ESQC 2026

Mathematical Methods Lecture 1

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Material for mathematics course

- Lecture notes
- Exercise book
- Roadmap
- Slides
- Where to find it:
  - https://simenkva.github.io/esqc_math

Introduction

Why learn mathematics?

- Quantum chemistry requires mathematics
- From applications of DFT …
- … to invention of new methods
- Mathematics is the language of science
- Mathematics is *fun and useful*

Mathematics, you see, is not a spectator sport. To understand mathematics means to be able to do mathematics.

(From “How To Solve It”)

George Pólya (1887–1985)
Hungarian-American mathematician

Mathematics at ESQC

- One cannot *teach* mathematics in 5 hours
  - We can give an overview
  - Inspiration
- One cannot *learn* mathematics in 5 hours
  - Soak up the inspiration!
  - Do not despair – exercise!
- Exercises:
  - The math exercises are *today!*
  - Exercises focus on important topics

Real and complex numbers

What we work with every day

Real numbers

$$\mathbb{R} = \{\text{all infinite decimal expansions}\}$$

The real numbers form a *complete ordered field:*

- **Field**: Closed under addition and multiplication, and
- every number except 0 has a **multiplicative inverse**
- **Ordered**: We always have $a \leqslant b$ or $b \leqslant a$
- **Completeness**: Cauchy sequences converge to numbers in $\mathbb{R}$

Complex numbers

$$\mathbb{C} = \{\, x + \mathrm{i}y \mid x, y \in \mathbb{R} \,\}, \qquad \mathrm{i}^2 = -1$$

- An *algebraic extension* of reals
- For $z = x + \mathrm{i}\,y$:

