ESQC 2024

Mathematical Methods Lecture 1

By Simen Kvaal

Where to find the material

SCAN ME

- Alternative 1:
  - www.esqc.org, go to“lectures”
  - Find links there
- Alternative 2:
  - Scan QR code
  - simenkva.github.io/esqc_material

About these lectures

What to expect

Why learn mathematics?

- Quantum chemistry requires mathematics
- From applications of DFT …
- … to invention of new methods
- 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”)

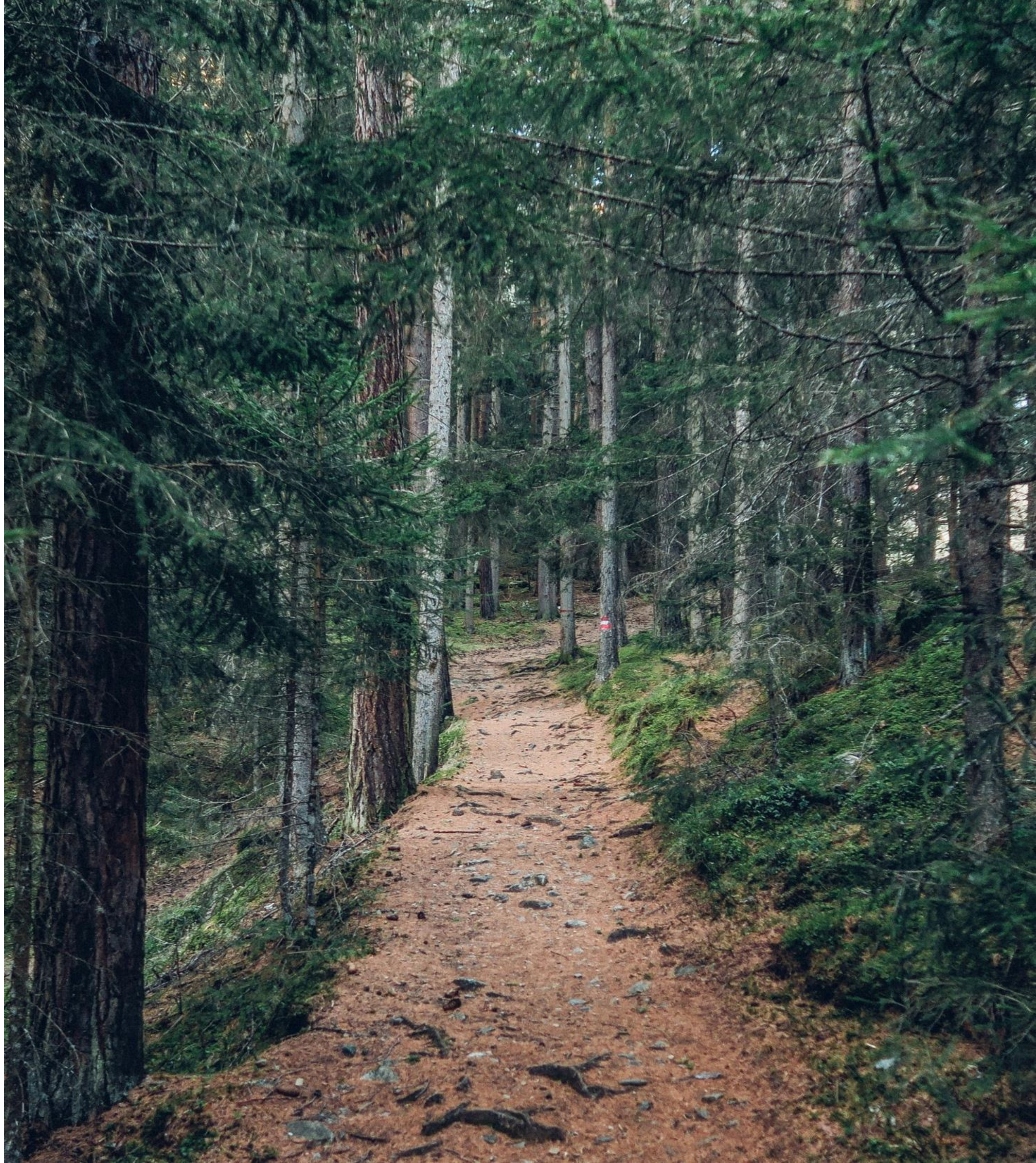
George Pólya (1887–1985)
Hungarian-American mathematician

Idea behind lectures

- One cannot *teach* mathematics in 5 hours
  - Overview
  - Inspiration
- One cannot *learn* mathematics in 5 hours
  - Needs practice
  - Get a feeling for concepts
  - Learn where to look
- Exercises:
  - The math exercises are *today!*
  - Use the lecture notes when needed

A mathematical roadmap

- How are mathematical topics connected?
- Which topics are useful for quantum chemists?
- Feedback welcome!



