of matrix inverse to rectangular and singular matrices.

### Definition (Moore-Penrose inverse)

For a given matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$ , the pseudo-inverse  $\mathbf{A}^\dagger \in \mathbb{F}^{n \times m}$  is **unique** and such that

- $\mathbf{A}^\dagger$  is consistent with  $\mathbf{A}$ :  $\mathbf{AA}^\dagger \mathbf{A} = \mathbf{A}$
- $\mathbf{A}^\dagger$  is consistent with  $\mathbf{A}^\dagger$ :  $\mathbf{A}^\dagger \mathbf{AA}^\dagger = \mathbf{A}^\dagger$
- $\mathbf{A}^\dagger \mathbf{A}$  is Hermitian:  $(\mathbf{AA}^\dagger)^H = \mathbf{AA}^\dagger$
- $\mathbf{AA}^\dagger$  is Hermitian:  $(\mathbf{A}^\dagger \mathbf{A})^H = \mathbf{A}^\dagger \mathbf{A}$

- If  $\mathbf{A}$  is invertible, then  $\mathbf{A}^\dagger = \mathbf{A}^{-1}$ .
- Pseudo-inverses are used to provide **alternative solutions to linear systems which admit no standard solution**, or **infinitely many solutions**.

# Different methods for different types of linear systems

Methods for solving linear systems depend on the system's characteristics:

► Systems with **square matrices**:

- **Full-rank (invertible)** matrices:
  - Direct methods: Gaussian elimination, LU decomposition.
  - Iterative methods: Fixed-point methods, Krylov subspace methods.
- **Singular** matrices but **consistent** systems:
  - Low-rank approximation (SVD, pseudoinverse).
  - Specialized iterative methods that exploit the structure of fundamental subspaces.

► Over-determined systems (**tall-and-skinny matrices**):

- **Full column-rank** matrices:
  - **Consistent** systems: QR decomposition or transformation to normal equations.
  - **Inconsistent** systems: Least squares problems.
- **Rank-deficient** matrices: Least squares problems with regularization.

► Under-determined systems (**short-and-fat matrices**):

- **Consistent** systems: Low-rank approximation (SVD, pseudoinverse).
- **Inconsistent** systems: Least squares problems with regularization.

► Least squares problems:

- direct methods (through QR factorization), or iterative methods (LSQR, LSMR).

## Types of matrices

- ▶ Normal matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  s.t.  $\mathbf{A}\mathbf{A}^H = \mathbf{A}^H\mathbf{A}$ :
  - Diagonal matrices, i.e.,  $\mathbf{D} = \text{diag}(d_1, \dots, d_n)$ .
  - Hermitian matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  s.t.  $\mathbf{A}^H = \mathbf{A}$ .
  - Symmetric matrices, i.e.,  $\mathbf{A} \in \mathbb{R}^{n \times n}$  s.t.  $\mathbf{A}^T = \mathbf{A}$ .
  - Unitary matrices, i.e.,  $\mathbf{U} \in \mathbb{F}^{n \times n}$  s.t.  $\mathbf{U}\mathbf{U}^H = \mathbf{U}^H\mathbf{U} = \mathbf{I}_n$ , i.e.,  $\mathbf{U}^{-1} = \mathbf{U}^H$ .
  - Skew-Hermitian matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  s.t.  $\mathbf{A}^H = -\mathbf{A}$ .
  - Skew-symmetric matrices, i.e.,  $\mathbf{A} \in \mathbb{R}^{n \times n}$  s.t.  $\mathbf{A}^T = -\mathbf{A}$ .
- ▶ Orthogonal matrices:  $\mathbf{Q} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_n$ .
- ▶ Tridiagonal matrices: 
- ▶ Triangular matrices:
  - Lower-triangular matrices: 
  - Upper-triangular matrices: 
- ▶ Hessenberg matrices:
  - Lower Hessenberg matrices: 
  - Upper Hessenberg matrices: 
- ▶ Block diagonal matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  s.t.  $\mathbf{A} = \text{diag}(\mathbf{A}_1, \dots, \mathbf{A}_{n_b})$ .
- ▶ ...

# Projections in $\mathbb{F}^n$

- ▶ Projections, and their abstract representation, play an important role in formulating and understanding methods in NLA.

## Definition (Projection in $\mathbb{F}^n$ & projector)

- A projection in  $\mathbb{F}^n$  is an **idempotent linear map**  $x \in \mathbb{F}^n \mapsto Px \in \mathbb{F}^n$ , i.e., such that  $P^2x = Px \forall x \in \mathbb{F}^n$ . The matrix  $P \in \mathbb{F}^{n \times n}$  is called a **projector**.
- The range of a non-trivial projector is a proper subset of  $\mathbb{F}^n$ , i.e.,  $\text{rank}(P) < n$ .

## Proposition (Complementary projector)

If  $P \in \mathbb{F}^{n \times n}$  is a projector, then  $I_n - P$  is a projector onto  $\text{null}(P)$ .

## Proof.

- $I_n - P$  is idempotent, i.e.,  $(I_n - P)^2 = I_n - P - P + P^2 = I_n - 2P + P = I_n - P$ .
- $\text{range}(I_n - P) = \text{null}(P)$ :
  - $x = Px + (I_n - P)x \forall x \in \mathbb{F}^n$ , so that  $Px = 0 \implies x = (I_n - P)x \implies \text{null}(P) \subseteq \text{range}(I_n - P)$ .
  - $P(I_n - P)x = (P - P^2)x = (P - P)x = 0 \forall x \in \mathbb{F}^n \implies \text{range}(I_n - P) \subseteq \text{null}(P)$ .