$$\operatorname{Re} z = x, \qquad \operatorname{Im} z = y$$

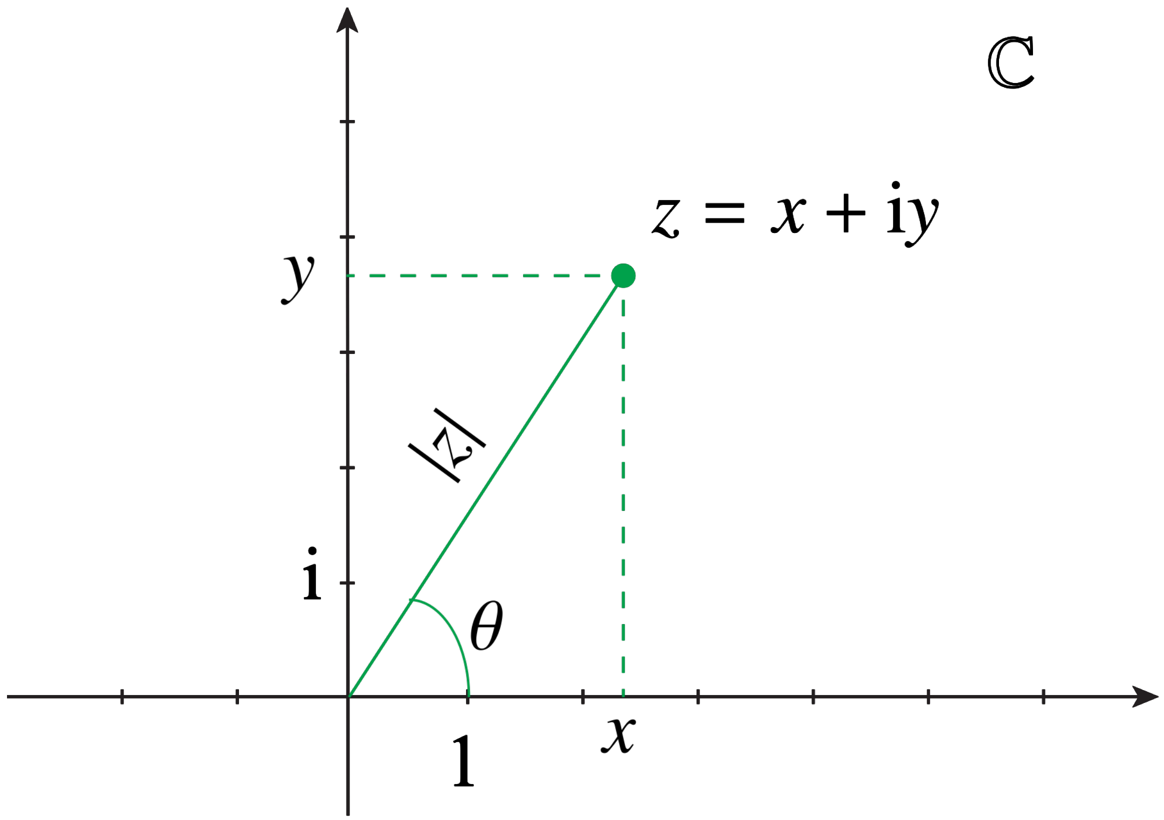
$$\bar{z} = x - \mathrm{i}y$$

$$|z|^2 = \bar{z}z = (\operatorname{Re} z)^2 + (\operatorname{Im} z)^2$$

These numbers have no use, they are *imaginary*

René Descartes (1596–1650)

Geometric interpretation



- Discovered by the Norwegian mathematician and cartographer Caspar Wessel (1797)
- Multiplication rule:

$$w = z_1 z_2, \quad |w| = |z_1| \cdot |z_2|$$

$$\theta_w = \theta_1 + \theta_2$$

Fundamental theorem of algebra

Theorem : Fundamental theorem of algebra

Every polynomial p of degree n over $\mathbb{C}$ have exactly n roots in $\mathbb{C}$, i.e., there is a nonzero $C \in \mathbb{C}$ and n numbers $r_i \in \mathbb{C}$, such that

$$p(z) = C(z - r_1)(z - r_2)\cdots(z - r_n).$$

The complex numbers are a field like the reals, but we can «do more stuff» with complex numbers

An introduction to linear algebra

Perhaps the most important mathematical tool in science

1. Liner algebra in 2D

Points in the plane

- We start by considering points in the plane

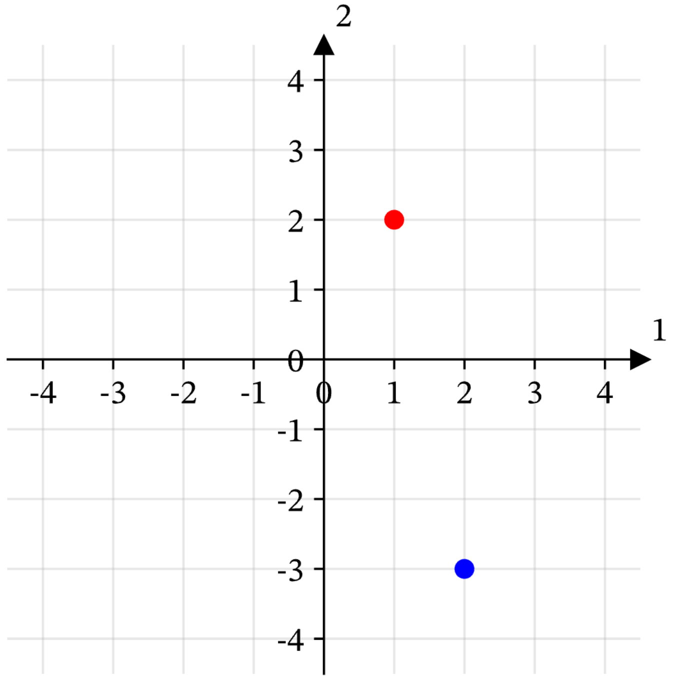
$$\mathbf{p} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \qquad \mathbf{q} = \begin{bmatrix} 2 \\ -3 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- We can **add** two points

$$\mathbf{p} + \mathbf{q} = \begin{bmatrix} 1+2 \\ 2-3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \end{bmatrix} \qquad \mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \end{bmatrix}$$