A look at the roadmap

- We look at the web browser
- https://simenkva.github.io/esqc_material

At the core: Logic and set theory

All of mathematics can be built using sets

Naïve set theory

- In our lectures, like in most mathematics, we will use *naïve set theory*
- Sets are specified as:
  - List of elements

$$C = \{\text{Romeo}, \text{Pallina}, \text{Micio}, \text{Luna}\} \subset \{\text{Italian cats}\} \subset \{\text{all cats}\}$$

  - Conditions on other sets

$$\{n \in \mathbb{N} \mid n \text{ is even}\}$$

  - Words, descriptions, but be careful!

“cat” is slang for jazz musicians

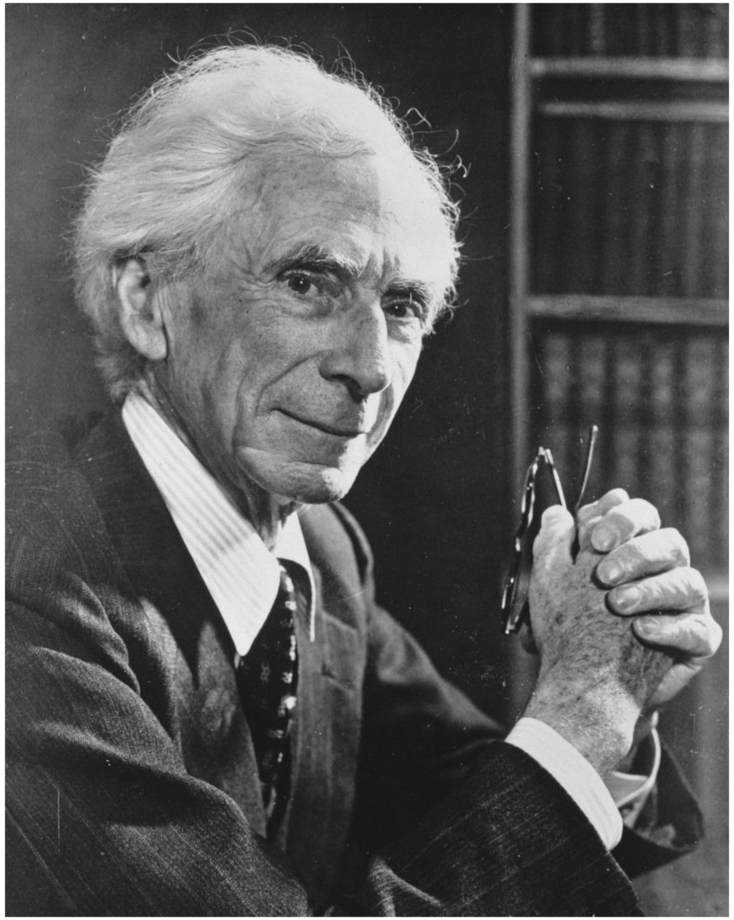
Russell’s paradox (next slide)

Russell’s paradox (1902)

- In a town, there is a hairdresser who cuts the hair of everyone who does not cut their own hair.

- Does the hairdresser cut their own hair?

$$A = \{x \mid x \notin x\}$$



Bertrand Russell in 1957 (from Wikipedia)

More set operations

- Union of two sets:

$$A \cup B = \{x \mid x \in A \text{ or } x \in B\}$$

- Intersection of two sets:

$$A \cap B = \{x \mid x \in A \text{ and } x \in B\}$$

- Set difference/relative complement:

$$A \setminus B = \{x \in A \mid x \notin B\}$$

- Cartesian product:

$$A \times B = \{(a, b) \mid A \in A,\ b \in B\}$$

Zermelo-Fraenkel set theory with axiom of choice (ZFC)