# Projections in $\mathbb{F}^n$ , cont'd

## Theorem (Decomposition of $\mathbb{F}^n$ via projection)

Given a projector  $\mathbf{P} \in \mathbb{F}^{n \times n}$ , every  $\mathbf{x} \in \mathbb{F}^n$  is uniquely decomposed into a sum  $\mathbf{x} = \mathbf{Px} + (\mathbf{I}_n - \mathbf{P})\mathbf{x}$  with  $\mathbf{Px} \in \text{range}(\mathbf{P})$  and  $(\mathbf{I}_n - \mathbf{P})\mathbf{x} \in \text{null}(\mathbf{P})$ :

$$\mathbb{F}^n = \text{range}(\mathbf{P}) \oplus \text{null}(\mathbf{P})$$

$$n = \text{rank}(\mathbf{P}) + \text{rank}(\mathbf{I}_n - \mathbf{P}).$$

## Proof.

- $\text{range}(\mathbf{P}) \cap \text{null}(\mathbf{P}) = \{\mathbf{0}\}$ .

Let  $\mathbf{y} \in \text{range}(\mathbf{P}) \cap \text{null}(\mathbf{P})$ , then

- Since  $\mathbf{P}$  is idempotent and  $\mathbf{y} \in \text{range}(\mathbf{P})$ , we have  $\mathbf{Py} = \mathbf{y}$ .
- From  $\mathbf{y} \in \text{null}(\mathbf{P})$ , we have  $\mathbf{Py} = \mathbf{0}$ .  
 $\implies \mathbf{y} = \mathbf{0}$ .  $\square$

- Since  $\mathbf{x} = \mathbf{Px} + (\mathbf{I}_n - \mathbf{P})\mathbf{x} \forall \mathbf{x} \in \mathbb{F}^n$ , in which  $\mathbf{x} \mapsto \mathbf{Px}$  is onto  $\text{range}(\mathbf{P})$ , while  $\mathbf{x} \mapsto (\mathbf{I}_n - \mathbf{P})\mathbf{x}$  is onto  $\text{null}(\mathbf{P})$ , and  $\text{range}(\mathbf{P}) \cap \text{null}(\mathbf{P}) = \{\mathbf{0}\}$ , we have that the decomposition of  $\mathbf{x}$  via projection is unique.  $\square$

## Abstract and geometric formulation of projections in $\mathbb{F}^n$

- ▶ For every pair  $(\mathcal{M}, \mathcal{S})$  of linear subspaces of  $\mathbb{F}^n$  such that  $\mathbb{F}^n = \mathcal{M} \oplus \mathcal{S}$ , there exists a unique projector  $\mathbf{P} \in \mathbb{F}^{n \times n}$  such that

$$\mathcal{M} = \text{range}(\mathbf{P}) \text{ and } \mathcal{S} = \text{null}(\mathbf{P}).$$

- ▶ In general,  $\mathbf{y} \in \mathcal{S} = \text{null}(\mathbf{P}) \iff \mathbf{y} \perp \mathcal{M} = \text{range}(\mathbf{P})$ .
- ▶ For every such pair  $(\mathcal{M}, \mathcal{S})$ , the linear map  $\mathbf{x} \mapsto \mathbf{u} := \mathbf{P}\mathbf{x}$  is recast into:

$$\text{Find } \mathbf{u} \in \mathcal{M}$$

$$\text{s.t. } \mathbf{x} - \mathbf{u} \in \mathcal{S}.$$

Since  $\mathbf{y} \in \mathcal{S} \iff \mathbf{y} \perp \mathcal{L}$  where  $\mathcal{L} := \mathcal{S}^\perp$ , the projection is recast into

Find $\mathbf{u} \in \mathcal{M}$ where $\mathcal{M} = \text{range}(\mathbf{P})$	(1)
--	-----

s.t. $\mathbf{x} - \mathbf{u} \perp \mathcal{L}$	$\mathcal{L} = \text{null}(\mathbf{P})^\perp$	(2)
--	---	-----

where  $\mathcal{L}$  is the **orthogonality subspace** (or **space of constraints**).

We say that Eqs. (1)-(2) define a projector  $\mathbf{P}$  onto  $\mathcal{M}$  **perpendicular to  $\mathcal{L}$**  (or **along  $\mathcal{L}$** ). An advantage of this reformulation is that  $\dim(\mathcal{L}) = \dim(\mathcal{M})$ .

# Orthogonal and oblique projections in $\mathbb{F}^n$

- ▶ Every projection induced by the decomposition of  $\mathbb{F}^n$  into complementary subspaces  $\mathcal{M}, \mathcal{L}^\perp \subset \mathbb{F}^n$  is either orthogonal, or oblique.

## Definition (Orthogonal projections & oblique projections)

- The projection in  $\mathbb{F}^n$  induced by the linear subspaces  $\mathcal{M}, \mathcal{L} \subset \mathbb{F}^n$  such that  $\mathbb{F}^n = \mathcal{M} \oplus \mathcal{L}^\perp$ , is **orthogonal** if the space of constraints  $\mathcal{L}$ , is the approximation space  $\mathcal{M}$ , i.e.,  $\mathcal{L} = \mathcal{M}$ . Then, for every  $\mathbf{x} \in \mathbb{F}^n$ , the projection  $\mathbf{x} \mapsto \mathbf{u} := \mathbf{P}\mathbf{x}$  is the solution of

$$\begin{aligned} \text{Find } \quad \mathbf{u} \in \mathcal{M} \\ \text{s.t. } \mathbf{x} - \mathbf{u} \perp \mathcal{M}. \end{aligned}$$

- A projection in  $\mathbb{F}^n$  that is not orthogonal, is **oblique**. Then, for every  $\mathbf{x} \in \mathbb{F}^n$ , the projection  $\mathbf{x} \mapsto \mathbf{u} := \mathbf{P}\mathbf{x}$  is the solution of

$$\begin{aligned} \text{Find } \quad \mathbf{u} \in \mathcal{M} \\ \text{s.t. } \mathbf{x} - \mathbf{u} \perp \mathcal{L} \end{aligned}$$

where the space of constraints  $\mathcal{L}$  is different from the approximation space  $\mathcal{M}$ , i.e.,  $\mathcal{L} \neq \mathcal{M}$ .

## Optimality of orthogonal projections in $\mathbb{F}^n$

- Orthogonal projections have important approximation properties.

