# Linear Algebra for Machine Learning

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- Introduction
- Vector Spaces
- Linear Transformations
- Change of Basis
- Diagonalization
- Application of Diagonalization
- Application to Statistics: Least Square and SVD

# Motivations for Linear Algebra Review

- Computational engine of mathematics:
  - → Numerical Analysis (Finite Elements); Algebraic Geometry (Hodge Decomposition); Statistics (Covariance Matrix, Data Shape)
- Data science practitioners: diverse backgrounds
- Refresh key concepts often forgotten (e.g., eigenvalues)

## Goal: develop dexterity with

- ✓ Linear Equations, Gaussian Elimination, Matrices
- ✓ Vector Spaces, Transformations, Basis Changes
- √ Diagonalization, Webpage Ranking, Covariance
- √ Orthogonality, Least Squares, SVD

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### Example: Smoking in Smallville

Each year: 30% of nonsmokers start smoking, 20% of smokers quit. Initial population: 8000 smokers, 2000 nonsmokers. Questions:

- Numbers after 100 years?
- Numbers after *n* years?
- Is there a stable equilibrium?

## Core points (why and how)

 Goal: reduce to fewer equations/variables via elimination.

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$
  
 $a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$ 

- Basic elimination step (column 1):
  - ① Pivot: swap so  $a_{11} \neq 0$ .
  - ② Normalize:  $L_1 \leftarrow \frac{1}{a_{1,1}} L_1$ .
  - **3** Zero below: for  $i \ge 2$ ,  $L_i \leftarrow L_i a_{i1}L_1$ .
- Iterate on remaining submatrix; back-substitute or continue to RREF.

# Operations (preserve solution set of Ax = b):

Reason: Each operation equals left-multiplication by an invertible elementary matrix E, hence

$$Ax = b \iff (EA)x = Eb.$$

- Row swap:  $L_i \leftrightarrow L_j$
- Scale:  $L_i \leftarrow \lambda L_i$ ,  $\lambda \neq 0$
- Row add:  $L_i \leftarrow L_i + \lambda L_j$

Gaussian Elimination: Key Ideas II

## Exercise

Solve the system

$$\begin{cases} x+y+z=3\\ 2x+y=7\\ 3x+2z=5 \end{cases}$$

Matrices: Definition and Properties

#### Definition

A matrix is an  $m \times n$  array of elements, where m is the number of rows and n is the number of columns.

$$A \in \mathcal{M}_{m \times n}(\mathbb{K})$$
 (matrix with entries in a field  $\mathbb{K}$ , e.g.,  $\mathbb{R}$ ,  $\mathbb{C}$ ).

We also write  $A \in \mathbb{R}^{m \times n}$  for  $\mathbb{K} = \mathbb{R}$ .

## Key properties of $\mathcal{M}_{m \times n}(\mathbb{K})$

- ullet Vector space over  $\mathbb{K}$ : addition and scalar multiplication are defined entrywise.
- Dimension:  $\dim \mathcal{M}_{m \times n}(\mathbb{K}) = mn$ .
- Matrix multiplication defined if inner dimensions match  $(A \in \mathcal{M}_{m \times n}, B \in \mathcal{M}_{n \times p})$ .
- Multiplication is associative but not commutative in general.
- Identity matrix  $I_n \in \mathcal{M}_{n \times n}(\mathbb{K})$ :  $AI_n = I_m A = A$ .
- Invertibility only for square matrices  $A \in \mathcal{M}_{n \times n}(\mathbb{K})$ , with  $\det(A) \neq 0$ .

Matrix Multiplication as Composition of Linear Systems I

# ldea

 $\label{lem:multiplication} \mbox{Matrix multiplication corresponds to composing two linear systems:}$ 

$$C = AB \iff \mathsf{Apply}\ B \ \mathsf{first}, \ \mathsf{then}\ A.$$

# Example (two $2 \times 2$ systems)

Let

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 2 & 0 \\ 1 & 3 \end{bmatrix}.$$

First system (apply B to  $\begin{pmatrix} x \\ y \end{pmatrix}$ ):

$$\begin{cases} \mathbf{z} = 2\mathbf{x} + 0\mathbf{y} \\ \mathbf{w} = \mathbf{x} + 3\mathbf{y} \end{cases}$$

Second system (apply A to  $\begin{pmatrix} z \\ w \end{pmatrix}$ ):

$$\begin{cases} u = z + 2w = 4x + 6y \\ v = w = 1x + 3y \end{cases}$$

Overall transformation  $\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} u \\ v \end{pmatrix}$  is given by

$$C = AB = \begin{bmatrix} 4 & 6 \\ 1 & 3 \end{bmatrix}.$$

### Definition: Dot Product

For vectors  $\mathbf{v} = [a_1, \dots, a_n]$  and  $\mathbf{w} = [b_1, \dots, b_n]$ , the dot product is

$$\mathbf{v} \cdot \mathbf{w} = \sum_{i=1}^{n} a_i b_i$$
, and  $|\mathbf{v}| = \sqrt{\mathbf{v} \cdot \mathbf{v}}$ .

By the law of cosines, vectors  $\mathbf{v}$ ,  $\mathbf{w}$  are orthogonal iff  $\mathbf{v} \cdot \mathbf{w} = 0$ .

### Matrix Multiplication

Let  $A \in \mathcal{M}_{m \times n}(\mathbb{K})$  and  $B \in \mathcal{M}_{p \times q}(\mathbb{K})$ . Matrix multiplication AB is defined when n = p. If  $(AB)_{ij}$  denotes the (i,j) entry, then

$$(AB)_{ij} = \operatorname{row}_i(A) \cdot \operatorname{col}_j(B).$$

Interpretation: Each matrix represents a linear map in a chosen basis. Therefore, multiplication of matrices (composition of linear maps) and the dot product (row · column) only make sense within the same basis. We will formalize this with the notions of *linear maps* and *basis*, introduced next.

Dot Product and Matrix Multiplication II

Exercise

$$\begin{bmatrix} 2 & 7 \\ 3 & 3 \\ 1 & 5 \end{bmatrix} \cdot \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix} = \begin{bmatrix} 37 & 46 & 55 & 64 \\ * & * & * & * \\ * & * & * & * \end{bmatrix}$$

Fill in the missing entries.

#### **Definitions**

- Transpose:  $(A^{\top})_{ii} = A_{ii}$ .
  - Linearity:  $(\alpha A + \beta B)^{\top} = \alpha A^{\top} + \beta B^{\top}$ . Involution:  $(A^{\top})^{\top} = A$ .

  - Product rule:  $(AB)^{\top} = B^{\top}A^{\top}$ .
- A is symmetric if  $A^{\top} = A$ .
- A is diagonal if  $A_{ii} \neq 0 \Rightarrow i = j$ .
  - If A, B diagonal  $\in \mathcal{M}_{n \times n}(\mathbb{K})$ : AB = BA,  $(AB)_{ii} = a_{ii} b_{ii}$ .
- Identity:  $I_n = \operatorname{diag}(1, \dots, 1)$ ,  $I_n A = A = A I_m$ .
- Inverse:  $A \in \mathcal{M}_{n \times n}$  is invertible  $\iff \exists B \text{ s.t. } BA = AB = I_n$ . Denote  $A^{-1} = B$ .

## Transpose, Symmetry, and Inverses

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### Exercise

- Find  $2 \times 2$  matrices (A, B) with  $AB \neq BA$ .
- Show  $(AB)^{\top} = B^{\top}A^{\top}$ . Deduce that  $A^{\top}A$  is symmetric.

# Transpose, Symmetry, and Inverses

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# Matrix form of a linear system

A system of n linear equations in m unknowns is written as

Diagonalization: Motivation via Smoking Example I

Smoking in Smallville

Let  $(n_t, s_t)^{\top} = (\# \text{ nonsmokers }, \# \text{ smokers})$  at year t. Transition rule:

$$\begin{bmatrix} n_{t+1} \\ s_{t+1} \end{bmatrix} = \begin{bmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{bmatrix} \begin{bmatrix} n_t \\ s_t \end{bmatrix}.$$

By iteration:

$$\begin{bmatrix} n_t \\ s_t \end{bmatrix} = \left( \begin{bmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{bmatrix} \right)^t \begin{bmatrix} n_0 \\ s_0 \end{bmatrix}.$$

To study  $t\gg 0$ , we need to compute  $A^t$  with

$$A = \begin{bmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{bmatrix}.$$

Diagonalization: Motivation via Smoking Example II

## Key Trick: Diagonalization

There exists a change-of-basis matrix  ${\cal B}$  such that

$$BAB^{-1} = D$$
 (diagonal).