- Consistent and powerful foundation for mathematics
- Almost all of mathematics can be built with ZFC
  - Some people take unconventional stances, hence ”almost all”
- Example: von Neumann’s construction of natural numbers:

$$0 = \emptyset, \quad 1 = \{\emptyset\}, \quad 2 = \{\emptyset, \{\emptyset\}\}, \ldots$$

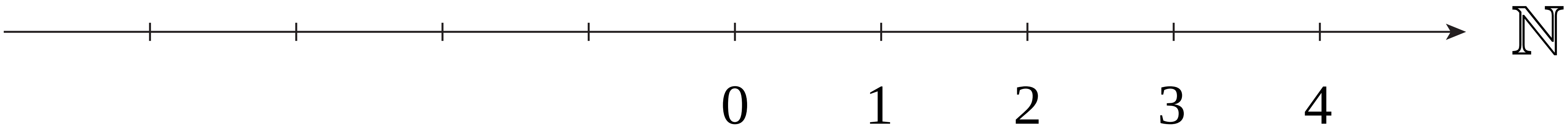
$$n + 1 = n \cup \{n\}$$

Number systems

Foundation for large areas of mathematics

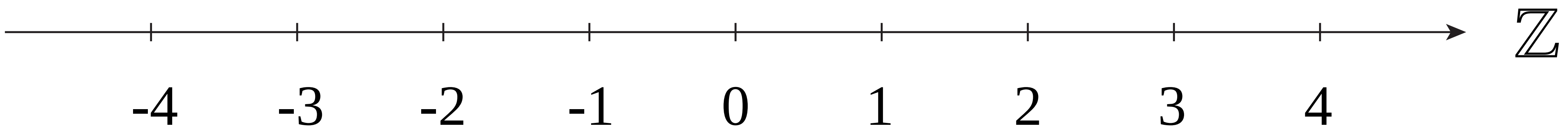
Natural numbers

$$\mathbb{N} = \{0, 1, 2, 3, \ldots\}$$



Integers

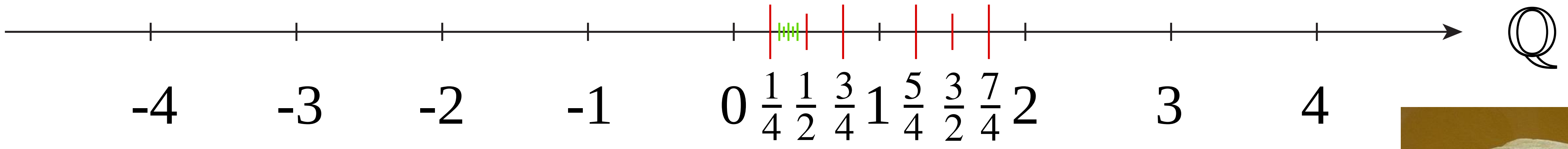
$$\mathbb{Z} = \{\ldots -3, -2, 1, 0, 1, 2, 3, \ldots\}$$

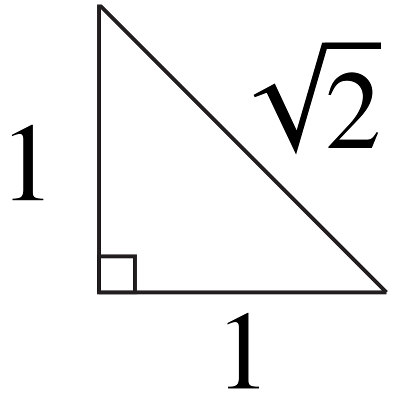


- First occurs in Chinese mathematics <300 AD (Han Period or before)
- Called "absurd numbers" in Europe until 16th century!
- In Europe, first satisfactory account by Cardano (1545)

Rational numbers

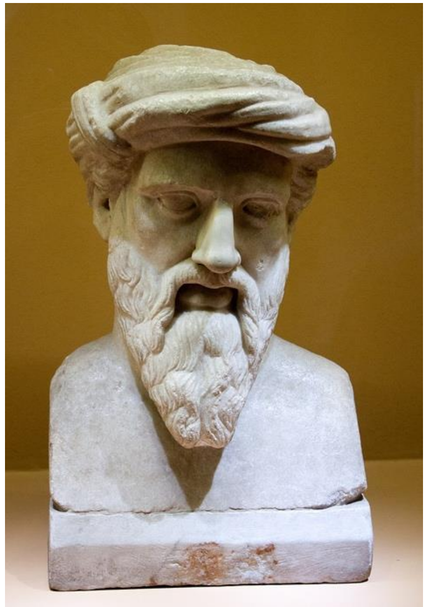
$$\mathbb{Q} = \left\{ \frac{p}{q} \mid p, q \in \mathbb{Z},\ \ q > 0 \right\}$$





Pythagoras of Samos

To the Pythagorean school, ”everything is number”. And by number, they meant *rational* number.



