ESQC 2026

Mathematical Methods Lecture 3

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Today's agenda:

- Two «roadmaps»:
  - Mathematical topics
  - Quantum chemistry and relevant mathematics

- Set theory
- Calculus and vector calculus

A mathematical roadmap

- How are mathematical topics connected?
- Which topics are useful for quantum chemists?
- We look at these 2 diagrams in the browser
- Feedback welcome!

At the core: 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*
- Informal, intuitive formalism developed late 1800s
- Contrast: *axiomatic set theory*
  - A matheatical theory with specific **axioms**
  - Everything derived from that
- Standard foundation for *all* of mathematics:
  - ZFC = Zermelo-Fraenkel set theory with axiom of choice

Basics of (naïve) set theory

- A **set** is an **unordered** collection of objects:

$$S = \{1, 2, 3\} \qquad C = \{\text{red}, \text{green}, \text{blue}\} \qquad \emptyset = \{\}$$

- The objects are **elements:**

$$1 \in S \qquad \text{cyan} \notin S$$

- **Unrestricted comprehension** generates new sets by assigning *conditions on a set*:

$$\{n \in S \mid n \text{ is even}\} = \{2\}$$

Operations on sets

- **Union** of two sets:

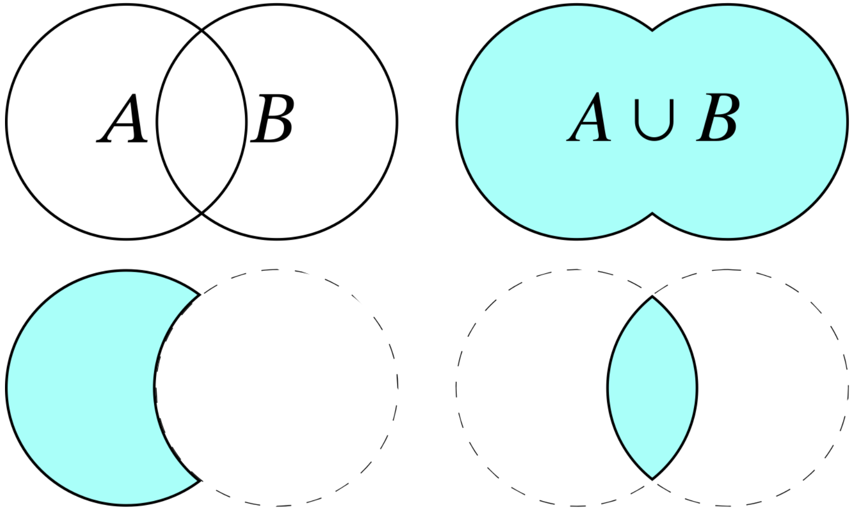
$$A = \{1, 2, 3\} \qquad B = \{2, 3, 4\} \qquad A \cup B = \{1, 2, 3, 4\}$$

- **Intersection:**

$$A \cap B = \{2, 3\}$$

- **Set difference:**

$$A \setminus B = \{1\}$$



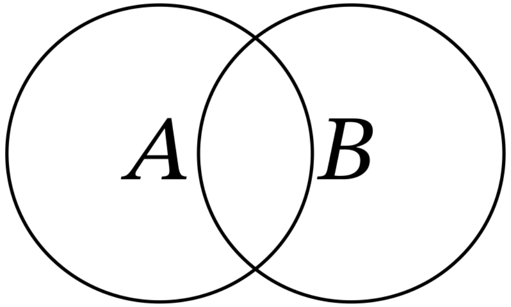
$A \setminus B$ $\qquad$ $A \cap B$

Subsets

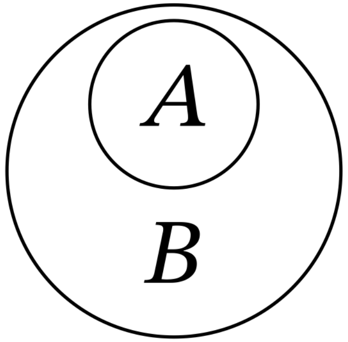
- A set can be **contained** in another set, i.e., be a **subset:**

$$A \subset B$$

$$x \in A \implies x \in B$$



$A \not\subset B$



$A \subset B$

Sets need not be simple …

- Infinite sets:

$$\mathbb{N} = \{0, 1, 2, 3, 4, \ldots\} \qquad \mathbb{R} = \{\text{all real numbers}\}$$

