ESQC Mathematics Lecture 1

By Simen Kvaal

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*

About these lectures

- One cannot *teach* mathematics in 5 hours
    - Give a refresher
    - Good resources
    - Overview of material that is relevant
    - Inspiration to learning mathematics back home
- One cannot *learn* mathematics in 5 hours
    - One can get a feeling for concepts, how they are connected
    - Learn where to look for information when needed later
- Exercises:
    - The math exercises are *today!*
    - Use the lecture notes when needed

Where to find the material

- All lectures (slides) and lecture notes available from Dropbox folder
- Lectures also on esqc.org
- https://www.dropbox.com/sh/g1939ggypzpu4nu/AAD7JruTlirzUndzWcQvDxoNa
- Updated all the time

What *is* mathematics?

Or, what I think it is

Quote from Wikipedia

- **Mathematics** (from Ancient Greek μαθημα; máthēma: ‘knowledge, study, learning’) is an area of knowledge that includes such topics as numbers (**arithmetic and number theory**), formulas and related structures (**algebra**), shapes and the spaces in which they are contained (**geometry**), and quantities and their changes (**calculus and analysis**). Most mathematical activity involves the use of **pure reason to discover or prove** the properties of abstract objects, which consist of either abstractions from nature or—in modern mathematics—entities that are stipulated with certain properties, called **axioms**. A mathematical **proof** consists of a succession of applications of some deductive rules to already known results, including previously proved theorems, axioms and (in case of abstraction from nature) some basic properties that are considered as true starting points of the theory under consideration.

https://en.wikipedia.org/w/index.php?title=Mathematics

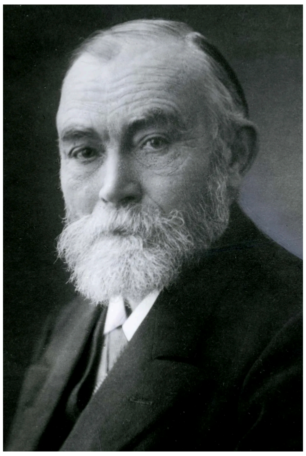
The language of science

- Models to describe outcomes of experiment
- Mathematics is the language of these models
- Example: The postulates of quantum mechanics
- Isn’t it strange, that mathematics can accurately describe nature?
- Mathematics today is based in logic
- Logic: self-evident, “not derivable”, we strongly *believe* it describes reality

The foundational crisis of mathematics

- Prior to the 20th century, mathematics was kind of *disconnected.*
- *Example:* The integers described with the Peano axioms. But there was no description of the integers based on some "fundamental mathematics"
- A common foundation for mathematics was sought
- Many schools of thought
- Gottlob Frege's *logicism*:
- Axiom of *schema of comprehension:*

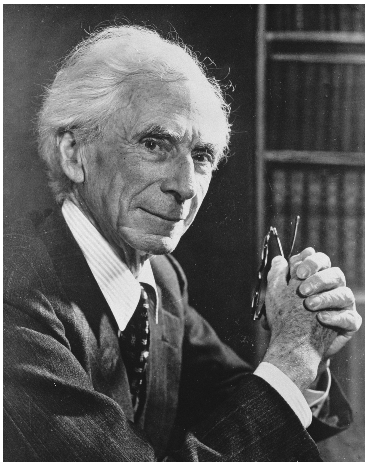
  If φ is a property, then there exists a set $Y = \{X \mid \varphi(X)\}$
- *This is false!*



Gottlob Frege (1848–1925)

Russell's paradox (1902)

By a set, we mean any collection of objects — for example the set of all even integers or the set of all saxophone players in Brooklyn. The objects that make up a set are called its members or elements. Sets may themselves be members of sets; for example the set of all sets of integers has sets as its members. Most sets are not members of themselves; the set of cats, for example, is not a member of itself because the set of cats is not a cat. However, there may be sets that do not belong to themselves— perhaps, for example, a set containing all sets. Now, consider the set A of all those sets X such that X is not a member of X. Clearly, by definition, A is a member of A if and only if A is not a member of A. So, if A is a member of A, then A is also not a member of A; and if A is not a member of A, then A is a member of A. In any case, A is a member of A and A is not a member of A.