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: Every Cauchy sequence converges to a number in $\mathbb{R}$

There are *much more real numbers* than natural numbers

Complex numbers

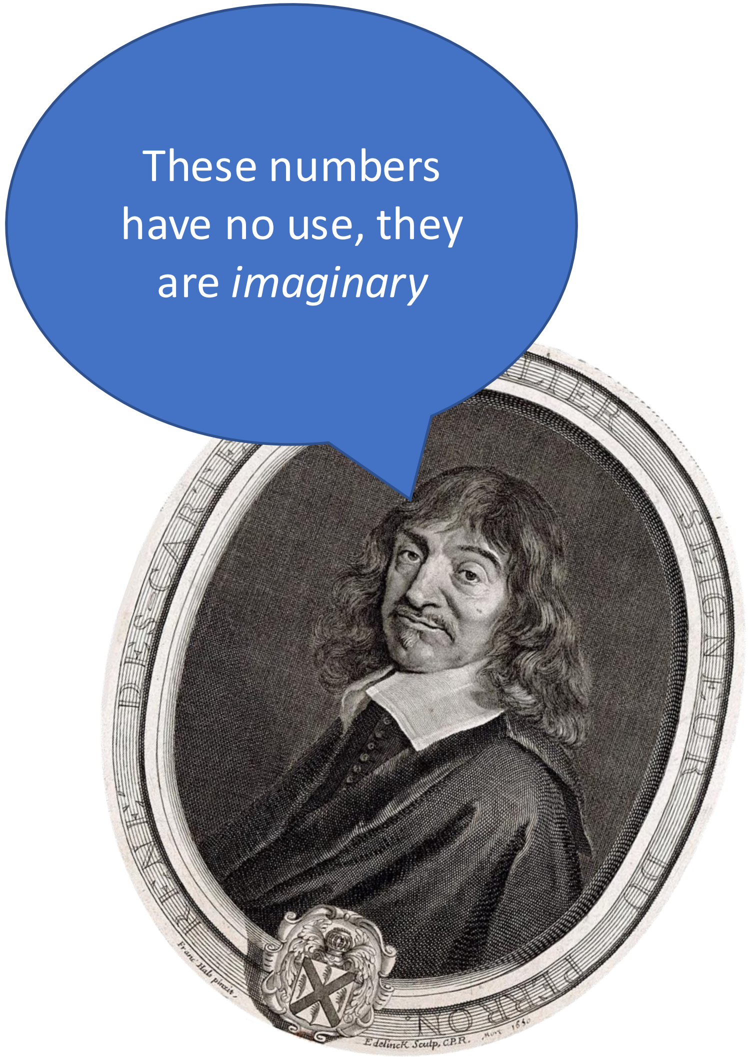
$$\mathbb{C} = \{\, x + \mathrm{i}y \;|\; x, y \in \mathbb{R} \,\},$$