### Theorem (Optimality of orthogonal projections in $\mathbb{F}^n$ )

Let  $\mathbf{x} \mapsto \mathbf{Px}$  be the orthogonal projection induced by the linear subspace  $\mathcal{M} \subset \mathbb{F}^n$ . Then, for every  $\mathbf{x} \in \mathbb{F}^n$ ,  $\mathbf{Px}$  is the best approximation of  $\mathbf{x}$  in  $\mathcal{M}$ :

$$\|\mathbf{x} - \mathbf{Px}\| = \min_{\mathbf{u} \in \mathcal{M}} \|\mathbf{x} - \mathbf{u}\| \quad \forall \mathbf{x} \in \mathbb{F}^n.$$

### Proof.

- Every orthogonal projection  $\mathbf{x} \mapsto \mathbf{Px}$  is such that  $\text{range}(\mathbf{P})^\perp = \text{null}(\mathbf{P})$ .
- Then, for all  $(\mathbf{x}, \mathbf{u}) \in \mathbb{F}^n \times \mathcal{M}$ , we have:

$$\|\mathbf{x} - \mathbf{u}\| = \|(\mathbf{I}_n - \mathbf{P})\mathbf{x} + \mathbf{Px} - \mathbf{u}\| = \|(\mathbf{I}_n - \mathbf{P})\mathbf{x}\| + \|\mathbf{Px} - \mathbf{u}\|$$

where we use the fact that  $\text{range}(\mathbf{I}_n - \mathbf{P}) \perp \mathcal{M}$  and  $\mathbf{u} \in \mathcal{M} = \text{range}(\mathbf{P})$ , and we assume  $\|\cdot\|$  is induced by the inner product from the definition of orthogonality.

- Then, we have  $\|\mathbf{x} - \mathbf{u}\| \geq \|\mathbf{x} - \mathbf{Px}\| \quad \forall \mathbf{u} \in \mathcal{M}$ .
- Moreover,  $\|\mathbf{x} - \mathbf{u}\|$  is minimized when  $\mathbf{u} = \mathbf{Px}$ .



## Matrix form of orthogonal projections in $\mathbb{F}^n$

- ▶ Let the linear subspace  $\mathcal{M} \subset \mathbb{F}^n$  of an orthogonal projection  $\mathbf{x} \mapsto \mathbf{Px}$  have dimension  $m$ , i.e.,  $\dim(\mathcal{M}) = m < n$ .
- ▶ Then, there exists a basis  $\mathbf{v}_1, \dots, \mathbf{v}_m \in \mathcal{M}$  such that, for every  $\mathbf{u} \in \mathcal{M}$ , there is a unique  $\hat{\mathbf{u}} \in \mathbb{F}^m$  such that  $\mathbf{u} = \mathbf{V}\hat{\mathbf{u}}$ , where  $\mathbf{V} := [\mathbf{v}_1, \dots, \mathbf{v}_m]$ .
- ▶ Then, from the geometric definition of an orthogonal projection onto  $\mathcal{M}$  given by  $\mathbf{x} \mapsto \mathbf{u} := \mathbf{Px}$ , for every  $\mathbf{x} \in \mathbb{F}^n$ , there exists  $\hat{\mathbf{u}} \in \mathbb{F}^m$  such that  $\mathbf{u} \in \mathcal{M}$ ,  $\mathbf{x} - \mathbf{u} \perp \mathcal{M} \iff \mathbf{u} = \mathbf{V}\hat{\mathbf{u}}$ ,  $(\mathbf{v}_i, \mathbf{x} - \mathbf{V}\hat{\mathbf{u}}) = 0$  for  $i = 1, \dots, m$ .
- ▶ Let the inner product  $(\cdot, \cdot)$  be a dot product, in which case we have

$$\mathbf{V}^H(\mathbf{x} - \mathbf{V}\hat{\mathbf{u}}) = \mathbf{0}$$

$$\mathbf{V}^H\mathbf{x} = \mathbf{V}^H\mathbf{V}\hat{\mathbf{u}}$$

so that  $\hat{\mathbf{u}} = (\mathbf{V}^H\mathbf{V})^{-1}\mathbf{V}^H\mathbf{x}$ , and  $\mathbf{u} = \mathbf{Px}$ , where

$$\boxed{\mathbf{P} = \mathbf{V}(\mathbf{V}^H\mathbf{V})^{-1}\mathbf{V}^H}.$$

- ▶ Note that the basis  $\mathbf{v}_1, \dots, \mathbf{v}_m$  does not need to be orthogonal for  $\mathbf{x} \mapsto \mathbf{Px}$  to be an orthogonal projection. But if it is, then  $\mathbf{P} = \mathbf{V}\mathbf{V}^H$ .

## Matrix form of oblique projections in $\mathbb{F}^n$

- ▶ Let the linear subspaces  $\mathcal{M}, \mathcal{L} \subset \mathbb{F}^n$  of an oblique projection  $\mathbf{x} \mapsto \mathbf{Px}$  have dimension  $m$ , i.e.,  $\dim(\mathcal{M}) = \dim(\mathcal{L}) = m < n$  and  $\mathcal{M} \oplus \mathcal{L}^\perp = \mathbb{F}^n$ .
- ▶ Then, there exist two bases  $\mathbf{v}_1, \dots, \mathbf{v}_m \in \mathcal{M}$  and  $\mathbf{w}_1, \dots, \mathbf{w}_m \in \mathcal{L}$ . The first one is such that, for every  $\mathbf{u} \in \mathcal{M}$ , there is a unique  $\hat{\mathbf{u}} \in \mathbb{F}^m$  such that  $\mathbf{u} = \mathbf{V}\hat{\mathbf{u}}$ , where  $\mathbf{V} := [\mathbf{v}_1, \dots, \mathbf{v}_m]$ .
- ▶ From the definition of an oblique projection onto  $\mathcal{M}$  perpendicular to  $\mathcal{L}$  given by  $\mathbf{x} \mapsto \mathbf{u} := \mathbf{Px}$ , for every  $\mathbf{x} \in \mathbb{F}^n$ , there exists  $\hat{\mathbf{u}} \in \mathbb{F}^m$  such that