- Sets containing sets:

$$S = \{\{0, 1, 2\}, \{\text{red, green}\}\}$$

- Sets that are not explicitly known:

$$\mathcal{A} = \{\text{the set of all } v\text{-representable densities in DFT}\}$$

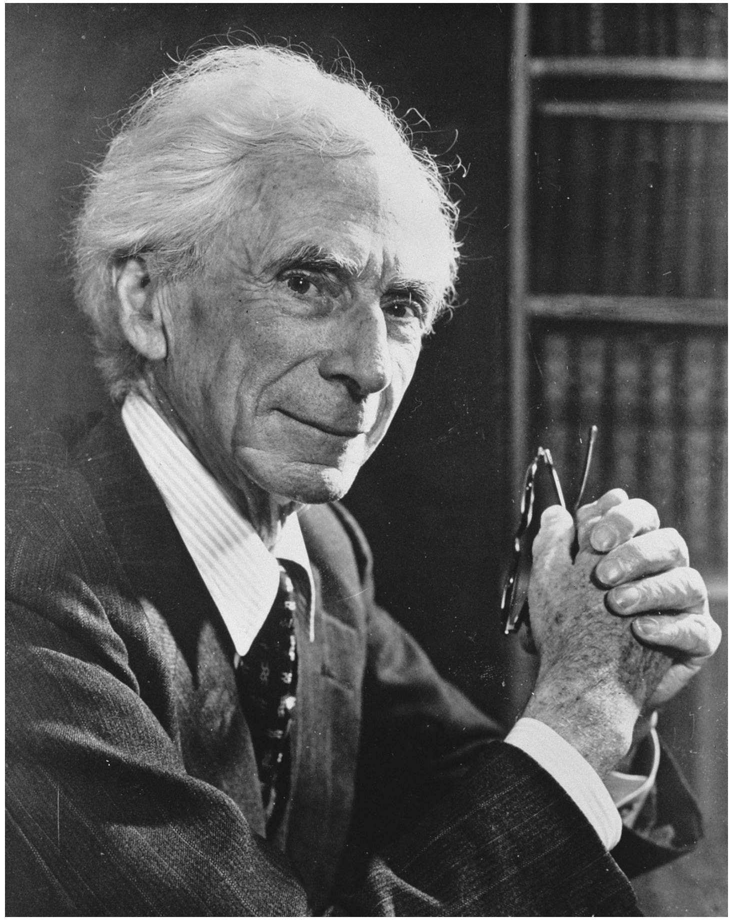
Russell's paradox (1902)

- 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?

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

- **Naive set theory has pitfalls**



Bertrand Russell in 1957 (from Wikipedia)