- We can also **scale** a point

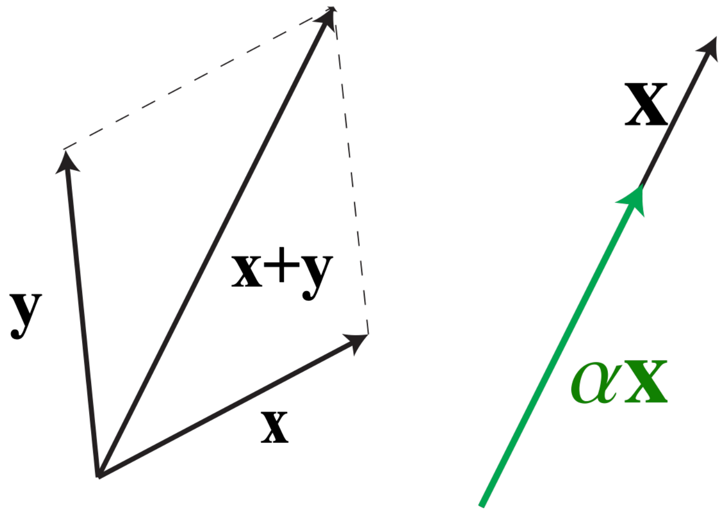
$$7\mathbf{p} = \begin{bmatrix} 7 \cdot 1 \\ 7 \cdot 2 \end{bmatrix} = \begin{bmatrix} 7 \\ 14 \end{bmatrix} \qquad \alpha\mathbf{x} = \begin{bmatrix} \alpha x_1 \\ \alpha x_2 \end{bmatrix}$$



Points as arrows: Vectors

- We visualize a point as an **arrow from the origin**
- **Adding and scaling become geometric operations**
- Points/vectors in the plane form
  a 2D vector space:

$$\mathbb{R}^2$$



Inner product and norm

- Every arrow has a length: **norm**
- Two arrows span an **angle**
- Norm and angle comes from **Euclidean inner product**

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x} \cdot \mathbf{y} = x_1 y_1 + x_2 y_2 \qquad ||x|| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} \qquad \cos\theta = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{||\mathbf{x}||||\mathbf{y}||}$$

- We obtain a **Hilbert space** $(\mathbb{R}^2, \langle \cdot, \cdot \rangle)$

- **Demo:** `lecture-1-plane-geometry.ipynb`

Linear transformations in the plane

- An important class of transformations is **linear transformations**
- **Intuition:** straight lines go to straight lines (or to points)
- Computational machinery: **matrix algebra**

$$\mathbf{y} = \mathbf{A}\mathbf{x} \qquad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \underbrace{\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}}_{\mathbf{A}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 \\ A_{21}x_1 + A_{22}x_2 \end{bmatrix}$$

Example of **matrix vector product**

- **Demo:** `lecture-1-plane-transformation.ipynb`

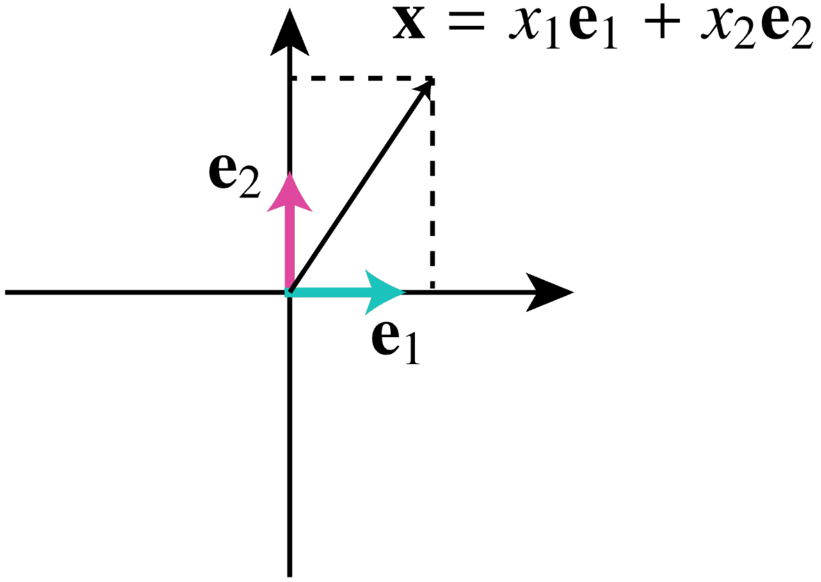
Linear transformations are extremely important in quantum chemistry

The standard basis

- A **basis** is a set of vectors in which **all vectors can be expanded**
- Here is the **standard basis:**

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} 4 \\ 5 \end{bmatrix} = 4\mathbf{e}_1 + 5\mathbf{e}_2$$