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

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

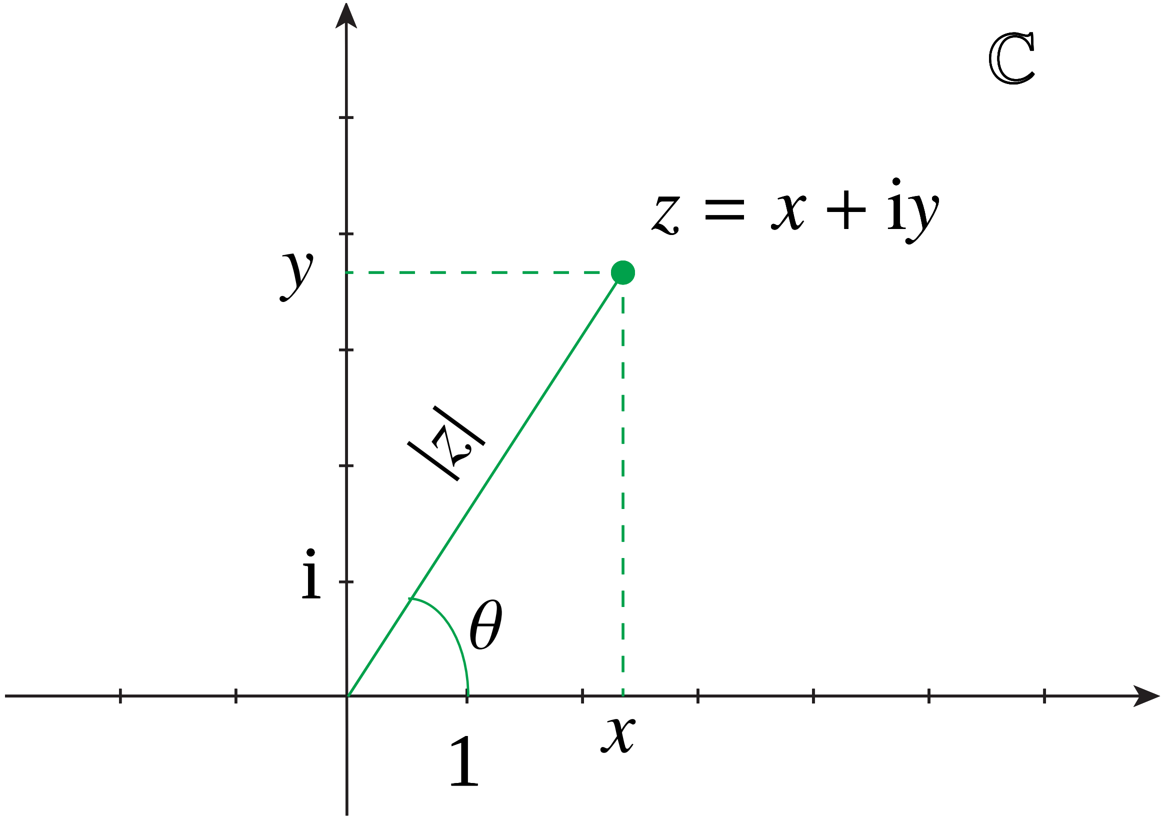
$$\bar{z} = x - \mathrm{i}y$$

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



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

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

Euclidean space

The foundation of physics

Tuples of real or complex numbers

$$(x, y) \in \mathbb{R}^2, \quad x, y \in \mathbb{R}$$

$$(x, y, z) \in \mathbb{R}^3, \quad x, y$$

$$(x_1, x_2, \cdots ,$$

$$(z_1, z_2, \cdots , z_n$$

Time evolution, magnetic fields require complex numbers!

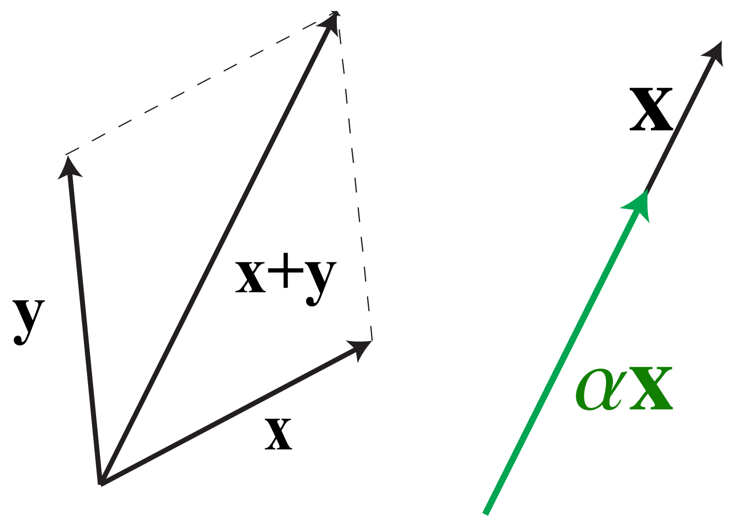
$\mathbb{F}$ either $\mathbb{R}$ or $\mathbb{C}$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

All the variables of a quantum chemical method

Vectors

- By elementwise addition and scalar multiplication, we obtain a *vector space*
- By introducing an *inner product* we obtain an *inner product space* – *Euclidean space*