Calculus

Functions, integration and differentiation, in one and several variables

Calculus: The local and the global

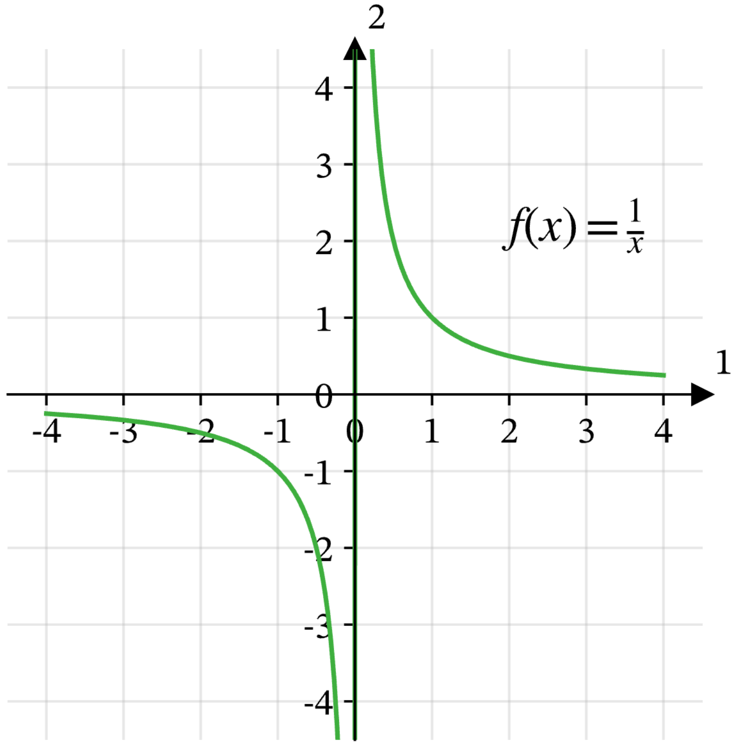
- In calculus we try to understand **functions of one variable:**

$$f : \mathbb{R} \to \mathbb{R}$$

- Two fundamental operations:
  differentiate = local change *vs.* integrate = global accumulation

$$\frac{dE(R)}{dR} \qquad \int |\psi(x)|^2 \, dx \qquad \int \phi_\mu(x) \hat{H} \phi_\nu(x) \, dx$$

Limits



- **Limits** are important in calculus

$$\lim_{x \to a} f(x) = L$$

- $f(x)$ **approaches (the limit)** L as x approaches a
- The limit L **may** not exist.
- *Examples:*

$$\lim_{x \to 4}(x^2 + 1) = 17 \qquad \lim_{x \to +\infty} \frac{1}{x} = 0 \qquad \lim_{x \to 0} \frac{1}{x} = \;??$$

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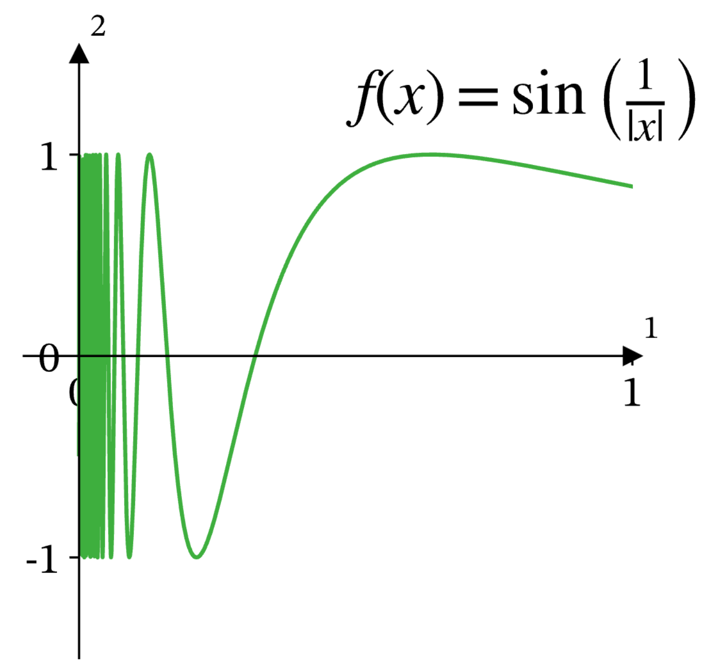
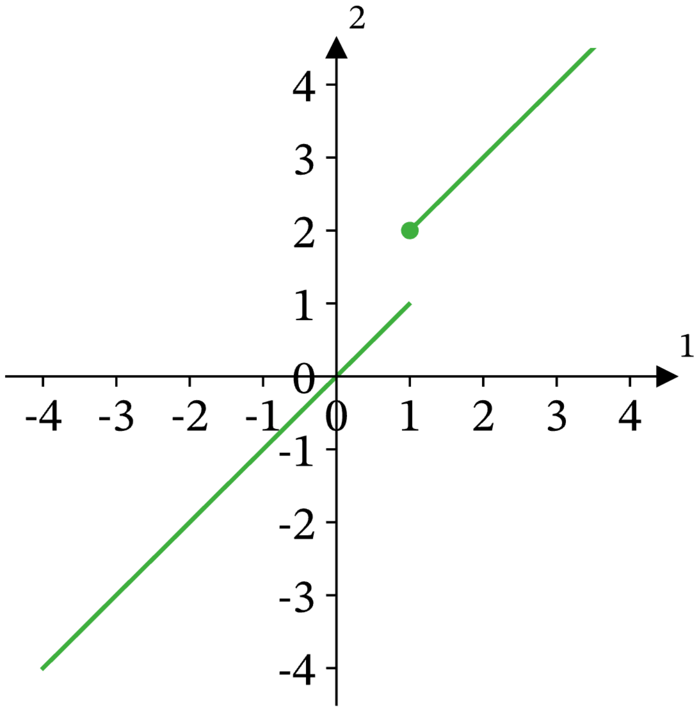
Continuity