Bertrand Russell in 1957 (from Wikipedia)

Today

- Crisis is settled (mostly)
- Most common foundation taken to be Zermelo—Fraenkel set theory (ZF) with axiom of choice (ZFC)
- But there are also others. Not all equivalent.
- ZF: ”Predicate logic with binary relation ∈ for set membership”
- Example: Natural numbers as sets (von Neumann)
- Model of *Peano axioms for natural numbers*

Natural numbers

- Zero is the empty set

$$0 := \{\,\} = \emptyset$$

- We are allowed to take unions of sets, so n+1 is defined as

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

- This gives

$$0 := \emptyset, \quad 1 := \{\emptyset\}, \quad 2 := \{\emptyset, \{\emptyset\}\}$$
$$3 := \{\emptyset, \{\emptyset\}, \{\emptyset, \{\emptyset\}\}\} \quad \ldots$$

- The natural numbers $\mathbb{N}$ is defined as the smallest set closed under ”addition of 1” that contains all n

Now for the mathematics

Set theory and functions

Naïve set theory

- In our lectures, like in most mathematics, we will use *naïve set theory*
- Sets are specified as
  - List of elements
    $C = \{\text{Romeo, Pallina, Micio, Luna}\} \subset \{\text{Italian cats}\} \subset \{\text{all cats}\}$
  - Conditions on other sets
    $$\{n \in \mathbb{N} \mid n \text{ is even}\}$$
  - Words, descriptions, but be careful!

    "cat" is slang for jazz musician
- Cartesian product
  $$A \times B = \{(a, b) \mid A \in A,\ b \in B\}$$

More set operations

- Union of two sets:

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

- Intersection of two sets:

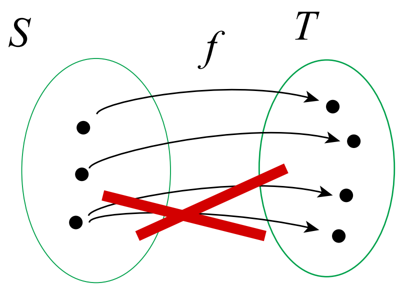
$$A \cap B = \{x \mid x \in A \text{ and } x \in B\}$$

- Set difference/relative complement:

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

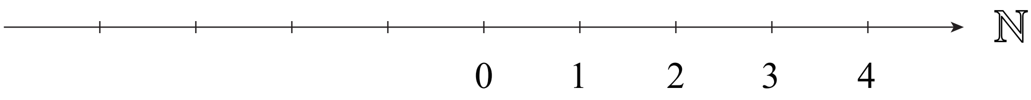
Functions

- Given two sets S *(domain)* and T *(codomain)*
- A function $f : S \to T$ is a rule, that to every $s \in S$ *assigns a unique* $t \in T$, written $t = f(s)$
- Domain: Possible input
- Codomain: Possible output
- Range: Set of actual outputs
- *Surjective*/onto: all of T is reached
- *Injective*/one-to-one: Only one s maps to a given t
- *Bijective:* Surjective and injective



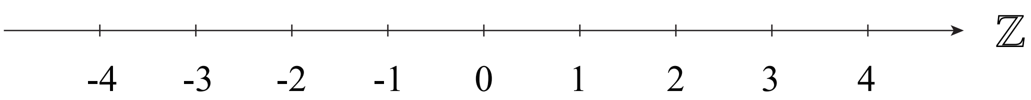
Natural numbers

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



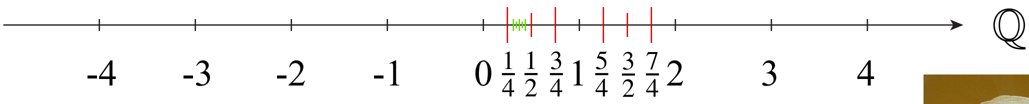
Integers

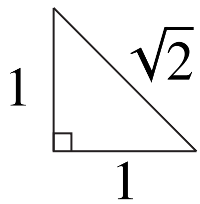
$$\mathbb{Z} = \{\ldots - 3, -2, 1, 0, 1, 2, 3, \ldots\}$$



Rational numbers

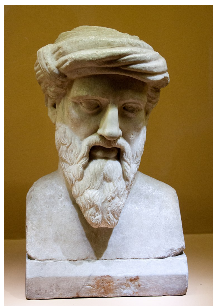
$$\mathbb{Q} = \left\{ \frac{p}{q} \mid p, q \in \mathbb{Z},\ q > 0 \right\}$$





Pythagoras of Samos

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



Real numbers

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

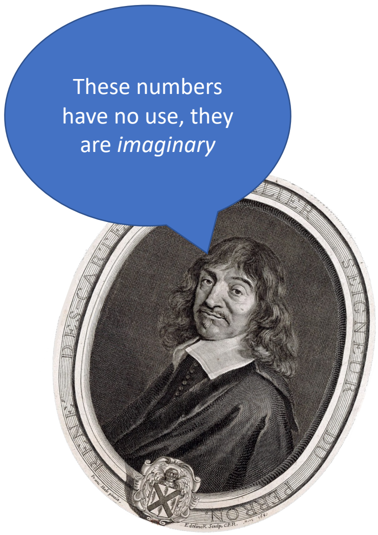
The real numbers form a *complete ordered field:*