Definition : Euclidean space

Let $\mathbb{F}$ be either $\mathbb{R}$ or $\mathbb{C}$. Let $\mathbb{F}^n$ be the set of n-tuples of $\mathbb{F}$-numbers $\mathbf{x} = (x_1, \cdots, x_n)$, on which we define the following operations: For $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$ define

$$\mathbf{x} + \mathbf{y} \in \mathbb{F}^n, \quad (\mathbf{x} + \mathbf{y})_i = x_i + y_i \qquad \textbf{\textit{addition}}, \tag{1}$$

for all $1 \leq i \leq n$. and for any $\alpha \in \mathbb{F}$,

$$\alpha\mathbf{x} \in \mathbb{F}^n, \quad (\alpha\mathbf{x})_i = \alpha x_i \qquad \textbf{\textit{scalar multiplication}}. \tag{2}$$

We also define the Euclidean *inner prooduct*

$$\langle \mathbf{x}, \mathbf{y} \rangle = \bar{\mathbf{x}} \cdot \mathbf{y} = \sum_i \bar{x}_i y_i \in \mathbb{F} \qquad \textbf{\textit{Euclidean inner product}} \tag{3}$$

and the Euclidean norm

$$||\mathbf{y}|| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} \in \mathbb{R}. \qquad \textbf{\textit{Euclidean norm}} \tag{4}$$

Definition : Standard basis

The *standard basis* for $\mathbb{F}^n$ is the set of vectors $\{\mathbf{e}_i \mid 1 \leq i \leq n\}$ such that

$$(\mathbf{e}_i)_j = \delta_{ij}, \qquad \textit{Kronecker delta symbol} \tag{1}$$

i.e.,

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \quad \text{etc.} \tag{2}$$

It now follows that for every $\mathbf{x} \in \mathbb{F}^n$,

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i. \tag{3}$$

It is easy to see, that

$$x_i = \langle \mathbf{e}_i, \mathbf{x} \rangle . \tag{4}$$

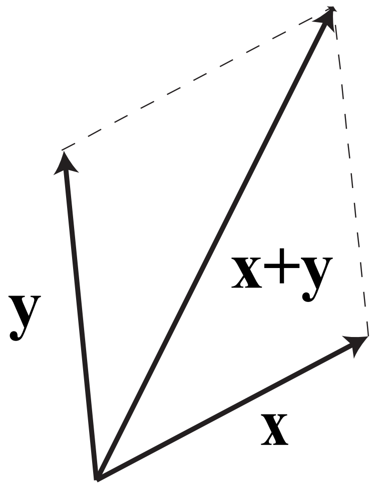
Example: inner product with std basis

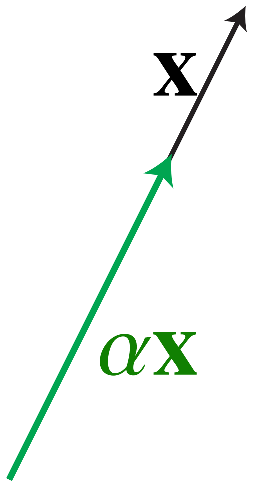
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\langle \mathbf{e}_2, \mathbf{x} \rangle = \mathbf{e}_2 \cdot \mathbf{x} = 0 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3 = x_2$$

Example: scalar multiplication and addition

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad \alpha\mathbf{x} = \begin{bmatrix} \alpha x_1 \\ \alpha x_2 \end{bmatrix}$$





$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \end{bmatrix}$$

Linear transformation

Definition 4: Linear transformation

Let $A : \mathbb{F}^n \to \mathbb{F}^m$ be a function. We say that A is a *linear transformation* if it conserves the vector addition and scalar multiplication laws, i.e., for all $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$

$$A(\mathbf{x} + \mathbf{y}) = A(\mathbf{x}) + A(\mathbf{y}), \tag{2.11}$$

and for all $\alpha \in \mathbb{F}$,

$$A(\alpha\mathbf{x}) = \alpha A(\mathbf{x}). \tag{2.12}$$

If a $n = m$, i.e., the special case when domain and codomain both are the same space, we often say that A is a *linear operator*

Examples

- Rotations
- Reflections
- Scaling along some axis
- Any combination of linear operations!

Linear transformations and matrices

- A linear transformation is *determined by a matrix and vice versa*

$$A(\mathbf{x})_i = \sum_{j=1}^{n} A_{ij} x_j$$

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}$$

$$A(\mathbf{x}) = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

End of lecture 1

- That’s it for today!