Then, for any integer m, we get

$$A^m = B^{-1} D^m B,$$

and computing  $\mathbb{D}^m$  is easy (just raise diagonal entries).

 $\Rightarrow$  Expensive repeated multiplications become trivial if A is diagonalizable.

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### **Number Sets**

- Natural numbers:  $\mathbb{N} = \{0, 1, 2, 3, \dots\}$ , non-negative integers.
- Integers:  $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$ , all negative and positive whole numbers, including 0.
- Rational numbers:  $\mathbb{Q}=\left\{rac{p}{q}\,:\,p\in\mathbb{Z},\;q\in\mathbb{Z}^*,\;q
  eq0
  ight\}$ , ratios of integers.
- Real numbers:  $\mathbb{R}$  is the *completion* of  $\mathbb{Q}$ ; a totally ordered complete field.  $\pi$ , e,  $\sqrt{2}$ ,  $\varphi = \frac{1+\sqrt{5}}{2}$  are real numbers that are irrational.
- Complex numbers:  $\mathbb{C} = \{x + iy : x, y \in \mathbb{R}, i^2 = -1\}$ , an algebraic extension of  $\mathbb{R}$ .

# Hierarchy

$$\mathbb{N}\subset\mathbb{Z}\subset\mathbb{Q}\subset\mathbb{R}\subset\mathbb{C}$$

# Binary Operation (Internal Law)

Let E be a set. An internal binary operation on E is a map

$$\star : E \times E \rightarrow E, \qquad (x, y) \mapsto x \star y.$$

Examples: + and  $\times$  on  $\mathbb{Z}$ .

# Group

A group is a pair  $(G, \star)$  where  $\star$  is an internal binary operation satisfying:

- Associativity:  $(x \star y) \star z = x \star (y \star z)$ .
- **Identity element:** there exists  $e \in G$  such that  $x \star e = e \star x = x$ .
- Inverse: every  $x \in G$  has an inverse  $x^{-1}$  with  $x \star x^{-1} = e$ .

If  $x \star y = y \star x$  for all x, y, the group is abelian.

Name some familiar examples!

Fundamental Algebraic Structures II

# Example

 $(\mathbb{Z},+)$  is an abelian group.  $(\mathbb{Z},\times)$  is *not* a group: not every integer has a multiplicative inverse in  $\mathbb{Z}$ .

# Ring

A *ring*  $(A, +, \times)$  is a set with two operations:

- $\bullet$  (A, +) is an abelian group.
- ullet x is associative and has a multiplicative identity 1.
- × distributes over +.

### Field

A  $\mathit{field}$  is a ring  $(K,+,\times)$  in which every nonzero element has a multiplicative inverse.

### Examples

 $\mathbb{Q},\ \mathbb{R},\ \mathbb{C}$  are fields.  $\mathbb{Z}$  is a ring but not a field.

Exercise: A Nonstandard Binary Operation on  $\ensuremath{\mathbb{Z}}$ 

### Problem

Define, for  $a, b \in \mathbb{Z}$ , the operation

$$a \star b = a + b + 1.$$

- **9** Show that  $\star$  is an *internal* binary operation on  $\mathbb{Z}$ .
- Check associativity and commutativity of \*.
- **3** Determine the identity element e for  $\star$ .
- **9** For a given  $a \in \mathbb{Z}$ , find the inverse of a with respect to  $\star$ .
- **⑤** Conclude: is  $(\mathbb{Z}, \star)$  a group? Is it abelian?

Your solution?

To fully grasp and master the notion of matrices, we need to introduce the formal framework that governs them: vector spaces and linear maps.

## Definition (Vector Space)

Let  $\mathbb{K}$  be a field (e.g.,  $\mathbb{R}$  or  $\mathbb{C}$ ). A vector space over  $\mathbb{K}$  is a set V equipped with:

• an internal operation + (vector addition)

$$(x, y) \mapsto x + y,$$

• an external operation (scalar multiplication)

$$\mathbb{K} \times V \to V, \qquad (\lambda, x) \mapsto \lambda x,$$

such that the following axioms hold for all  $x, y, z \in V$  and  $\lambda, \mu \in \mathbb{K}$ :

- $lackbox{0}\ (V,+)$  is an abelian group (associativity, commutativity, neutral element 0, inverses).
- ② Scalar compatibility:  $(\lambda \mu)x = \lambda(\mu x)$ .
- **③** Neutral element of scalars:  $1_{\mathbb{K}}x = x$ .
- **1** Distributivity:  $(\lambda + \mu)x = \lambda x + \mu x$ , and  $\lambda(x + y) = \lambda x + \lambda y$ .

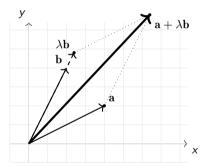
### Examples of Vector Spaces

•  $\mathbb{K}^n$  (the *n*-tuples of scalars from  $\mathbb{K}$ ) is a vector space. Indeed:

$$\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} + \lambda \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} a_1 + \lambda b_1 \\ \vdots \\ a_n + \lambda b_n \end{pmatrix} \in \mathbb{K}^n$$

- The set  $\mathbb{R}[X]$  of real-coefficient polynomials is a vector space over  $\mathbb{R}$ .
- The set  $C^0([a,b],\mathbb{R})$  of continuous functions from [a,b] to  $\mathbb{R}$  is a vector space.

$$\begin{pmatrix} \mathsf{a}_1 \\ \mathsf{a}_2 \end{pmatrix} + \lambda \begin{pmatrix} \mathsf{b}_1 \\ \mathsf{b}_2 \end{pmatrix} = \begin{pmatrix} \mathsf{a}_1 + \lambda \mathsf{b}_1 \\ \mathsf{a}_2 + \lambda \mathsf{b}_2 \end{pmatrix} \in \mathbb{R}^2$$



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### Definition (Subspace)

Let V be a vector space over  $\mathbb{K}$ . A subset  $F \subset V$  is a *subspace* if:

- $0_V \in F$ ,
- $\forall x, y \in F$ , then  $x + y \in F$  (closed under addition),
- $\forall \lambda \in \mathbb{K}, x \in F$ , then  $\lambda x \in F$  (closed under scalar multiplication).

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## Examples

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### **Properties**

- If F, G are subspaces of V, then  $F \cap G$  is also a subspace.
- The **sum** of subspaces is

$$F + G = \{x + y : x \in F, y \in G\},\$$

which is again a subspace.

Span, Linear Independence, and Basis

### Span of a Set

Given a subset  $A \subset V$ , the set of all finite linear combinations of elements of A forms a subspace of V, denoted

$$\mathrm{Span}(A) = \{\lambda_1 v_1 + \cdots + \lambda_k v_k \mid k \in \mathbb{N}, \ v_i \in A, \ \lambda_i \in \mathbb{K}\}.$$

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### Linear Independence and Generating Set

• A family  $(v_1, \ldots, v_p)$  is *linearly independent* if the only relation

$$\lambda_1 \mathbf{v}_1 + \cdots + \lambda_p \mathbf{v}_p = 0 \Rightarrow \forall i, \ \lambda_i = 0.$$

ullet It is a generating set of V if

$$\operatorname{Span}(\mathbf{v}_1,\ldots,\mathbf{v}_p)=V.$$

#### Definition

Let V be a vector space over a field  $\mathbb{K}$ .

- A basis of V is a family of vectors  $(\mathbf{v}_1, \dots, \mathbf{v}_n)$  in V that is
  - linearly independent,
  - ② and generates V (i.e.,  $Span(\mathbf{v}_1, \dots, \mathbf{v}_n) = V$ ).
- The **dimension** of V, denoted  $\dim(V)$ , is the number of vectors in any basis of V.

**Remark.** The definition is well-posed: every two bases of a finite-dimensional vector space V have the same number of elements.

# Theorem (Dimension of a Subspace)

Let F be a subspace of a finite-dimensional vector space V. Then

$$\dim(F) \leq \dim(V)$$
.

Moreover, if  $F \neq V$ , the inequality is strict.

#### Grassmann Formula

If F, G are finite-dimensional subspaces of V, then

$$\dim(F+G) = \dim(F) + \dim(G) - \dim(F \cap G).$$

#### Exercise

Consider the set

$$\mathcal{F} = \{[1,0], [0,1], [2,3]\} \subset \mathbb{R}^2.$$

- Is F linearly independent?
- Is  $\mathcal{F}$  a generating family of  $\mathbb{R}^2$ ?
- ullet What is the cardinality of a maximal linearly independent subfamily of  $\mathcal{F}$ , i.e., the dimension of  $\mathrm{Span}(\mathcal{F})$ ?