$$\mathbf{u} \in \mathcal{M}, \mathbf{x} - \mathbf{u} \perp \mathcal{L} \iff \mathbf{u} = \mathbf{V}\hat{\mathbf{u}}, (\mathbf{w}_i, \mathbf{x} - \mathbf{V}\hat{\mathbf{u}}) = 0 \text{ for } i = 1, \dots, m$$

$$\mathbf{W}^H(\mathbf{x} - \mathbf{V}\hat{\mathbf{u}}) = \mathbf{0}$$

$$\mathbf{W}^H\mathbf{x} = \mathbf{W}^H\mathbf{V}\hat{\mathbf{u}}.$$

where the inner product is a dot product, so that  $\hat{\mathbf{u}} = (\mathbf{W}^H\mathbf{V})^{-1}\mathbf{W}^H\mathbf{x}$ , and  $\mathbf{u} = \mathbf{Px}$ , where

$$\boxed{\mathbf{P} = \mathbf{V}(\mathbf{W}^H\mathbf{V})^{-1}\mathbf{W}^H}$$

where  $\mathbf{W}^H\mathbf{V}$  is not singular because, by definition, we have  $\mathcal{M} \cap \mathcal{L}^\perp = \{\mathbf{0}\}$ .

# Matrix norms

- Matrix norms are abstract measures of the strength of a transformation.

## Definition (Matrix norm)

A matrix norm is a function  $\mathbb{F}^{m \times n} \rightarrow \mathbb{R}$  such that

1.  $\|\cdot\|$  is positive-definite:  $\|\mathbf{A}\| \geq 0$  and  $\|\mathbf{A}\| = 0 \iff \mathbf{A} = \mathbf{0}$
2.  $\|\cdot\|$  is homogeneous:  $\|\alpha\mathbf{A}\| = |\alpha|\|\mathbf{A}\| \forall \mathbf{A} \in \mathbb{F}^{m \times n}, \alpha \in \mathbb{F}$
3.  $\|\cdot\|$  satisfies the triangular inequality:  $\|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\| \forall \mathbf{A}, \mathbf{B} \in \mathbb{F}^{m \times n}$

- Some matrix norms are naturally induced by vector norms.

## Definition (Induced norms)

Let  $\|\cdot\|_\beta : \mathbb{F}^m \rightarrow \mathbb{R}$  and  $\|\cdot\|_\alpha : \mathbb{F}^n \rightarrow \mathbb{R}$  be vector norms. The **induced norm** (or subordinate norm, or operator norm)  $\|\cdot\| : \mathbb{F}^{m \times n} \rightarrow \mathbb{R}$  is the matrix norm defined as

$$\|\mathbf{A}\| = \sup_{\mathbf{x} \in \mathbb{F}^n \setminus \{\mathbf{0}\}} \frac{\|\mathbf{Ax}\|_\beta}{\|\mathbf{x}\|_\alpha} \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n}.$$

## Properties of matrix norms

- A number of properties of matrix norms can come in handy, in particular

### Definition (Consistency of matrix norms)

- The matrix norms  $\|\cdot\|_\alpha : \mathbb{F}^{m \times n} \rightarrow \mathbb{R}$ ,  $\|\cdot\|_\beta : \mathbb{F}^{n \times p} \rightarrow \mathbb{R}$  and  $\|\cdot\|_\gamma : \mathbb{F}^{m \times p} \rightarrow \mathbb{R}$  are mutually **consistent** if

$$\|\mathbf{AB}\|_\gamma \leq \|\mathbf{A}\|_\alpha \|\mathbf{B}\|_\beta \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n}, \mathbf{B} \in \mathbb{F}^{n \times p}.$$

- In case  $m = n = p$  and  $\gamma = \beta = \alpha$ , we say that the matrix norm  $\|\cdot\|_\alpha$  is **sub-multiplicative**.
- All **induced norms are consistent**, i.e., mutually consistent with themselves.
- The **Frobenius norm**, which is **not induced by any vector norm**, and is defined as

$$\|\mathbf{A}\|_F := \left( \sum_{i=1}^m \sum_{j=1}^n a_{ij}^2 \right)^{1/2}$$

is consistent.

## Properties of matrix norms, cont'd

- A number of properties of matrix norms can come in handy, in particular

### Definition (Consistency of matrix and vector norms)

- A matrix norm  $\|\cdot\| : \mathbb{F}^{m \times n} \rightarrow \mathbb{R}$  is **consistent with** the vector norms  $\|\cdot\|_\beta : \mathbb{F}^m \rightarrow \mathbb{R}$  and  $\|\cdot\|_\alpha : \mathbb{F}^n \rightarrow \mathbb{R}$  if

$$\|\mathbf{Ax}\|_\beta \leq \|\mathbf{A}\| \|\mathbf{x}\|_\alpha \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n}, \mathbf{x} \in \mathbb{F}^n.$$

- In case  $m = n$  and  $\beta = \alpha$ , we say the matrix norm  $\|\cdot\|$  is **compatible with**  $\|\cdot\|_\alpha$ .
- All **induced norms** are **consistent** with their underlying vector norms **by definition**.

- The **Frobenius norm** is **consistent with vector 2-norms**.
- For every matrix norm  $\|\cdot\| : \mathbb{F}^{m \times n} \rightarrow \mathbb{R}$  induced by the vector norms  $\|\cdot\|_\beta : \mathbb{F}^m \rightarrow \mathbb{R}$  and  $\|\cdot\|_\alpha : \mathbb{F}^n \rightarrow \mathbb{R}$ , and every matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$ , there exists  $\mathbf{x} \in \mathbb{F}^n$  s.t.  $\|\mathbf{Ax}\|_\beta = \|\mathbf{A}\| \|\mathbf{x}\|_\alpha$ .

