

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

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

- ▶ 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.,

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

- ▶ 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 $(\mathbf{x}, \mathbf{x}) = 0 \iff \mathbf{x} = \mathbf{0}$

$\overline{\alpha} := \Re\{\alpha\} - i\Im\{\alpha\}$ 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:

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

$\mathbf{x}^H := \overline{\mathbf{x}}^T$ 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: $\|\mathbf{x}\| \geq 0 \ \forall \mathbf{x} \in \mathcal{V}$ and $\|\mathbf{x}\| = 0 \iff \mathbf{x} = \mathbf{0}$
2. $\|\cdot\|$ is homogeneous: $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\| \ \forall \mathbf{x} \in \mathcal{V}, \alpha \in \mathbb{F}$
3. $\|\cdot\|$ satisfies the triangular inequality: $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\| \ \forall \mathbf{x}, \mathbf{y} \in \mathcal{V}$

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

- 1-norm: $\|\mathbf{x}\|_1 := \sum_{i=1}^n |x_i| \ \forall \mathbf{x} \in \mathcal{V}$.
- 2-norm: $\|\mathbf{x}\|_2 := \left(\sum_{i=1}^n |x_i|^2 \right)^{1/2} \ \forall \mathbf{x} \in \mathcal{V}$.
 - 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 $\|\mathbf{x}\| := (\mathbf{x}, \mathbf{x})^{1/2} \ \forall \mathbf{x} \in \mathcal{V}$.
- p -norm: $\|\mathbf{x}\|_p := \left(\sum_{i=1}^n |x_i|^p \right)^{1/p} \ \forall \mathbf{x} \in \mathcal{V}$.
- ∞ -norm: $\|\mathbf{x}\|_\infty := \max_{1 \leq i \leq n} |x_i| \ \forall \mathbf{x} \in \mathcal{V}$.

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:

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

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 ($m = n$):

- $\mathrm{tr}(\mathbf{A}) = \sum_i \lambda_i$ (λ_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 $\mathbf{A}\mathbf{x} = \mathbf{0}$.
 - For all $\mathbf{y} \in \mathbb{F}^m$, we then have $\mathbf{y}^H \mathbf{A}\mathbf{x} = \mathbf{x}^H \mathbf{A}^H \mathbf{y} = \mathbf{0}$, 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

$$\left\{ \begin{array}{l} a_{11}x_1 + \cdots + a_{1n}x_n = b_1 \\ \vdots \quad \vdots \quad \vdots \quad \vdots \\ a_{m1}x_1 + \cdots + a_{mn}x_n = b_m \end{array} \right.$$

- ▶ 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., $\text{dim}(\text{range}(\mathbf{A})) = n$.
On the other hand, if $\text{dim}(\text{range}(\mathbf{A})) < n$, 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

$$\mathbf{B}\mathbf{A} = \mathbf{A}\mathbf{B} = \mathbf{I}_n.$$

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} : $\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}$
- \mathbf{A}^\dagger is consistent with \mathbf{A}^\dagger : $\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger$
- $\mathbf{A}^\dagger\mathbf{A}$ is Hermitian: $(\mathbf{A}\mathbf{A}^\dagger)^H = \mathbf{A}\mathbf{A}^\dagger$
- $\mathbf{A}\mathbf{A}^\dagger$ 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** $\mathbf{x} \in \mathbb{F}^n \mapsto \mathbf{Px} \in \mathbb{F}^n$, i.e., such that $\mathbf{P}^2\mathbf{x} = \mathbf{Px} \forall \mathbf{x} \in \mathbb{F}^n$. The matrix $\mathbf{P} \in \mathbb{F}^{n \times n}$ is called a **projector**.
- The range of a non-trivial projector is a proper subset of \mathbb{F}^n , i.e., $\text{rank}(\mathbf{P}) < n$.

Proposition (Complementary projector)

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

Proof.

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



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:

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

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 λ_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 $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1}$, where $\mathbf{\Lambda}$ 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 λ , 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 λ of \mathbf{A} , there is a number of associated Jordan blocks in \mathbf{J} given by the geometric multiplicity of λ , whereas the sizes of these blocks add up to the algebraic multiplicity of λ .

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

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

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

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