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### Canonical Example

In  $\mathbb{R}^n$ , the canonical family

$$e_1 = (1, 0, \dots, 0), \dots, e_j = (0, \dots, 1, \dots, 0), \dots, e_n = (0, \dots, 0, 1)$$

is a basis of  $\mathbb{R}^n$ , and its dimension is n.

## Theorem (Incomplete Basis Theorem)

Let V be a finite-dimensional vector space with dim(V) = n. Suppose

$$(v_1, \ldots, v_p), \quad p < n,$$

is a linearly independent family of vectors in V.

Then there exist additional vectors  $v_{p+1}, \ldots, v_n \in V$  such that

$$(v_1,\ldots,v_p,v_{p+1},\ldots,v_n)$$

is a basis of V.

In other words, any linearly independent family can be extended to a basis.

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### Example

In  $\mathbb{R}^3$ , consider  $\{(1,0,0),(0,1,0)\}$ . This family is linearly independent but not a basis (only p=2 < n=3). Adding (0,0,1) yields

$$\{(1,0,0), (0,1,0), (0,0,1)\},\$$

which forms the canonical basis of  $\mathbb{R}^3$ .

## Theorem (Extracted Basis Theorem)

Let V be a finite-dimensional vector space with dim(V) = n. Suppose

$$(v_1,\ldots,v_p), \quad p\geq n,$$

is a generating family of V.

Then there exists a subfamily

$$(v_{i_1},\ldots,v_{i_n})$$

that forms a basis of V.

In other words, any generating family contains a basis.

### Example

In  $\mathbb{R}^3$ , consider the generating family

$$\{(1,0,0),\ (0,1,0),\ (0,0,1),\ (1,1,1)\}.$$

This set spans  $\mathbb{R}^3$ . By removing the redundant vector (1,1,1), we obtain the canonical basis

$$\{(1,0,0), (0,1,0), (0,0,1)\},\$$

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## Conceptual Motivation

A linear transformation is a mapping between vector spaces that preserves their structure. It takes a vector as input and produces another vector, in such a way that:

- vector addition is preserved,
- scalar multiplication is preserved.

These maps are fundamental because they capture the essence of "structure-preserving" operations in linear algebra.

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#### Definition

Let V and W be vector spaces. A map  $T: V \to W$  is a linear transformation if

$$T(c\mathbf{v}_1 + \mathbf{v}_2) = c T(\mathbf{v}_1) + T(\mathbf{v}_2), \quad \forall \mathbf{v}_1, \mathbf{v}_2 \in V, \ c \in \mathbb{K}.$$

#### Linear Transformations

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#### Exercise

Check whether the map  $\mathcal T$  is a linear transformation, where  $\mathcal T:\mathbb R^2 o\mathbb R^2$  is defined by

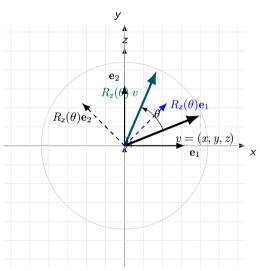
$$T(x, y) = (2x + y, -x + 3y)$$

## Canonical Examples

Let  $V = \mathbb{R}^3$ .

- Identity  $Id: \mathbb{R}^3 \to \mathbb{R}^3$ ,  $Id(\mathbf{x}) = \mathbf{x}$ . Matrix:  $I_3$ .
- Homothety (Scaling)  $H_{\alpha}(\mathbf{x}) = \alpha \mathbf{x}$  for  $\alpha \in \mathbb{R}$ . Matrix:  $\alpha I_3$ .
- Rotation about the z-axis by angle  $\theta$

$$R_{z}(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R_{z}(\theta) \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \cos \theta - y \sin \theta \\ x \sin \theta + y \cos \theta \\ z \end{bmatrix}.$$



$$R_{z}(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta & 0\\ \sin \theta & \cos \theta & 0\\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{array}{c|c} x & x & x \\ \hline y = (x, y, z) \\ \hline \mathbf{e}_1 & x \end{array} \quad \begin{array}{c} R_z(\theta) \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \cos \theta - y \sin \theta \\ x \sin \theta + y \cos \theta \\ z \end{bmatrix}$$

#### **Definitions**

Let V, W be vector spaces.

- $\mathcal{L}(V, W) := \text{set of linear maps } T: V \to W.$
- Endomorphism:  $T \in \mathcal{L}(V, V)$ .
- **Isomorphism**: bijective linear map  $T \in \mathcal{L}(V, W)$ .
- **Automorphism**: bijective endomorphism  $T \in \mathcal{L}(V, V)$ .

## Algebraic Structure

On  $\mathcal{L}(V) := \mathcal{L}(V, V)$ ,

- With pointwise addition + and composition  $\circ$ ,  $(\mathcal{L}(V), +, \circ)$  is a (not-necessarily commutative) ring with identity Id.
- Distributivity:  $T \circ (S_1 + S_2) = T \circ S_1 + T \circ S_2$  and  $(S_1 + S_2) \circ T = S_1 \circ T + S_2 \circ T$ .

#### **Definitions**

For  $T \in \mathcal{L}(V, W)$ :

$$\ker(T) := \{ \mathbf{v} \in V \mid T(\mathbf{v}) = \mathbf{0}_W \}, \qquad \operatorname{Im}(T) := \{ T(\mathbf{v}) \mid \mathbf{v} \in V \} \subseteq W.$$

## **Key Properties**

- T is injective  $\iff \ker(T) = \{\mathbf{0}_V\}.$
- If  $(\mathbf{v}_i)_{i \in I}$  generates V, then  $\operatorname{Im}(T) = \operatorname{Span}(T(\mathbf{v}_i) : i \in I)$ .

# Rank-nullity theorem

Let  $T \in \mathcal{L}(V, W)$  with  $\dim(V) < \infty$ . Then

$$\underbrace{\dim \ker(T)}_{\text{nullity}} + \underbrace{\dim \operatorname{Im}(T)}_{\text{rank}} = \dim(V).$$

#### Consequences

- T injective  $\iff$   $\dim \ker(T) = 0 \iff \operatorname{rank}(T) = \dim(V)$ .
- If  $\dim(W) < \infty$ , then T surjective  $\iff \operatorname{rank}(T) = \dim(W)$ .
- If  $\dim(V) = \dim(W)$ , then: injective  $\iff$  surjective  $\iff$  T is an isomorphism.

#### Setup

Let  $T \in \mathcal{L}(\mathbb{R}^n) \equiv \mathbb{R}^{n \times n}$  be endomorphism with  $\mathrm{rank}(T) = 1$ . Then there exist  $u, v \in \mathbb{R}^n$  such that

$$T = v u^{\top}$$
 (i.e.,  $T(x) = (u^{\top}x) v$  for all  $x \in \mathbb{R}^n$ ).

# Image and Kernel

Since  $u^{\top}x$  is a scalar,

$$\text{Im}(T) = \text{span}\{v\}, \quad \ker(T) = \{x \in \mathbb{R}^n : u^{\top}x = 0\} = u^{\perp}.$$

In particular,  $\dim \operatorname{Im}(T) = 1$  and  $\dim \ker(T) = n - 1$  (rank-nullity).

# Quick Properties

- $T^2 = (u^\top v) \ T$  (so T is diagonalizable with eigenvalues  $\{0, \ u^\top v\}$ ).
- $\bullet$  tr $(T) = u^{\top}v$  and  $\det(T) = 0$ .
- If  $u^{\top}v = 1$  and v is a unit vector, then T is the orthogonal projection onto  $\operatorname{span}\{v\}$  along  $u^{\perp}$ .

**Note:** The subspace denoted by the orthogonal complement symbol  $^{\perp}$  will be formally introduced in the final chapter of this course.

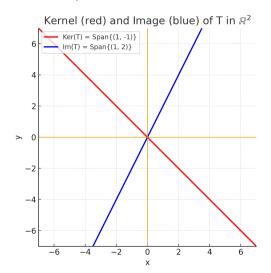
In  $\mathbb{R}^2$ 

Consider the following linear map:

$$T: \mathbb{R}^2 \to \mathbb{R}^2$$
$$(x, y) \mapsto (x + y, \ 2x + 2y)$$

- lacktriangle What type of morphism is T (e.g.,, injective, surjective, isomorphism)? Prove the linear aspect.
- ② Determine  $\ker(T)$  and  $\operatorname{Im}(T)$ . Is the rank-null theorem verified ?
- ullet Plot  $\ker(T)$  in red and  $\operatorname{Im}(T)$  in blue in the Cartesian plane, and provide their equations. Interpret your result.