## Equivalence of matrix norms

- ▶ A sequence of matrices  $\{\mathbf{A}_k\}_{k \in \mathbb{N}} \subset \mathbb{F}^{m \times n}$  converges to a matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  under the norm  $\|\cdot\|$  defined on  $\mathbb{F}^{m \times n}$  if, for any real  $\epsilon > 0$ , there exists  $K$  s.t.  $\|\mathbf{A}_k - \mathbf{A}\| < \epsilon$  for all  $k > K$ .
- ▶ Two matrix norms  $\|\cdot\|$  and  $\|\cdot\|'$  are equivalent if convergence under one norm implies convergence under the other. This can be checked by

### Theorem (Equivalent matrix norms)

Two matrix norms  $\|\cdot\|$  and  $\|\cdot\|'$  on  $\mathbb{F}^{m \times n}$  are equivalent iff there exist real constants  $C_1, C_2 > 0$  s.t.  $C_1\|\mathbf{A}\| \leq \|\mathbf{A}\|' \leq C_2\|\mathbf{A}\| \forall \mathbf{A} \in \mathbb{F}^{m \times n}$ .

- ▶ All matrix norms defined on  $\mathbb{F}^{m \times n}$  are equivalent. In particular,

- $\frac{1}{\sqrt{n}}\|\mathbf{A}\|_\infty \leq \|\mathbf{A}\|_2 \leq \sqrt{m}\|\mathbf{A}\|_\infty \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n},$
- $\frac{1}{\sqrt{m}}\|\mathbf{A}\|_1 \leq \|\mathbf{A}\|_2 \leq \sqrt{n}\|\mathbf{A}\|_1 \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n},$
- $\frac{1}{\sqrt{\min(m,n)}}\|\mathbf{A}\|_F \leq \|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_F \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n},$
- $\max_{i,j} |a_{ij}| \leq \|\mathbf{A}\|_2 \leq \sqrt{mn} \max_{i,j} |a_{ij}| \quad \forall \mathbf{A} \in \mathbb{F}^{m \times n}.$

# Eigenvalues and eigenvectors

Section 2.4 in Darve & Wootters (2021)

## Eigenvalue and eigenvectors

- ▶ **Eigenvalues and eigenvectors** reveal how a square matrix transforms space by identifying invariant directions (along eigenvectors) and their scaling factors (eigenvalues).

### Definition (Eigenvalues, eigenvectors & spectrum)

- A scalar  $\lambda \in \mathbb{C}$  is an eigenvalue of  $\mathbf{A} \in \mathbb{F}^{n \times n}$  if there is a non-zero vector  $\mathbf{u} \in \mathbb{C}^n$  such that  $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$ .
- $\mathbf{u}$  is called an **eigenvector** of  $\mathbf{A}$ .
- The set of all the eigenvalues of  $\mathbf{A}$ , denoted by  $\text{Sp}(\mathbf{A})$ , is the **spectrum** of  $\mathbf{A}$ .

- ▶ Equivalently,  $\lambda \in \mathbb{C}$  is an eigenvalue of  $\mathbf{A} \in \mathbb{F}^{n \times n}$  if it is a root of the characteristic polynomial:

$$p_{\mathbf{A}} : \lambda \in \mathbb{C} \mapsto \det(\mathbf{A} - \lambda \mathbf{I}_n) \in \mathbb{F}.$$

### Definition (Left eigenpair)

- A scalar  $\vartheta \in \mathbb{C}$  and a non-zero vector  $\mathbf{v} \in \mathbb{C}^n$  such that  $\mathbf{v}^H \mathbf{A} = \vartheta \mathbf{v}^H$  is called a **left eigenpair** of  $\mathbf{A}$ .

## Multiplicity of eigenvalues

- ▶ Eigenvalues have two types of multiplicities: **algebraic** and **geometric**.
- ▶ **Algebraic multiplicity**: The number of times an eigenvalue appears as a root of the characteristic polynomial.
- ▶ **Geometric multiplicity**: The dimension of the eigenspace corresponding to the eigenvalue, i.e., the number of linearly independent eigenvectors associated with that eigenvalue.

$$1 \leq \text{geometric multiplicity} \leq \text{algebraic multiplicity}$$

- ▶ An eigenvalue is **semisimple** if its **geometric mult.** = its **algebraic mult.**.
- ▶ An eigenvalue with **geometric mult.** < **algebraic mult.** has fewer independent eigenvectors than the size of the eigenspace implied by the algebraic multiplicity.
- ▶ If a matrix has at least one eigenvalue with **geometric mult.** < **algebraic mult.**, then it is **defective**, i.e., it does not have a full set of linearly independent eigenvectors.
- ▶ **defective**  $\not\iff$  **singular**

## Characterization of normal matrices

- A square matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is called **normal** if it satisfies:

$$\mathbf{A}\mathbf{A}^H = \mathbf{A}^H\mathbf{A}.$$

- Common examples of normal matrices are

- Diagonal matrices, i.e.,  $\mathbf{A} = \text{diag}(a_{11}, \dots, a_{nn})$ .
- Hermitian matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  such that  $\mathbf{A}^H = \mathbf{A}$ .
- Symmetric matrices, i.e.,  $\mathbf{A} \in \mathbb{R}^{n \times n}$  such that  $\mathbf{A}^T = \mathbf{A}$ .
- Unitary matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  such that  $\mathbf{A}\mathbf{A}^H = \mathbf{A}^H\mathbf{A} = \mathbf{I}_n$ .
- Skew-Hermitian matrices, i.e.,  $\mathbf{A} \in \mathbb{F}^{n \times n}$  such that  $\mathbf{A}^H = -\mathbf{A}$ .
- Skew-symmetric matrices, i.e.,  $\mathbf{A} \in \mathbb{R}^{n \times n}$  such that  $\mathbf{A}^T = -\mathbf{A}$ .

### Theorem

A *normal triangular matrix must be diagonal*.