- 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

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

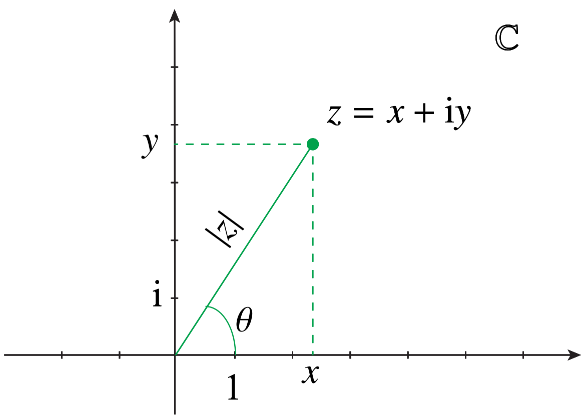


René Descartes (1596–1650)

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

$$\operatorname{Re} z = x, \qquad \operatorname{Im} z = y$$
$$\bar{z} = x - \mathrm{i}y$$
$$|z|^2 = \bar{z}z = (\operatorname{Re} z)^2 + (\operatorname{Im} z)^2$$

Geometric interpretation



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

$$w = z_1 z_2, \qquad |w| = |z_1| \cdot |z_2|$$
$$\theta_w = \theta_1 + \theta_2$$

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

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

Recommendations

- YouTube channel of Michael Penn
- YouTube channel *Bright Side of Mathematics*
- See the Lecture Notes for links and textbook recommendations

Euclidean space

Vectors and matrices

Tuples of real or complex numbers

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

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

$(x_1, x_2, \cdots,$

$(z_1, z_2, \cdots, z_n$

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

Time evolution, magnetic fields require complex numbers!

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

All the variables of a quantum chemical method

The Schrödinger equation

$$H\mathbf{x} = E\mathbf{x}$$

Matrix eigen value equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

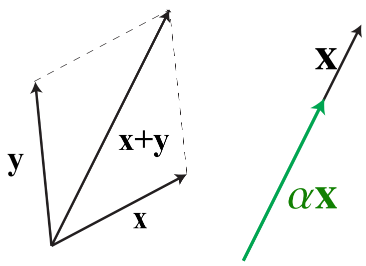
Bra-ket notation

$$\mathrm{i}\frac{\partial}{\partial t}\,|\psi\rangle = \hat{H}\,|\psi\rangle$$

Time-dependent Schrödinger eq.

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

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

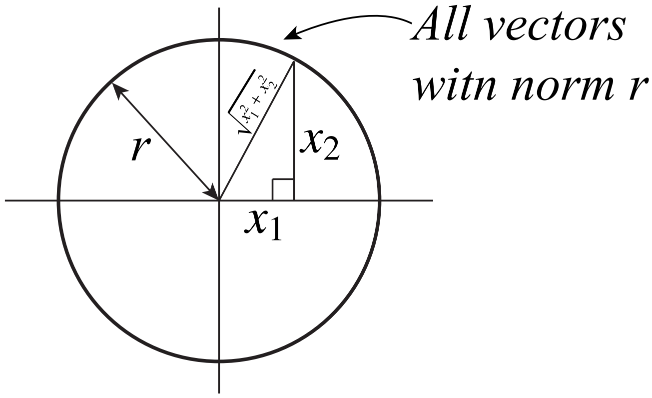
Example: inner product with std basis

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

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

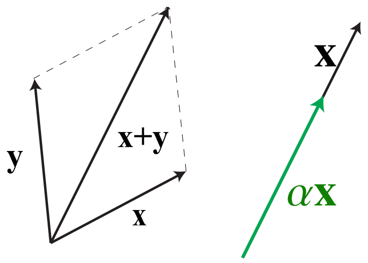
Example: Norm of vector

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \|\mathbf{x}\|^2 = \mathbf{x} \cdot \mathbf{x} = x_1^2 + x_2^2 + x_3^2$$



Example: scalar multilpication

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



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

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

Linear operators/transformations

Definition : Linear operator

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

$$A(\mathbf{x} + \mathbf{y}) = A(\mathbf{x}) + A(\mathbf{y}), \tag{1}$$

and

$$A(\alpha\mathbf{x}) = \alpha A(\mathbf{x}). \tag{2}$$

Examples

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

Linear operators and matrices

- A linear operator over Euclidean space is *determined by a matrix*

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

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

End of lecture 1

- That’s it for today!