- **There are infinitely many bases!**

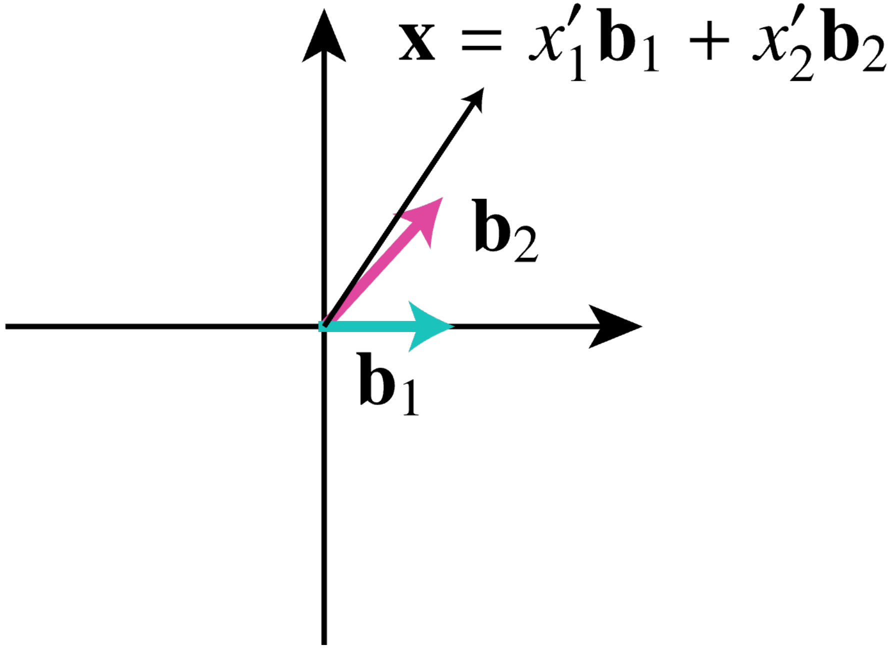
Other bases

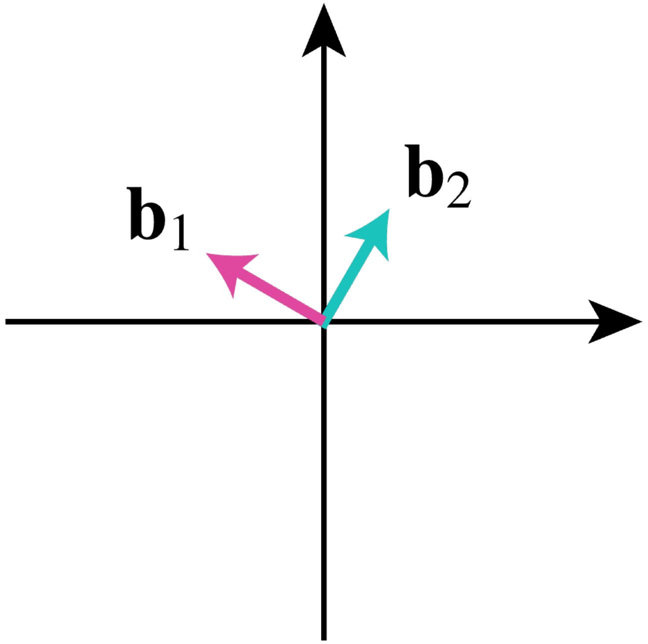
- Example:

$$\mathbf{b}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbf{b}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- **Othonormal bases** have orthogonal vectors that have unit norm:

$$||\mathbf{b}_1|| = ||\mathbf{b}_2|| = 1 \quad \langle \mathbf{b}_1, \mathbf{b}_2 \rangle = 0$$





Eigenvalue problem

- Given a matrix A, an important problem is:

  Find $\mathbf{x}$ and λ such that:

Eigenvalue

$$A\mathbf{x} = \lambda\mathbf{x}$$

Eigenvector

- **Interpretation:** The action of an otherwise stretching, rotating, reflecting operation - on $\mathbf{x}$ it is **just a scaling**
- Sometimes, one can find a **basis of eigenvectors**

$$A\mathbf{x}_1 = \lambda_1\mathbf{x}_1, \quad A\mathbf{x}_2 = \lambda_2\mathbf{x}_2$$