### Theorem (Spectral characterization of normal matrices)

A matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is normal if and only if each of its eigenvectors is also an eigenvector of  $\mathbf{A}^H$ . That is,  $\mathbf{A}$  is normal if and only if for every eigen-pair  $(\lambda, \mathbf{u}) \in \mathbb{C} \times \mathbb{C}^n$  such that  $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$ , we have  $\mathbf{u}^H\mathbf{A} = \lambda\mathbf{u}^H$ .

## Characterization of Hermitian matrices

- A square matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is called **Hermitian** if it satisfies  $\mathbf{A}^H = \mathbf{A}$ .

### Theorem

- The eigenvalues of a Hermitian matrix are real.
- A normal matrix whose eigenvalues are real is Hermitian.

- The ordered eigenvalues  $\lambda_1 \geq \dots \geq \lambda_n$  of a Hermitian matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  are characterized by optimality properties of the **Rayleigh quotient**

$$\mu_{\mathbf{A}} : \mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\} \mapsto \frac{\mathbf{x}^H \mathbf{A} \mathbf{x}}{\mathbf{x}^H \mathbf{x}} \in \mathbb{R}.$$

### Theorem (Courant-Fisher min-max principle)

The ordered eigenvalues of a Hermitian matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  are such that

$$\begin{aligned}\lambda_k &= \min_{\mathcal{S} \subseteq \mathbb{C}^n, \dim(\mathcal{S})=n-k+1} \max_{\mathbf{x} \in \mathcal{S} \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x}) \\ &= \min_{\mathcal{S} \subseteq \mathbb{C}^n, \dim(\mathcal{S})=k} \max_{\mathbf{x} \in \mathcal{S} \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x}).\end{aligned}$$

## Characterization of Hermitian matrices, cont'd

- A corollary of the (Courant-Fisher) min-max principle is that the largest and smallest eigenvalues of a Hermitian matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  are such that

$$\lambda_1 = \max_{\mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x}) \quad \text{and} \quad \lambda_n = \min_{\mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x}).$$

- Another way to characterize the optimality of the ordered eigenvalues  $\lambda_1 \geq \dots \geq \lambda_n$  of a Hermitian matrix is

### Theorem (Courant characterization)

*The largest eigenvalue  $\lambda_1$  of a Hermitian matrix  $\mathbf{A}$  with a corresponding eigenvector  $\mathbf{u}_1$  is such that*

$$\lambda_1 = \mu_{\mathbf{A}}(\mathbf{u}_1) = \max_{\mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x})$$

*and the other eigenvalues  $\lambda_2 \geq \dots \geq \lambda_n$ , with corresponding eigenvectors, are such that*

$$\lambda_k = \mu_{\mathbf{A}}(\mathbf{u}_k) = \max_{\mathbf{x} \in \text{range}([\mathbf{u}_1, \dots, \mathbf{u}_{k-1}])^\perp \setminus \{\mathbf{0}\}} \mu_{\mathbf{A}}(\mathbf{x}).$$

## Characterization of Hermitian (semi)positive-definite matrices

- A matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is **Hermitian semipositive-definite** if  $\mathbf{A}^H = \mathbf{A}$  and

$$\mathbf{x}^H \mathbf{A} \mathbf{x} \geq 0 \quad \forall \mathbf{x} \in \mathbb{F}^n \setminus \{\mathbf{0}\}. \quad (3)$$

The **eigenvalues** of such matrices are **non-negative**, i.e.,  $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ .

- If Eq. (3) is strictly satisfied, the matrix is **Hermitian positive-definite**, or **symmetric positive-definite**, i.e., **SPD**, if  $\mathbb{F} = \mathbb{R}$ .

The **eigenvalues** of such matrices are **positive**, i.e.,  $\lambda_1 \geq \dots \geq \lambda_n > 0$ .

- Hermitian positive definite matrices are **invertible**.

They admit **Cholesky decompositions** of the form  $\mathbf{A} = \mathbf{L} \mathbf{L}^H$  where  $\mathbf{L}$  is lower-triangular.

- Hermitian (semi)positive-definite matrices are common in practice:

- **Low-rank approximation**:  $\mathbf{A}^H \mathbf{A}$  and  $\mathbf{A} \mathbf{A}^H$ .
- **Optimization**: Hessian matrices.
- **Machine learning**: Covariance matrices, kernel matrices.
- **Computational physics**: Discretized PDEs.
- **Statistics**: Fisher information matrices.

# Matrix canonical forms

Section 2.4 in Darve & Wootters (2021)

## Similarity transformations

- ▶ Similarity is an equivalence relation between linear maps induced by a change of basis, that preserves key properties of the underlying linear operator.

### Definition (Similar matrices)

Two square matrices  $\mathbf{A}, \mathbf{B} \in \mathbb{F}^{n \times n}$  are **similar** if there exists an invertible matrix  $\mathbf{X} \in \mathbb{F}^{n \times n}$  such that  $\mathbf{A} = \mathbf{X}\mathbf{B}\mathbf{X}^{-1}$ .

- ▶ The mapping  $\mathbf{A} \mapsto \mathbf{B}$  is a **similarity transformation**, which recasts the matrix representation of a linear map in a different basis.
- ▶ Similar matrices have the same **rank**, **characteristic polynomial** and underlying properties (i.e., **determinant**, **eigenvalues** and their **algebraic multiplicities**, **trace**, ...), **geometric multiplicities**, ...
- ▶ An eigenvector  $\mathbf{v}$  of  $\mathbf{B}$  is transformed into an eigenvector  $\mathbf{u} := \mathbf{X}\mathbf{v}$  of the similar  $\mathbf{A} = \mathbf{X}\mathbf{B}\mathbf{X}^{-1}$ .
- ▶ Similarity is crucial for finding canonical forms, such as the **diagonal form**, the **Jordan form** and the **Schur form**, which provide simplified representations useful in solving and analyzing numerical linear algebraic problems.

## Diagonal form and eigen-decomposition

- The simplest similar form into which a matrix may be reduced is the diagonal form, i.e.,  $\mathbf{A} = \mathbf{X}\mathbf{D}\mathbf{X}^{-1}$ , for some diagonal matrix  $\mathbf{D}$ .