- A function is **continuous** at a if:

$$f(a) = \lim_{x \to a} f(x)$$



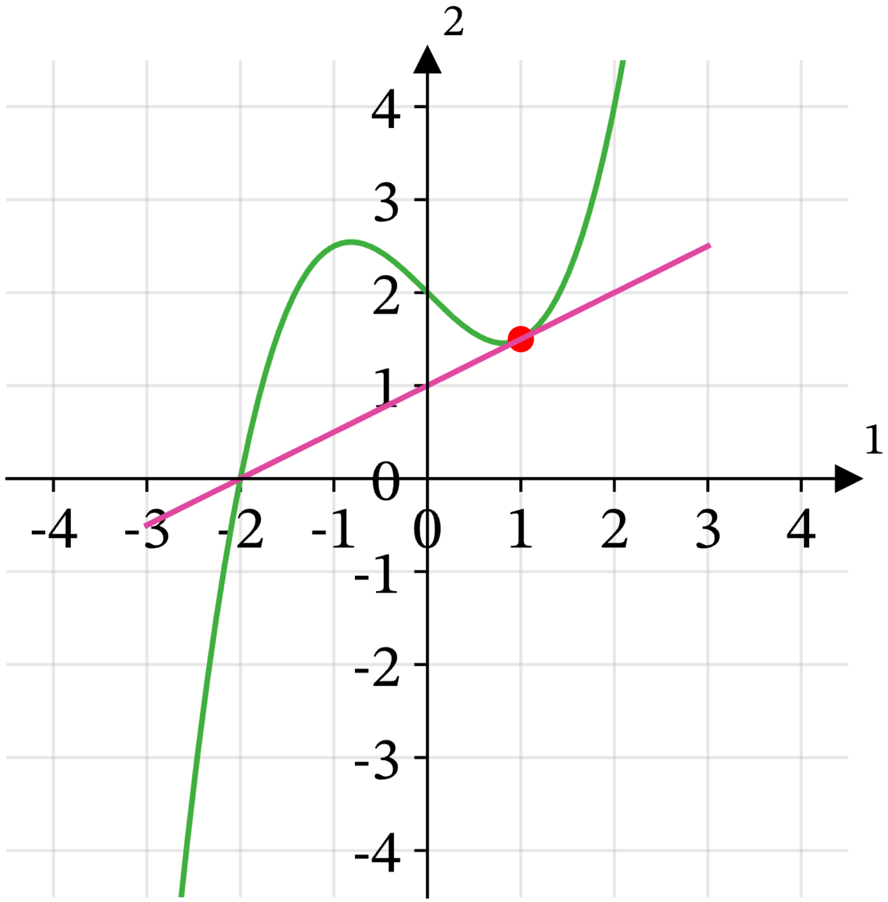


The derivative

- The **derivative** is defined as a limit

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

- The derivative is the **slope** of a line tangent to the graph
- **Demo:** `lecture-3-zoom.ipynb`