  - We like this because **in a basis of eigenvectors A is really simple!**

2. Higher dimensions

Higher dimensions

- Nothing special about 2 dimensions (easy to visualize, though)
- Vectors in **any dimension** are defined similarly

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n \qquad \mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ x_3 + y_3 \\ \vdots \\ x_n + y_n \end{bmatrix} \qquad \alpha\mathbf{x} = \begin{bmatrix} \alpha x_1 \\ \alpha x_2 \\ \alpha x_3 \\ \vdots \\ \alpha x_n \end{bmatrix}$$

- **Complex vectors** are also common

$\mathbb{F}$ means $\mathbb{R}$ or $\mathbb{C}$

Basis in higher dimensions

- A basis in *n* dimensions:

$$\mathbf{b}_1, \quad \mathbf{b}_2, \quad \mathbf{b}_3, \; \cdots, \quad \mathbf{b}_n$$

- Can expand **any vector:**

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

- An **orthonormal basis** is an *n-dimensional* axis cross:

$$||\mathbf{b}_1|| = ||\mathbf{b}_2|| = \ldots = ||\mathbf{b}_n|| = 1 \qquad \langle \mathbf{b}_1, \mathbf{b}_2 \rangle = \langle \mathbf{b}_1, \mathbf{b}_3 \rangle = \ldots = 0$$

Linear transformations in higher dimensions

- A **linear transformation** is a function between vector spaces:

$$A : \mathbb{F}^n \to \mathbb{F}^m$$

- Linear transformations **preserve scalar multiplication and addition:**

$$A(\alpha \mathbf{x}) = \alpha(A\mathbf{x}) \qquad A(\mathbf{x} + \mathbf{y}) = (A\mathbf{x}) + (A\mathbf{y})$$

- Essentially the same as in 2D - just harder to visualize

Demo: blurring an image

- We show an example of a linear transformation
- Very high dimension, yet visual ...

- **Demo:** `lecture-1-blurring.ipynb`

Matrices

- A **matrix** is a table of numbers

rows

cols

$$A \in \mathbb{F}^{m \times n} = M(m, n; \mathbb{F})$$

$$m\left\{\vphantom{\begin{bmatrix} A_{11} \\ A_{21} \\ \vdots \\ A_{m1} \end{bmatrix}}\right. A = \overbrace{\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}}^{n}$$

- Vectors are also matrices!

$$\mathbf{x} \in \mathbb{F}^{n} = \mathbb{F}^{n \times 1} = M(n, 1; \mathbb{F})$$

The matrix-vector product

- A matrix and a vector can be **multiplied together**

$$A \in M(m, n, \mathbb{F}) \qquad \mathbf{x} \in \mathbb{F}^n \qquad A\mathbf{x} \in \mathbb{F}^m$$

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \qquad (A\mathbf{x})_i = \sum_{j=1}^{n} A_{ij} x_j$$

Matrices = linear transformations

- The matrix-vector product **is linear**
- Therefore it defines a linear transformation (from n to m dimensions)
- Conversely, any linear transformation can be written as a matrix-vector product
- **A powerful result!**