### Theorem

A square matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is diagonalizable iff it has  $n$  linearly independent eigenvectors or, equivalently, iff it is not defective.

- In particular, every diagonalizable matrix  $\mathbf{A}$  can be recast into an eigen-decomposition of the form  $\mathbf{A} = \mathbf{U}\Lambda\mathbf{U}^{-1}$ , where  $\Lambda$  is a diagonal matrix of eigenvalues, and the columns of  $\mathbf{U}$  are normalized eigenvectors.  
If  $\mathbf{A}$  is normal, then  $\mathbf{U}^{-1} = \mathbf{U}^H$ . All normal matrices are diagonalizable.
- An invertible matrix is not necessarily diagonalizable, e.g.:

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \text{ is invertible, but defective.}$$

- A diagonalizable matrix is not necessarily invertible, e.g.:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \text{ is diagonal, but singular.}$$

## Jordan form

- For defective matrices, an alternative representation is the **Jordan form**.

### Definition (Jordan block)

A Jordan block is either a scalar  $\lambda$ , or a matrix of the form:

$$\mathbf{J} = \begin{bmatrix} \lambda & 1 & 0 & \dots & 0 \\ 0 & \lambda & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & \lambda & 1 \\ 0 & 0 & \dots & 0 & \lambda \end{bmatrix}.$$

### Theorem (Reduction to Jordan form)

- For every matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$ , there exist  $\mathbf{X}, \mathbf{J} \in \mathbb{C}^{n \times n}$  such that  $\mathbf{A} = \mathbf{X}\mathbf{J}\mathbf{X}^{-1}$ , where  $\mathbf{J}$  is a block-diagonal matrix of Jordan blocks, i.e.,  $\mathbf{J} = \text{diag}(\mathbf{J}_1, \dots, \mathbf{J}_k)$ .
  - For each distinct eigenvalue  $\lambda$  of  $\mathbf{A}$ , there is a number of associated Jordan blocks in  $\mathbf{J}$  given by the geometric multiplicity of  $\lambda$ , whereas the sizes of these blocks add up to the algebraic multiplicity of  $\lambda$ .
- The Jordan form is a generalization of the eigen-decomposition, mostly used for the analysis of defective matrices.

## Schur form/decomposition

- ▶ A Jordan form exists for every square matrix, but its computation can be challenging, and the associated basis ill-conditioned.
- ▶ An alternative to the Jordan form, which also exists for every square matrix, is the **Schur form** (or **decomposition**).

### Theorem (Schur decomposition)

For every matrix  $\mathbf{A} \in \mathbb{F}^{n \times n}$ , there exist  $\mathbf{Q}, \mathbf{R} \in \mathbb{C}^{n \times n}$  such that

$$\mathbf{A} = \mathbf{Q}\mathbf{R}\mathbf{Q}^H$$

where  $\mathbf{R}$  is upper triangular, and  $\mathbf{Q}$  is unitary, i.e.,  $\mathbf{Q}^{-1} = \mathbf{Q}^H$ .

- ▶ Since  $\mathbf{R}$  is a triangular matrix, its eigenvalues are listed on the diagonal. And since  $\mathbf{R}$  and  $\mathbf{A}$  are similar, the values listed on the diagonal of  $\mathbf{R}$  are also the eigenvalues of  $\mathbf{A}$ .

Matrix decompositions with eigenvalues on the diagonal:

For diagonalizable matrices:  Eigendecomposition

For normal matrices:  Eigendecomposition  
 $Q$  is unitary

For any square matrix:  Jordan form.

For any square matrix:  Schur decomposition  
 $Q$  is unitary

## Matrix functions

- ▶ A **matrix function**  $f(\mathbf{A})$  extends scalar functions like  $e^x$ ,  $\sin(x)$ , or  $\log(x)$  to matrices  $\mathbf{A} \in \mathbb{F}^{n \times n}$ .
- ▶ The previously introduced canonical forms can be used to define the application of matrix functions. In particular, for
  - **Diagonalizable matrices:** If  $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^{-1}$  where  $\mathbf{D}$  is diagonal, then

$$f(\mathbf{A}) = \mathbf{U}f(\mathbf{D})\mathbf{U}^{-1} \quad \text{where} \quad f(\mathbf{D}) = \text{diag}(f(d_{11}), \dots, f(d_{nn})).$$

- **Jordan forms:** If  $\mathbf{A} = \mathbf{X}\mathbf{J}\mathbf{X}^{-1}$  where  $\mathbf{J}$  is a Jordan matrix, then

$$f(\mathbf{A}) = \mathbf{X}f(\mathbf{J})\mathbf{X}^{-1}$$

where  $f(\mathbf{J})$  is block diagonal, with each block corresponding to a Jordan block. Computing functions of Jordan blocks requires handling the non-diagonal terms via derivatives of the scalar function.

- **Schur form:** If  $\mathbf{A} = \mathbf{Q}\mathbf{R}\mathbf{Q}^H$  where  $\mathbf{R}$  is upper triangular, then:

$$f(\mathbf{A}) = \mathbf{Q}f(\mathbf{R})\mathbf{Q}^H$$

For upper triangular matrices, matrix functions can be computed recursively based on the entries of  $\mathbf{R}$ .

# Singular value decomposition

Section 2.5 in Darve & Wootters (2021)

## Singular value decomposition

- Eigenvalues and related canonical forms are for square matrices only.  
But singular value decompositions exist for all matrices.

### Theorem (Singular value decomposition (SVD))

- For every matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$ , there exist decompositions of the form

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

where  $\mathbf{U} \in \mathbb{F}^{m \times m}$  and  $\mathbf{V} \in \mathbb{F}^{n \times n}$  are unitary matrices, and the only non-zero entries of  $\Sigma \in \mathbb{R}^{m \times n}$  are on the diagonal.