## Geometric interpretation



- Every vector  $v \in \mathbb{R}^2$  is sent onto the blue line:  $T(v) \in \operatorname{im}(T) = \operatorname{Span}\{(1,2)\}...$
- ... except vectors on the red line that are mapped to the origin:

$$T(v) = 0 \iff v \in \ker(T) = \operatorname{Span}\{(1, -1)\}.$$

Hence T is a rank-1 linear map that collapses the plane onto  $\mathrm{Span}\{(1,2)\}$  along  $\mathrm{Span}\{(1,-1)\}.$ 

#### Definitions

Let U, V be subspaces of a vector space E.

$$U + V = \{u + v : u \in U, v \in V\}.$$

We say that *E* is the direct sum of *U* and *V*, written  $E = U \oplus V$ , if

$$E = U + V$$
 and  $U \cap V = \{0\}.$ 

In this case, every decomposition x = u + v is unique.

#### Criteria and Dimensions

For finite-dimensional spaces:

$$E = U \oplus V \iff E = U + V \text{ and } U \cap V = \{0\}.$$
  $\dim(U \oplus V) = \dim U + \dim V.$ 

Paul MINCHELLA, Stéphane CHRÉTIEN

## Rank-nullity theorem

Let  $T: E \to E$  be linear with dim  $E < \infty$ .

$$\dim \ker T + \underbrace{\dim \operatorname{im} T}_{\operatorname{rg}(T)} = \dim E.$$

If moreover  $\ker T \cap \operatorname{im} T = \{0\}$ , then

$$E = \ker T \oplus \operatorname{im} T$$
.

#### Useful cases:

- If T is a **projection** ( $T^2 = T$ ), then  $E = \ker T \oplus \operatorname{im} T$ .
- If T is symmetric (real matrix A with  $A^{\top} = A$ ), then  $(\operatorname{im} T)^{\perp} = \ker T$  and thus  $E = \ker T \stackrel{\perp}{\oplus} \operatorname{im} T$ .

Check the previous example to see an application of this theorem with  $\mathbb{R}^2 = \ker T \oplus \operatorname{im} T!$ 

#### Definition

Let  $T: V \to W$  be a linear transformation, where V and W are vector spaces with bases  $\mathcal{B}_V = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  and  $\mathcal{B}_W = \{\mathbf{f}_1, \dots, \mathbf{f}_m\}$ , respectively.

The matrix of T with respect to these bases is the  $m \times n$  matrix

$$M_{ij}$$
 such that  $T(\mathbf{e}_j) = \sum_{i=1}^m M_{ij} \mathbf{f}_i$ .

Equivalently, the j-th column of the matrix is the coordinate vector of  $T(\mathbf{e}_j)$  in the basis  $\mathcal{B}_W$ .

# Examples

What are the matrix of the following linear maps?

- $\bullet \mathbb{R}^2 \to \mathbb{R}^2 \colon T(x, y) = (2x + y, -x + 3y)$
- $\bullet \mathbb{R}^3 \to \mathbb{R}^3 \colon T(x, y, z) = (x + z, y, 2z)$
- $\bullet \mathbb{R}^2 \to \mathbb{R}^3$ : T(x, y) = (x, y, x + y)

# Key Idea in 3D

A linear map  $T:\mathbb{R}^3 \to \mathbb{R}^3$  associates each vector with another vector.

- If T is **bijective** (invertible), its image is all of  $\mathbb{R}^3$ . Any direction in space can be reached.
- If T is not bijective, the image has lower dimension: a plane (dim 1), a line (dim 1), or just  $\{0\}$  (dim 0).

# Key Idea in 3D

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- If T is **bijective** (invertible), its image is all of  $\mathbb{R}^3$ . Any direction in space can be reached.
- If T is **not bijective**, the image has lower dimension: a plane (dim 2), a line (dim 1), or just  $\{0\}$  (dim 0).

## Example from Physics

- Projection of a 3D object onto a screen
  - $\bullet$   $\mathbb{R}^3 \to \mathsf{a}$  plane in  $\mathbb{R}^3$ .
  - Linear but not bijective: depth information is lost.
- Meteorology: wind coordinate change
  - Convert wind (u, v, w) into rotated/polar coordinates.
  - Invertible linear map (rotation, change of basis).
- Mechanics/Thermodynamics: unit conversion
  - Joules  $\leftrightarrow$  kilocalories, or forces  $\leftrightarrow$  stresses.
  - Invertible linear map (diagonal scaling matrix).

- Introduction
- Vector Spaces
- Linear Transformations
- Change of Basis
- Diagonalization
- Application of Diagonalization
- Application to Statistics: Least Square and SVD

Change of Basis via a Linear System (case n = 3) I

#### Motivation

A linear transformation is an abstract object, but once a basis is chosen it can be represented by a matrix. Different choices of basis yield different matrix representations. This motivates the study of the **change of basis**, a **bijective** correspondence between the coordinates of the same vector expressed in different bases.

# Setup

Let  $\mathcal{B}_1 = (b_1, b_2, b_3)$  and  $\mathcal{B}_2 = (c_1, c_2, c_3)$  be bases of  $\mathbb{R}^3$ . We want the change-of-basis matrix  $P_{21}$  that converts coordinates from  $\mathcal{B}_1$  to  $\mathcal{B}_2$ :

$$[\mathbf{x}]_{\mathcal{B}_2} = P_{21} [\mathbf{x}]_{\mathcal{B}_1}.$$

#### Linear system

Express each old basis vector  $b_j \in \mathbb{R}^3$  as a linear combination of the new basis vectors  $c_j$ :

$$\begin{cases} b_1 = \alpha_{11}c_1 + \alpha_{21}c_2 + \alpha_{31}c_3 & \leftarrow \textit{This is a system of 3 equations!} \\ b_2 = \alpha_{12}c_1 + \alpha_{22}c_2 + \alpha_{32}c_3 & \leftarrow \textit{same!} \\ b_3 = \alpha_{13}c_1 + \alpha_{23}c_2 + \alpha_{33}c_3 & \leftarrow \textit{same!} \end{cases}$$

# Matrix form (the matrix to invert)

 $\text{Let } C = [\textbf{\textit{c}}_1 \ \textbf{\textit{c}}_2 \ \textbf{\textit{c}}_3], \qquad B = [\textbf{\textit{b}}_1 \ \textbf{\textit{b}}_2 \ \textbf{\textit{b}}_3], \qquad A = \left(\alpha_{ij}\right)_{1 \leq \ i, \, j \, \leq 3}. \text{ Then the three systems above compactly read }$ 

$$CA = B \implies A = C^{-1}B$$
 (since  $C$  is invertible).

The change-of-basis matrix is precisely

$$P_{21} :\equiv A = C^{-1}B$$
.

Change of Basis via a Linear System (case n=3) III

## Augmented-matrix viewpoint

Gaussian elimination on the augmented matrix (where the first block contains the column vectors of  $\mathcal{B}_2$  and the second block those of  $\mathcal{B}_1$ ) simultaneously solves the three systems:

$$\left[ \begin{array}{c|c} \mathcal{B}_2 \mid \mathcal{B}_1 \end{array} \right] = \left[ \begin{array}{c|c} C \mid B \end{array} \right] \; \sim \; \left[ \begin{array}{c|c} I_d \mid C^{-1}B \end{array} \right] = \left[ \begin{array}{c|c} I_d \mid \textcolor{red}{P_{21}} \end{array} \right].$$

Example (to be solved)

Let  $B_1 = \{(1,0,0), (0,1,0), (0,0,1)\}$  and  $B_2 = \{(1,1,1), (1,-1,1), (2,1,1)\}$ . Find the coordinates of  $\mathbf{b} = (2,1,-1)$  in basis  $B_2$ .