Matrix-matrix product

- Suppose we have two matrices A and B

$$\mathbf{y} = A\mathbf{x} \quad \text{linear transformation}$$

$$\mathbf{z} = B\mathbf{y} \quad \text{linear transformation}$$

$$\mathbf{z} = B(A\mathbf{x}) \quad \text{also linear transformation}$$

$$\text{must have: } B(A\mathbf{x}) = C\mathbf{x}$$

- Leads to **matrix-matrix product** $C = AB$

Computing the matrix product

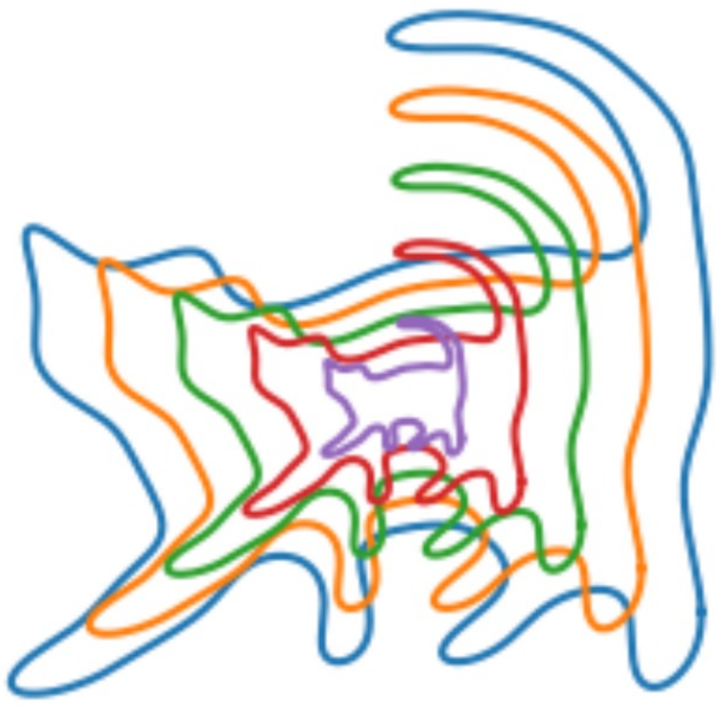
$$AB = C \qquad C_{ij} = \sum_k A_{ik} B_{kj}$$

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1o} \\ B_{21} & B_{22} & \cdots & B_{2o} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{no} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1o} \\ C_{21} & C_{22} & \cdots & C_{2o} \\ \vdots & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \cdots & C_{mo} \end{bmatrix}$$

Note: $A \times$ a column of B = a column of C

Eamples of linear transformations in 2D

- **Demo:** `lecture 1 – transforming a cat.ipynb`



Matrix multiplication is not commutative

- When multiplying real or complex numbers:

$$xy = yx$$

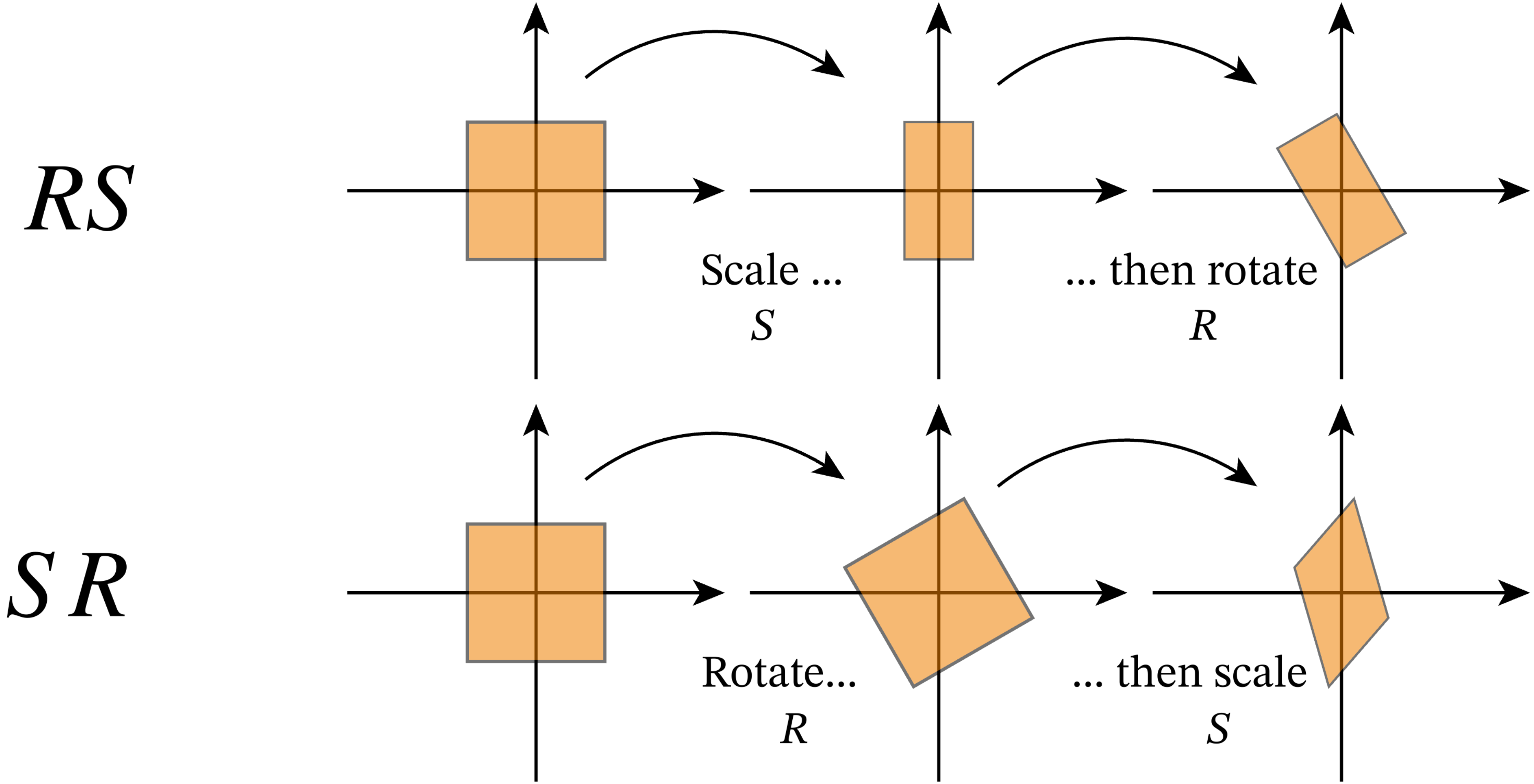
Scalar multiplication is «commutative»