Differentiability means local linearity

- As we zoomed in:

$$f(x) \approx f(x_0) + f'(x_0) \cdot (x - x_0)$$

- The two became indistinguishable
- A function is **diffferentiable at *x*** if it looks like a **linear function** when we zoom in

Standard identities one uses all the time

$$(x^n)' = nx^{n-1}, \qquad (e^x)' = e^x, \qquad (\ln x)' = \frac{1}{x},$$

$$(\sin x)' = \cos x, \qquad (\cos x)' = -\sin x.$$

Linearity

$$(f + g)' = f' + g',$$

Product rule

$$(fg)' = f'g + fg',$$

Chain rule

$$(f \circ g)'(x) = f'(g(x))g'(x).$$

Taylor series

- Repeated differentiation gives **Taylor series expansion**

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \cdots$$

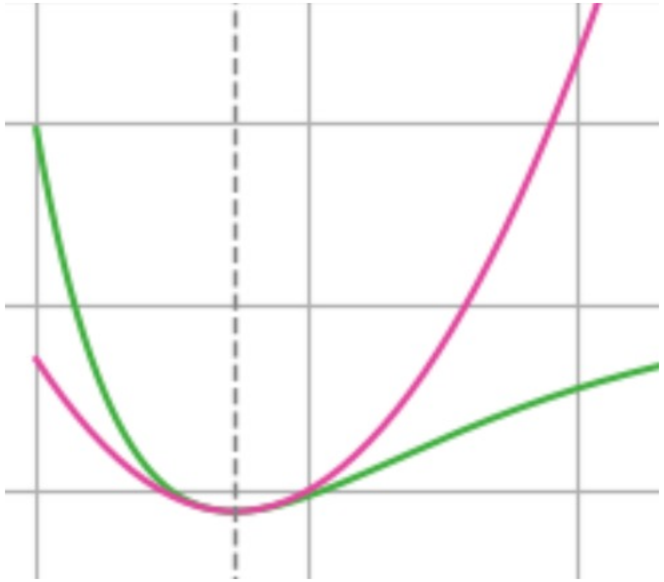
Slope Curvature

- When valid: **Approximation of a complicated function by a simple polynomial**
- **Demo:** `lecture-3-morse-taylor.ipynb`

Critical points and optimization

- Suppose we want to find a **local maximum or minimum**
- At such points **the slope is zero**