# Method 1: Direct System

Seek scalars  $\alpha, \beta, \gamma$  such that

$$\alpha(1,1,1) + \beta(1,-1,1) + \gamma(2,1,1) = (2,1,-1).$$

This gives the system:

$$\begin{cases} \alpha + \beta + 2\gamma = 2, \\ \alpha - \beta + \gamma = 1, \\ \alpha + \beta + \gamma = -1. \end{cases}$$

Solution:  $\alpha = -3, \ \beta = -1, \ \gamma = 3.$ 

$$[\mathbf{b}]_{B_2} = \begin{pmatrix} -3\\-1\\3 \end{pmatrix}.$$

#### Method 2: Gauss-Jordan

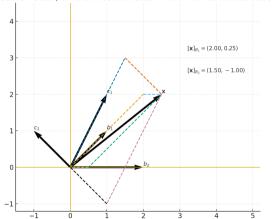
Form  $C = [c_1 \ c_2 \ c_3]$  and compute  $C^{-1}$ :

$$\mathbf{C} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbf{C}^{-1} = \begin{bmatrix} -1 & \frac{1}{2} & \frac{3}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \\ 1 & 0 & -1 \end{bmatrix}.$$

Thus  $P_{12} = C^{-1}$  and

$$[\mathbf{b}]_{B_2} = P_{12}[\mathbf{b}]_{B_1} = \begin{bmatrix} -3\\-1\\3 \end{bmatrix}.$$

#### Same vector, different coordinates in two non-canonical base



#### Exercise. Knowing

$$\mathcal{B}_{1} = \{b_{1}, b_{2}\} = \left\{ \begin{pmatrix} 1\\1 \end{pmatrix}, \begin{pmatrix} 2\\0 \end{pmatrix} \right\}$$
$$\mathcal{B}_{2} = \{c_{1}, c_{2}\} = \left\{ \begin{pmatrix} 1\\2 \end{pmatrix}, \begin{pmatrix} -1\\1 \end{pmatrix} \right\}$$
$$[\mathbf{x}]_{\mathcal{B}_{1}} = \begin{pmatrix} 2\\0.25 \end{pmatrix}$$

express the change-of-basis matrix  $P_{21}$  and find the coordinates of x in the basis  $\mathcal{B}_2$ .

$$[\mathbf{x}]_{\mathcal{B}_2} = ?$$

- Introduction
- Vector Spaces
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Eigenvalues and Eigenvectors: Motivation I

# Smallville Recap

We want to analyze the long-term behavior of the system:

- What happens after *n* years?
- Does the system converge to an equilibrium state?

Key idea: a matrix represents a linear transformation in some basis. Choosing a "better" basis can simplify the representation. Goal: compute

$$\lim_{t\to\infty}A^t.$$

## Definition: Eigenvalues and Eigenvectors

Let  $T: V \to V$ , with  $V = \mathbb{R}^n$ . If there exists a basis  $B = \{\mathbf{v}_1, \dots, \mathbf{v}_n\}$  such that

$$T(\mathbf{v}_i) = \lambda_i \mathbf{v}_i, \quad \lambda_i \in \mathbb{R},$$

then the matrix of T in basis B is diagonal:

$$M_{BB} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}.$$

#### Next Step

Given a matrix A representing T, we must find vectors  $\mathbf{v}$  and scalars  $\lambda$  such that

$$A\mathbf{v} = \lambda \mathbf{v} \iff (A - \lambda I_n) \cdot \mathbf{v} = 0.$$

## Key Idea

For a matrix A, an eigenvalue  $\lambda$  must satisfy

$$(A - \lambda I)\mathbf{v} = \mathbf{0}$$
 for some nonzero vector  $\mathbf{v}$ .

This means  $\ker(A - \lambda I) \neq \{0\}$ . Equivalently, since a square matrix has a nontrivial kernel iff its determinant vanishes:

$$\underbrace{\det(A-\lambda I)}_{\text{Characteristic polynomial }\chi_A(\lambda)}=0.$$

- The roots of  $\chi_A(\lambda)$  are the eigenvalues of A.
- The corresponding nonzero solutions v are the eigenvectors.
- The set of eigenvalues of A is called the **spectrum** of A, denoted by Sp(A).

## Eigenspace

Given an eigenvalue  $\lambda_i$ , the **eigenspace** associated with  $\lambda_i$  is

$$E_{\lambda_i} = \ker(A - \lambda_i I) = \{ \mathbf{v} \in \mathbb{R}^n \mid A\mathbf{v} = \lambda_i \mathbf{v} \}.$$

It is a subspace of  $\mathbb{R}^n$ , spanned by all eigenvectors corresponding to  $\lambda_i$ .

#### Remark

For each eigenvalue  $\lambda_i$  of a matrix A, there are two notions of multiplicity:

- The algebraic multiplicity of  $\lambda_i$  is its multiplicity as a root of the characteristic polynomial  $\chi_A(\lambda)$ .
- The **geometric multiplicity** of  $\lambda_i$  is the dimension of its eigenspace dim  $E_{\lambda_i}$ .

These satisfy

$$1 \leq \dim \mathcal{E}_{\lambda_i} \leq \text{algebraic multiplicity of } \lambda_i.$$

A matrix is **diagonalizable** precisely when, for **each eigenvalue**, the geometric and algebraic **multiplicities coincide**.

# Characteristic Equation - Examples

Example 1: Eigenvalues

Let

$$A = \begin{bmatrix} 7 & 2 \\ 3 & 8 \end{bmatrix}.$$

Compute  $det(A - \lambda I)$  and find the eigenvalues of A.

Example 2: Eigenvectors

For each eigenvalue  $\lambda$  of A, solve

$$(A - \lambda I)\mathbf{v} = \mathbf{0}.$$

Find a basis for the eigenspace corresponding to  $\lambda$ .

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## Example 2: Eigenvectors

For each eigenvalue  $\lambda$  of A, solve

$$(A - \lambda I)\mathbf{v} = \mathbf{0}.$$

Find a basis for the eigenspace corresponding to  $\lambda$ .

#### Observation

In Example [3], the eigenvalues appeared on the diagonal of the diagonalized matrix D. Next, we will see how the eigenvectors determine this change of basis.

Are they diagonalizable ?

So, are they ?

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 7 & -1 \\ 0 & 0 & 2 \end{pmatrix} \quad B = \begin{pmatrix} 7 & 2 & 3 \\ 0 & 7 & -1 \\ 0 & 0 & 7 \end{pmatrix} \quad C = \begin{pmatrix} 1 & 2 & 4 \\ -1 & -2 & -4 \\ 1 & 2 & 4 \end{pmatrix}$$

Are they diagonalizable ?

So, are they ?

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 7 & -1 \\ 0 & 0 & 2 \end{pmatrix} \quad B = \begin{pmatrix} 7 & 2 & 3 \\ 0 & 7 & -1 \\ 0 & 0 & 7 \end{pmatrix} \quad C = \begin{pmatrix} 1 & 2 & 4 \\ -1 & -2 & -4 \\ 1 & 2 & 4 \end{pmatrix}$$

A is; B is not; C is, even if it is not invertible.

# Change of Basis and Similarity

### Setup

Let  $T: V \to V$  be a linear endomorphism. Suppose  $B_1$  and  $B_2$  are two bases of V. We denote by  $M_{B_1B_1}$  and  $M_{B_2B_2}$  the matrices of T expressed in these bases.

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# Change of Basis Relation

Let  $P_{12}$  be the change-of-basis matrix from  $B_2$  to  $B_1$ :

$$\mathbf{v}_{B_1}=P_{12}\,\mathbf{v}_{B_2}.$$

Then the matrices of T in the two bases are related by

$$M_{B_2B_2} = P_{21} M_{B_1B_1} P_{12}$$
, where  $P_{21} = P_{12}^{-1}$ .

# Key Point

Two matrices  $M_{B_1B_1}$  and  $M_{B_2B_2}$  representing the same linear transformation in different bases are said to be **similar**. Similarity preserves eigenvalues and many structural properties, but the form of the matrix depends on the chosen basis.

# Diagonalization Formalism

#### Definition

A matrix  $A \in \mathbb{R}^{n \times n}$  is **diagonalizable** if there exists a basis  $B_2$  of eigenvectors of A. In that basis, the matrix of A is diagonal:

$$D = \operatorname{diag}(\lambda_1, \ldots, \lambda_n).$$

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## Change of Basis Relation

Let  $P:=M_{B_1B_2}$  invertible be the change-of-basis matrix from the eigenbasis  $B_2$  to the reference basis  $B_1$ . Then

$$A = PDP^{-1}.$$

## ${\sf Diagonalization}\ {\sf Formalism}$

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$$A = PDP^{-1}.$$

#### Theorem

For every integer  $p \geq 0$ ,

$$A^p = P D^p P^{-1}.$$

## Key Point

Diagonalization transforms a difficult computation  $(A^p)$  into a simple one (because simply  $D^p = \operatorname{diag}(\lambda_1^p, \ldots, \lambda_p^p)$ , just raising eigenvalues to powers).

#### Characterizations

Let  $A \in \mathbb{R}^{n \times n}$ . The following are equivalent:

- A is diagonalizable  $\iff$  there exists a basis of  $\mathbb{R}^n$  formed by eigenvectors of A.
- ullet A is similar to a diagonal matrix:

$$\exists P \text{ invertible}, \quad P^{-1}AP = D.$$

ullet The sum of the dimensions of all eigenspaces equals n.

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$$\exists P \text{ invertible}, \quad P^{-1}AP = D.$$

ullet The sum of the dimensions of all eigenspaces equals n.

#### **Practical Conditions**

- If A has n distinct eigenvalues  $\Rightarrow$  A is diagonalizable.
- ullet If A is symmetric (real entries), then A is diagonalizable (Spectral Theorem).
- Otherwise: compare algebraic multiplicity (from characteristic polynomial) and geometric multiplicity (dimension of eigenspace). Diagonalizability requires equality for every eigenvalue.