- When multiplying **matrices:**

$$\text{in general } AB \neq BA$$

Matrix multiplication is «non-commutative»

Example



The matrix zoo

- Matrices contain a lot of information!
- Can we tame that information?
- Usually, we are interested in special problems:
  - **Define important classes of matrices with common properties**
- For a given matrix, try to say as much as possible about it
  - **Study decompositions of matrices in terms of simpler matrices**

Important matrix operations

- *Transpose:*

$$(A^T)_{ij} = A_{ji} \qquad \begin{bmatrix} 0 & 1 \\ \mathrm{i} & 2 \\ 0 & -1 \end{bmatrix}^T = \begin{bmatrix} 0 & \mathrm{i} & 0 \\ 1 & 2 & -1 \end{bmatrix}$$

- *Hermitian adjoint:*

$$(A^H)_{ij} = \overline{A_{ji}} \qquad \begin{bmatrix} 0 & 1 \\ \mathrm{i} & 2 \\ 0 & -1 \end{bmatrix}^H = \begin{bmatrix} 0 & -\mathrm{i} & 0 \\ 1 & 2 & -1 \end{bmatrix}$$

- *Application: Inner product as matrix product:*

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^H \mathbf{y} \qquad \begin{bmatrix} \cdots & \mathbf{x}^H & \cdots \end{bmatrix} \begin{bmatrix} \vdots \\ \mathbf{y} \\ \vdots \end{bmatrix}$$

Class 1: Symmetric matrices

- Square matrices that are their own **transpose**

$$A = A^T \quad \Longleftrightarrow \quad A_{ij} = A_{ji}$$

$$A = \begin{bmatrix} 0 & 2 \\ 2 & -1 \end{bmatrix} \quad \text{is symmetric}$$

$$B = \begin{bmatrix} 0 & 2 \\ -2 & -1 \end{bmatrix} \quad \text{is not symmetric}$$

Class 2: Hermitian matrices (complex)

- Square matrices that are their own **conjugate transpose**

$$A = A^H \quad \Longleftrightarrow \quad A_{ij} = A^*_{ji}$$

$$A = \begin{bmatrix} 0 & 2 \\ 2 & -1 \end{bmatrix} \quad \text{is Hermitian and symmetric}$$

$$B = \begin{bmatrix} 0 & 2\mathrm{i} \\ -2\mathrm{i} & -1 \end{bmatrix} \quad \text{is Hermitian but not symmetric}$$

Class 3: Unitary/orthogonal matrices

- Matrices that **preserve orthogonality of vectors**
- Real matrices: «orthogonal»
- Complex matrices: «unitary»
- **Example:**
  - rotations preserve angles, and their matrices are orthogonal

- (There are many more classes of matrices)

End of lecture 1

- That’s it for today!

- Tutorial:
  - Bring laptop or mobile device to read the exercise book
  - Additional content for other tutorials the rest of the week: optional math exercises