- The diagonal entries  $\sigma_1 \geq \dots \geq \sigma_p \geq 0$  of  $\Sigma$  are called **singular values**.
  - The columns  $\mathbf{u}_1, \dots, \mathbf{u}_m \in \mathbb{F}^m$  of  $\mathbf{U}$  are called **left singular vectors**.
  - The columns  $\mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{F}^n$  of  $\mathbf{V}$  are called **right singular vectors**.
- 
- The singular values  $\sigma_1 \geq \dots \geq \sigma_p \geq 0$  are unique, but the matrices  $\mathbf{U}$  and  $\mathbf{V}$  of left and right singular vectors are not unique.
  - If  $\mathbf{A} \in \mathbb{F}^{m \times n}$  has rank  $r < p$  where  $p := \min(m, n)$ , then  $\sigma_k = 0$  for  $k = r + 1, \dots, p$ . Thus, the number of non-zero singular values equals the rank of  $\mathbf{A}$ .

## Relation between singular and eigenvalue problems

- If  $\mathbf{A} \in \mathbb{F}^{n \times n}$  is **Hermitian** with (real) eigenvalues ordered such that  $|\lambda_1| \geq \dots \geq |\lambda_n|$ , then the ordered singular values  $\sigma_1 \geq \dots \geq \sigma_n$  of  $\mathbf{A}$  are given by  $\sigma_i = |\lambda_i|$  for  $i = 1, \dots, n$ .
- If  $\mathbf{A} \in \mathbb{F}^{m \times n}$  is not Hermitian, or even square, then the singular values and singular vectors of  $\mathbf{A}$  can be characterized as eigen-pairs of Gram matrices.

### Theorem (Relation between the SVD and Gram matrices)

For every  $\mathbf{A} \in \mathbb{F}^{m \times n}$  with  $p := \min(m, n)$  singular values  $\sigma_1 \geq \dots \geq \sigma_p \geq 0$  and a proper SVD  $\mathbf{U}\Sigma\mathbf{V}^H$  with  $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_n]$  and  $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_m]$ ,

- $(\sigma_1, \mathbf{u}_1), \dots, (\sigma_p, \mathbf{u}_p) \in \mathbb{R} \times \mathbb{F}^n$  are eigen-pairs of  $\mathbf{A}^H \mathbf{A} \in \mathbb{F}^{n \times n}$ ,
- $(\sigma_1, \mathbf{v}_1), \dots, (\sigma_p, \mathbf{v}_p) \in \mathbb{R} \times \mathbb{F}^m$  are eigen-pairs of  $\mathbf{A} \mathbf{A}^H \in \mathbb{F}^{m \times m}$ .

- As a corollary, we have:  $\|\mathbf{A}\|_2 = \sigma_1(\mathbf{A}) = \sqrt{\lambda_{max}(\mathbf{A}^H \mathbf{A})} = \sqrt{\lambda_{max}(\mathbf{A} \mathbf{A}^H)}$

$$\text{and } \|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^p \sigma_i^2}.$$

## Compact singular value decomposition

- For rectangular matrices, we denote two types of structures of SVD:

Tall-and-skinny matrices ( $m > n$ )

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

Short-and-fat matrices ( $m < n$ )

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

- Due to the structure of  $\Sigma$ , a **compact SVD**  $A = \hat{U} \hat{\Sigma} \hat{V}^H$  is formed by discarding the zero block of  $\Sigma$ , and the corresponding blocks of singular vectors in  $\mathbf{U}$  or  $\mathbf{V}$ , leading to  $\hat{\mathbf{U}} \in \mathbb{F}^{m \times p}$ ,  $\hat{\Sigma} \in \mathbb{R}^{p \times p}$  and  $\hat{\mathbf{V}} \in \mathbb{F}^{n \times p}$ :

Tall-and-skinny matrices ( $m > n$ )

$$A = \hat{U} \hat{\Sigma} \hat{V}^H$$

Short-and-fat matrices ( $m < n$ )

$$A = \hat{U} \hat{\Sigma} \hat{V}^H$$

Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

## Low-rank approximation

- The factors of the SVD capture essential information about the action of  $\mathbf{A}$ :

### Theorem (Four fundamental subspaces and the SVD)

Every matrix  $\mathbf{A} \in \mathbb{F}^{m \times n}$  of rank  $r$  with left singular vectors  $\mathbf{u}_1, \dots, \mathbf{u}_n \in \mathbb{F}^n$ , and right singular vectors  $\mathbf{v}_1, \dots, \mathbf{v}_m \in \mathbb{F}^m$  is such that

$$\begin{aligned}\text{range}(\mathbf{A}) &= \text{span}\{\mathbf{u}_1, \dots, \mathbf{u}_r\}, & \text{null}(\mathbf{A}) &= \text{span}\{\mathbf{v}_{r+1}, \dots, \mathbf{v}_n\}, \\ \text{range}(\mathbf{A}^H) &= \text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_r\}, & \text{null}(\mathbf{A}^H) &= \text{span}\{\mathbf{u}_{r+1}, \dots, \mathbf{u}_m\}.\end{aligned}$$

### Theorem (Eckart-Young theorem)

Consider  $\mathbf{A} \in \mathbb{F}^{m \times n}$ , its  $p = \min(m, n)$  singular values  $\sigma_1 \geq \dots \geq \sigma_p \geq 0$  and corresponding left singular vectors  $\mathbf{u}_1, \dots, \mathbf{u}_{\min(p,m)}$  and right singular vectors  $\mathbf{v}_1, \dots, \mathbf{v}_{\min(p,n)}$ . Then, for  $r < p$ , the matrix  $\mathbf{B} := \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^H$  is such that

$$\|\mathbf{A} - \mathbf{B}\|_2 = \sigma_{r+1} \quad \text{and} \quad \|\mathbf{A} - \mathbf{B}\|_F = \sum_{i=r+1}^p \sigma_i^2.$$

Moreover,  $\mathbf{B}$  minimizes  $\|\mathbf{A} - \mathbf{B}\|_2$  and  $\|\mathbf{A} - \mathbf{B}\|_F$  among matrices of rank  $r$ .