IMPORTANT RESULTS: Trace, Determinant, and Spectrum I

## Trace

The **trace** of a square matrix  $A \in \mathcal{M}_n(\mathbb{R})$  is

$$\operatorname{tr}(A) = \sum_{i=1}^{n} a_{ii}.$$

If A is diagonalizable,  $A = PDP^{-1}$  with  $D = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$ , then

$$\operatorname{tr}(A) = \operatorname{tr}(D) = \lambda_1 + \cdots + \lambda_n.$$

#### Determinant

The **determinant** of a square matrix  $A = (a_{ij}) \in \mathcal{M}_n(\mathbb{R})$  is a scalar denoted  $\det(A)$ .

Formal recursive definition:

- For n = 1,  $det([a_{11}]) = a_{11}$ .
- For  $n \geq 2$ ,

$$\det(A) = \sum_{j=1}^{n} (-1)^{1+j} a_{1j} \det(M_{1j}),$$

where  $M_{1j}$  is the  $(n-1) \times (n-1)$  submatrix obtained by deleting row 1 and column j.

Geometric meaning:  $\det(A)$  represents the scaling factor of volumes induced by the linear transformation associated with A, with its sign indicating whether orientation is preserved or reversed. If A is diagonalizable as above, then

$$\det(A) = \det(D) = \lambda_1 \cdot \lambda_2 \cdots \lambda_n.$$

IMPORTANT RESULTS: Trace, Determinant, and Spectrum III

### Spectrum and Transpose

Since 
$$\det(A - \lambda I) = \det((A - \lambda I)^\top) = \det(A^\top - \lambda I)$$
, we have

$$\operatorname{Sp}(A) = \operatorname{Sp}(A^{\top}).$$

Let's once again consider

$$T: \mathbb{R}^2 \to \mathbb{R}^2$$
$$(x, y) \mapsto (x + y, \ 2x + 2y)$$

We showed in [37] that T is an endomorphism and not invertible.

- What is the matrix representation of T in the canonical basis of  $\mathbb{R}^2$ ? Let's denote it A.
- ② Is A diagonalizable? If so, what are its eigenvalues?
- **1** Determine a diagonal matrix D and an invertible matrix P (and  $P^{-1}$ ) such that

$$A = PDP^{-1}.$$

Diagonalization Method

Let

$$A = \begin{bmatrix} 0.7 & 0.2 \\ 0.3 & 0.8 \end{bmatrix}, \quad \begin{bmatrix} n_0 \\ s_0 \end{bmatrix} = \begin{bmatrix} 2000 \\ 8000 \end{bmatrix}.$$

Show that

$$\lim_{t \to \infty} A^t = \begin{bmatrix} 2/5 & 2/5 \\ 3/5 & 3/5 \end{bmatrix}.$$

Hence, what is the equilibrium ?

Solution ?

### Diagonalization Method

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Hence, what is the equilibrium?

#### Solution?

#### Observation

Since  $\begin{bmatrix} 2/5 & 2/5 \\ 3/5 & 3/5 \end{bmatrix} \begin{bmatrix} 2000 \\ 8000 \end{bmatrix} = \begin{bmatrix} 4000 \\ 6000 \end{bmatrix}$ , even though the initial population had far more smokers, the equilibrium state shifts toward more nonsmokers than at the start.

## Please note: you must master this type of exercise for the final exam.

### An example you have to work

Let us consider the linear map  $f: \mathbb{R}^3 \to \mathbb{R}^3$  represented in the canonical basis by the matrix

$$M = \begin{pmatrix} 3 & 1 & 3 \\ 1 & 3 & 3 \\ 3 & 3 & 1 \end{pmatrix}.$$

- lacktriangle Compute the **eigenvalues** of M.
  - → Hint: Try to avoid solving the full cubic polynomial. If necessary, look for an obvious root first to help factorize the degree-3 polynomial.
  - → Can you spot an obvious eigenvalue or eigenvector? What happens if you add up all the entries in each row (or in each column)?
  - → What equations can be derived from the trace and the determinant?
- For each eigenvalue, determine a basis of the associated eigenspace.
- $\odot$  Deduce whether M is **diagonalizable**, and if so, give an explicit diagonalization.

#### Definition

A square matrix  $Q \in \mathbb{R}^{n \times n}$  is called **orthogonal** if

$$Q^{\top} Q = Q Q^{\top} = I_n.$$

Equivalently,  $Q^{-1} = Q^{\top}$ .

#### Intuition

An orthogonal matrix represents a linear transformation that:

- preserves inner products and lengths,
- preserves orthogonality,
- is a composition of rotations and reflections.

## Remark: Isometry Property

Orthogonal matrices preserve lengths:

$$\|Q\mathbf{x}\|^2 = (Q\mathbf{x})^\top (Q\mathbf{x}) = \mathbf{x}^\top Q^\top Q\mathbf{x} = \mathbf{x}^\top \mathbf{x} = \|\mathbf{x}\|^2.$$

Thus,  $||Q\mathbf{x}|| = ||\mathbf{x}||$  for all  $\mathbf{x}$ .

# Why "orthogonal"?

If 
$$Q = [\mathbf{q}_1 \ \mathbf{q}_2 \ \dots \ \mathbf{q}_n]$$
, then

$$\mathbf{q}_i \cdot \mathbf{q}_j = \delta_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$$

so the column vectors form an **orthonormal basis** of  $\mathbb{R}^n$ .

# Example

The rotation matrix in  $\mathbb{R}^2$ ,

$$R(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix},$$

is orthogonal:  $R(\theta)^{\top}R(\theta) = I_2$ .

#### Remark

The set of all  $n \times n$  orthogonal matrices forms a group under multiplication, called the **orthogonal group** O(n). The subgroup of matrices with determinant 1 is the **special orthogonal group** SO(n), corresponding to pure rotations.

## Spectral Theorem

## Theorem (Spectral Theorem)

Every real symmetric matrix is diagonalizable. That is, if  $A \in \mathbb{R}^{n \times n}$  and  $A^{\top} = A$ , then there exists an orthogonal matrix Q such that

$$Q^{\top}AQ = D,$$

where D is diagonal.

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## Example

Consider

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

- ullet Show that A is symmetric.
- Compute its eigenvalues and eigenvectors.
- ullet Verify that A is diagonalizable via an orthogonal change of basis.

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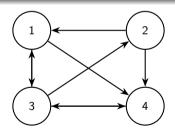
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**Remark:** Check your result for matrix M in Example [64], observing that  $M^{\top} = M!$ 

- Introduction
- Vector Spaces
- Linear Transformations
- Change of Basis
- Diagonalization
- Application of Diagonalization
- Application to Statistics: Least Square and SVD

#### Motivation

Model the web as a weighted, directed graph: vertices = websites, edges = links. If site j has  $\ell_j$  outgoing links, each outgoing edge carries weight  $1/\ell_j$ . This yields a column-stochastic transition matrix T; to allow random jumps, add a uniform "teleportation" matrix R.



# From Graph to Matrices

With  $\ell_j$  the out-degree of vertex j,

$$T_{ij} = egin{cases} rac{1}{\ell_j} & ext{if } j 
ightarrow i ext{ is an edge} \ 0 & ext{otherwise} \end{cases}.$$

Therefore, we construct this matrix:

$$T = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{3} & 0\\ 0 & 0 & \frac{1}{3} & 0\\ \frac{1}{2} & 0 & 0 & 1\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 0 \end{bmatrix}.$$

## Teleportation and the Google Matrix

The matrix 1 denotes the column vector of size n with all entries equal to 1. Hence  $\mathbf{11}^{\top}$  is the  $n \times n$  matrix of all 1's.

$$R = \frac{1}{n} \mathbf{1} \mathbf{1}^{\mathsf{T}}$$

is therefore the matrix where every entry is  $\frac{1}{n}$ . This models the fact that with probability p, a user may randomly jump to any website, independently of links.

The Google matrix combines both behaviors:

$$G = (1 - p) T + p R \in \mathbb{R}^{n \times n}$$
, with typical choice  $p \approx 0.15$ .

This construction ensures that G is stochastic, irreducible, and aperiodic, so it admits a unique stationary distribution. This stationary distribution reflects the long-term importance (rank) of each page, which is the core of Google's PageRank algorithm.

### Ranking Vector

We start with the uniform distribution:

$$\mathbf{v}(0) = \begin{bmatrix} \frac{1}{n}, & \frac{1}{n}, & \dots, & \frac{1}{n} \end{bmatrix}^{\top},$$

which represents an equal probability of being at any page initially.