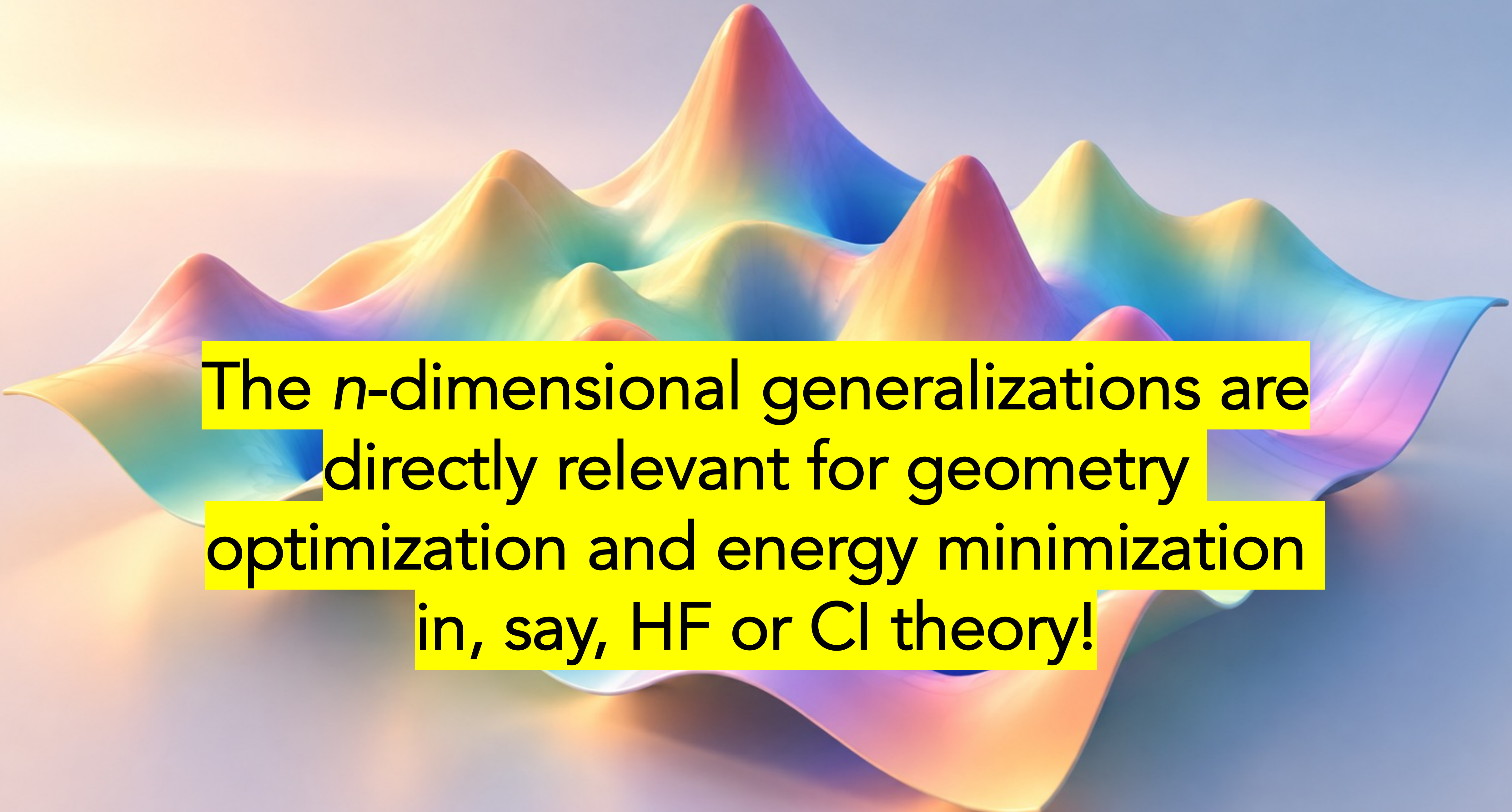
$$f'(x_*) = 0$$



  - Otherwise we would go up or down nearby!

$$f(x_* + h) \approx f(x_*) + \frac{h^2}{2} f''(x_*)$$

$f''(x_*) > 0$ local min $\qquad$ $f''(x_*) < 0$ local max



The *n*-dimensional generalizations are directly relevant for geometry optimization and energy minimization in, say, HF or CI theory!

From local to global: Integration

- The **definite integral** accumulates the function
  - «Area under graph»

$$\int_a^b f(x)\,dx = \lim_{n\to\infty} \sum_{i=1}^{n} f(x_i^*)\Delta x$$

- **Limit** of (signed) area of **small boxes**

- **Demo:** `lecture-3-riemann.ipynb`

Fundamental Theorem of Calculus

- Integration and differentiation are inverse operations
- Define

$$F(x) = \int_a^x f(t)\,dt.$$

- Then

$$F'(x) = f(x)$$

The anti-derivative

$$\int_a^b f(x)\,dx = F(b) - F(a).$$

End of lecture 3

- Next up: **Vector calculus**
- Calculus in **many dimensions**
- Some things stay the same, other things change