Iterating the process,

$$\mathbf{v}(t+1) = G\mathbf{v}(t),$$

converges to the unique fixed point

$$\mathbf{v}_{\infty} = \left(\lim_{t \to \infty} G^t\right) \cdot \mathbf{v}(0).$$

The vector  $\mathbf{v}_{\infty}$  is the **PageRank vector**: its *i*-th entry gives the long-term probability of a user visiting page *i*. Pages with larger entries are ranked higher in search results.

Paul MINCHELLA, Stéphane CHRÉTIEN

## Theorem (Perron-Frobenius)

If M is a column-stochastic matrix with all entries positive, then:

- ullet 1 is an eigenvalue of M,
- ullet the associated eigenvector  $v_{\infty}$  has strictly positive entries,
- ullet  $v_{\infty}$  can be normalized so that its entries sum to 1,
- the iteration  $M^t \mathbf{v}(0)$  converges to  $\mathbf{v}_{\infty}$ .

## Perron-Frobenius and PageRank

## Theorem (Perron-Frobenius)

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- the iteration  $M^t \mathbf{v}(0)$  converges to  $\mathbf{v}_{\infty}$ .

## Application to PageRank

The PageRank vector is defined by solving

$$G\mathbf{v}=\mathbf{v},$$

that is, finding the eigenvector of G associated with eigenvalue 1.

**Challenge:** for the web, n is in the billions. Direct eigenvector computation is infeasible.

**Practical solution:** approximate  $v_{\infty}$  by iterating

$$\mathbf{v}(m) = G^m \mathbf{v}(0),$$

for moderate m, until convergence is reached.

Data Application: Covariance Matrix and Diagonalization

## Setup

We have k observations of m variables:

$$X = \{p_1, \ldots, p_k\}, \quad p_i = (p_{i1}, \ldots, p_{im}) \in \mathbb{R}^m.$$

For each coordinate j, let  $\mu_j(X)$  be the mean. Define the centered data matrix:

$$N_{ij} = p_{ij} - \mu_j(X).$$

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### Questions of Interest

- How is the data spread across directions in  $\mathbb{R}^m$ ?
- Is the variance larger in some directions than others?
- Do subsets of the data cluster in certain patterns?

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#### Definition

The **covariance matrix** of X is

$$cov(X) = N^{\top} N.$$

Example: Centering, Covariance, and Eigenanalysis

Consider the dataset

$$X = \{(1,1), (2,2), (2,3), (3,2), (3,3), (4,4)\}.$$

Tasks:

- **①** Compute the coordinate-wise mean  $\mu = (\mu_1, \mu_2)$ .

$$N_{ij} = \mathbf{p}_{ij} - \mu_j$$
.

Compute the covariance matrix

$$\operatorname{cov}(X) = N^{\top} N$$
 (optionally normalized by  $\frac{1}{k}$  or  $\frac{1}{k-1}$ ).

• Find the eigenvalues and associated eigenvectors of cov(X).

### Covariance Matrix and Principal Directions

# Theorem (Variance along Eigenvectors)

Order the eigenvalues of cov(X) as

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_m$$
.

Then the data variance along each direction is proportional to the corresponding eigenvalue, in the direction of the associated eigenvector.

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### Interpretation

- ullet The largest eigenvalue  $\lambda_{
  m max}$  indicates the direction of greatest data spread.
- Smaller eigenvalues correspond to directions with less variation.
- For 2D data: eigenvectors give the principal axes of the ellipse approximating the data cloud, and eigenvalues determine their lengths.

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# Key Point: PCA

Theorem [13] is the foundation of **Principal Component Analysis (PCA)**, a fundamental tool in applied mathematics, statistics, and machine learning.

- Introduction
- Vector Spaces
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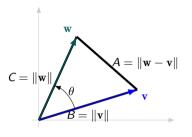
## Why orthogonality matters

In data science we approximate: we **minimize distance between model and data**. Squared distances are quadratic, so minimization leads to linear systems. Vector calculus links minimization with **orthogonal projections** onto subspaces.

# Law of Cosines (Al-Kashi)

For a triangle with side lengths A, B, C and opposite angles a, b, c,

$$A^2 = B^2 + C^2 - 2BC\cos(c).$$



$$A^2 = B^2 + C^2 - 2BC\cos(\theta)$$

# Exercise (warm-up)

Let  $\mathbf{v}, \mathbf{w}$  start at the origin and c be the angle between them. Apply the law of cosines to the triangle with sides  $A = \|\mathbf{w} - \mathbf{v}\|, \quad B = \|\mathbf{v}\|, \quad C = \|\mathbf{w}\|$  to show

$$\mathbf{v} \cdot \mathbf{w} = \|\mathbf{v}\| \|\mathbf{w}\| \cos(c).$$

Least Squares Approximation I

#### Motivation

Fitting data requires restricting model complexity: a good fit minimizes the error between data and model, without overfitting.

## **Key Point**

Least squares = **projection onto a subspace**. Understanding this requires the geometry of orthogonality.

Example: Line of Best Fit in  $\mathbb{R}^2$ 

Data set:  $X = \{(1,6), (2,5), (3,7), (4,10)\}.$ 

We want the line y = ax + b that minimizes the total squared error:

$$error = \sqrt{\sum_{(x_i,y_i) \in X} (y_i - (ax_i + b))^2}.$$

Minimizing the error is the same as minimizing the content of the square root.

Equivalently, solve the least squares system:

$$\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \\ 7 \\ 10 \end{bmatrix}.$$

Interpretation: we seek the projection of  $\begin{bmatrix} 6 & 5 & 7 & 10 \end{bmatrix}^{\top}$  onto the column space of the matrix.

Ordinary Least Squares: Computation and Interpretation I

# Ordinary Least Squares in Simple Linear Regression

We consider the model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \qquad i = 1, \dots, N,$$

where  $\varepsilon_i$  are random errors with zero mean. The aim is to estimate  $(\beta_0, \beta_1)$  by minimizing the total squared error.

## Derivation of the Optimal Coefficients

We minimize the quadratic error

$$f(\beta_0, \beta_1) = \sum_{i=1}^{N} (Y_i - (\beta_0 + \beta_1 X_i))^2.$$

First-order conditions:

$$\begin{cases} \frac{\partial f}{\partial \beta_0} = -2 \sum_{i=1}^{N} (Y_i - \beta_0 - \beta_1 X_i) = 0, \\ \frac{\partial f}{\partial \beta_1} = -2 \sum_{i=1}^{N} X_i (Y_i - \beta_0 - \beta_1 X_i) = 0. \end{cases}$$

Dividing by N and introducing

$$\bar{X} = \frac{1}{N} \sum_{i=1}^{N} X_i, \quad \bar{Y} = \frac{1}{N} \sum_{i=1}^{N} Y_i,$$

we obtain the system

$$\begin{cases} \bar{Y} = \beta_0 + \beta_1 \bar{X}, \\ \frac{1}{N} \sum_{i=1}^{N} X_i Y_i = \beta_0 \bar{X} + \beta_1 \frac{1}{N} \sum_{i=1}^{N} X_i^2. \end{cases}$$

#### Covariance and Variance Forms

Define

$$\operatorname{Cov}(X, Y) = \frac{1}{N} \sum_{i=1}^{N} (X_i - \bar{X})(Y_i - \bar{Y}), \qquad \operatorname{Var}(X) = \frac{1}{N} \sum_{i=1}^{N} (X_i - \bar{X})^2.$$

Useful expansions:

$$\frac{1}{N} \sum (X_i - \bar{X})(Y_i - \bar{Y}) = \frac{1}{N} \sum X_i Y_i - \bar{X} \bar{Y},$$
$$\frac{1}{N} \sum (X_i - \bar{X})^2 = \frac{1}{N} \sum X_i^2 - \bar{X}^2.$$

Therefore

$$\hat{\beta}_1 = \frac{\operatorname{Cov}(X, Y)}{\operatorname{Var}(X)}, \qquad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}.$$

Ordinary Least Squares: Computation and Interpretation IV

#### Final

Substituting the first into the second and rearranging yields

$$\hat{\beta}_1 = \frac{\frac{1}{N} \sum_{i=1}^{N} X_i Y_i - \bar{X} \bar{Y}}{\frac{1}{N} \sum_{i=1}^{N} X_i^2 - \bar{X}^2} = \frac{\text{Cov}(X, Y)}{\text{Var}(X)}.$$

Finally,

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}.$$

# Remark: Interpretation of $\hat{\beta}_1$

- Numerator Cov(X, Y): co-variation, the linear effect of X on Y.
- Denominator Var(X): variability of X itself.
- Hence  $\hat{\beta}_1$  measures the average change in Y per unit change in X, *i.e.*, the "linear effect" of X normalized by its own variability.

## Definition

Subspaces  $\mathit{W}, \mathit{W}' \subset \mathit{V}$  are **orthogonal** if

$$\mathbf{w} \cdot \mathbf{w}' = 0 \quad \forall \, \mathbf{w} \in W, \, \, \mathbf{w}' \in W'.$$

A set  $\{\mathbf{v}_1,\ldots,\mathbf{v}_n\}$  is orthonormal if  $\mathbf{v}_i\cdot\mathbf{v}_j=\delta_{ij}$ .

A matrix A is **orthonormal** when its columns are orthonormal vectors.

# Fundamental Subspaces of a Matrix

Let  $A \in \mathbb{R}^{m \times n}$ .

Column space (image):

$$C(A) \equiv \operatorname{Im}(A) = \{A\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^n\} \subset \mathbb{R}^m.$$

Dimension = rank of A.

• Null space (kernel):

$$N(A) \equiv \ker(A) = \{ \mathbf{x} \in \mathbb{R}^n \mid A\mathbf{x} = \mathbf{0} \} \subset \mathbb{R}^n.$$

Row space:

$$R(A) = \operatorname{Im}(A^{\top}) = \{\mathbf{y}^{\top}A, \ \mathbf{y} \in \mathbb{R}^{m}\} = [\operatorname{span} \ \operatorname{of} \ \operatorname{row} \ \operatorname{vectors} \ \operatorname{of} \ A] \subset \mathbb{R}^{n}.$$

• Rank-nullity theorem:

$$n = \dim N(A) + \dim R(A).$$

• Orthogonal complement: For a subspace  $W \subset V$ ,

$$W^{\perp} = \{ \mathbf{v} \in V \mid \mathbf{v} \cdot \mathbf{w} = 0, \ \forall \ \mathbf{w} \in W \}.$$

# Example

Let

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 1 & 1 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 3}.$$

- Compute  $C(A) = \operatorname{Im}(A)$ : span of the column vectors. Is it all of  $\mathbb{R}^3$ ?
- Compute  $C^{\perp}$ .
- Compute  $N(A) = \ker(A)$ : solve Ax = 0 explicitly.
- Determine R(A): span of row vectors. Compare  $\dim R(A)$  with  $\dim C(A)$ .
- Verify the rank-nullity theorem:

$$n = 3 = \dim N(A) + \dim R(A).$$

# Worked Example: Solution

Column Space

$$C(A) = \text{Span}\{(1,2,1)^{\top}, (2,4,1)^{\top}\}, \quad \dim = 2 < 3.$$

So  $C(A) \neq \mathbb{R}^3$ .

Orthogonal Complement

$$C(A)^{\perp} = \ker(A^{\top}) = \operatorname{Span}\{(-2, 1, 0)^{\top}\}.$$

Null Space

$$N(A) = \ker(A) = \text{Span}\{(1, -2, 1)^{\top}\}, \quad \dim = 1.$$

Row Space

$$R(A) = \text{Span}\{(1, 2, 3), (1, 1, 1)\}, \quad \dim = 2.$$

Note dim  $R(A) = \dim C(A) = 2$ .

Rank–Nullity Theorem

$$3 = \dim N(A) + \dim R(A) = 1 + 2.$$

Consistency: dim  $C(A)^{\perp} = 1$ , and indeed (-2, 1, 0) is orthogonal to both generators of C(A).

# Exercise

For A as above:

- Prove  $N(A) = R(A)^{\perp}$  and  $N(A^{\top}) = C(A)^{\perp}$ .
- **②** Prove any  $\mathbf{v} \in V$  decomposes uniquely as  $\mathbf{v} = \mathbf{w}' + \mathbf{w}''$  with  $\mathbf{w}' \in W$ ,  $\mathbf{w}'' \in W^{\perp}$ .
- **1** Prove that the closest vector in W to  $\mathbf{v}$  is exactly  $\mathbf{w}'$ .

Let A denote the matrix on the left in the last displayed equation in Example [80], and let  $\mathbf{b} = [6, 5, 7, 10]^{\mathsf{T}}$ . Then

$$A^{\top}A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

so

$$\left(\mathbf{A}^{\top}\mathbf{A}\right)^{-1} = \left[ \begin{array}{cc} 3/2 & -1/2 \\ -1/2 & 1/5 \end{array} \right]$$

Continuing with the computation, we have

$$A \cdot \left(A^{\top}A\right)^{-1} \cdot A^{\top} = \frac{1}{10} \left[ egin{array}{cccccc} 7 & 4 & 1 & -2 \ 4 & 3 & 2 & 1 \ 1 & 2 & 3 & 4 \ -2 & 1 & 4 & 7 \end{array} 
ight]$$

Putting everything together, we see that indeed

$$\mathbf{A} \cdot \left( \mathbf{A}^{\top} \mathbf{A} \right)^{-1} \cdot \mathbf{A}^{\top} \cdot \mathbf{b} = \begin{bmatrix} 4.9 \\ 6.3 \\ 7.7 \\ 9.1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \cdot \begin{bmatrix} 3.5 \\ 1.4 \end{bmatrix}$$

where  $\left[3.5, 1.4\right]$  is the solution we obtained using partials.

Exercise: Quadratic Least Squares and a Glimpse of SVD

## Quadratic fit for Example 4.2

Fit a degree–2 model  $y = ax^2 + bx + c$  to the data of Example 4.2. Set up the least–squares system

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix}}_{A} \begin{bmatrix} c \\ b \\ a \end{bmatrix} = \underbrace{\begin{bmatrix} 6 \\ 5 \\ 7 \\ 10 \end{bmatrix}}_{b}$$

and carry out the same analysis as for the linear fit:

- Derive the normal equations  $A^{\top}Ay = A^{\top}b$  (with  $y = [c, b, a]^{\top}$ ).
- Show that the solution y gives  $\mathbf{b}' = A\mathbf{y}$  equal to the projection of  $\mathbf{b}$  onto  $\operatorname{Col}(A)$ .
- Verify that this agrees with the solution found by minimizing via partial derivatives.

#### Towards SVD

Real-world problems often involve *non-square* matrices. **Singular Value Decomposition (SVD)** is "diagonalization for non-square matrices" and will generalize these ideas.

# Singular Value Decomposition Theoreme

Let M be an  $m \times n$  matrix of rank r. There exist matrices  $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  with orthonormal columns, and a diagonal matrix  $\Sigma \in \mathbb{R}^{m \times n}$  with nonzero entries  $\sigma_1, \ldots, \sigma_r$ , such that

$$M = U\Sigma V^{\top}.$$

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# Key Ideas of the Proof

- ullet  $M^{\top}M$  is symmetric  $\Rightarrow$  diagonalizable with orthonormal eigenvectors.
- If  $M^{\top}M\mathbf{v}_i = \lambda_i\mathbf{v}_i$ , define singular values  $\sigma_i = \sqrt{\lambda_i}$ .
- Construct  $\mathbf{q}_i = \frac{1}{\sigma_i} M \mathbf{v}_i$ ; these vectors are orthonormal in  $\mathbb{R}^m$ .
- Collect  $\{q_i\}$  as columns of U,  $\{v_i\}$  as columns of V.
- Then  $U^{\top}MV = \Sigma$ , hence  $M = U\Sigma V^{\top}$ .

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- Then  $U^{\top}MV = \Sigma$ , hence  $M = U\Sigma V^{\top}$ .

## Interpretation

SVD generalizes diagonalization to non-square matrices. It expresses any matrix as:

(orthogonal change of basis)  $\times$  (scaling)  $\times$  (orthogonal change of basis).

SVD: Examples and Exercises I

Example: Computing an SVD

Compute the Singular Value Decomposition of

$$M = \begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 2 & 0 \end{bmatrix}.$$

(Hint: start with  $M^{T}M$  and find eigenvalues/eigenvectors.)

Exercise: Verification and Rank-One Approximation

Check that indeed  $M = U \Sigma V^{T}$ . What is the best rank-one approximation of M?

Example: Decomposition into Rank-One Matrices

Write

$$M = \mathbf{u}_1 \sigma_1 \mathbf{v}_1^{\top} + \cdots + \mathbf{u}_r \sigma_r \mathbf{v}_r^{\top},$$

and interpret this as a decomposition into rank-one matrices. Discuss its use in applications such as image compression.

Exercise: Least Squares via SVD

Show that least squares approximation is an instance of SVD: minimizing  $\| Mx - b \|$  reduces to

$$\mathbf{y} = \mathbf{V}^{\mathsf{T}} \mathbf{x} = \frac{1}{\Sigma} \mathbf{U}^{\mathsf{T}} \mathbf{b}.$$