ESQC 2024

Mathematical Methods Lecture 3

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

Infinite Dimensions and Functional Analysis

Required for the formulation of physical laws

Functional analysis

- The study of (mostly) infinite dimensional vector spaces
  - Hilbert, Banach (and more)
  - *Function spaces*
- Linear transformations
  - In infinite dimensions strange things happen!
- Applications:
  - Quantum mechanics
  - Partial differential equations
  - Optimization and control theory

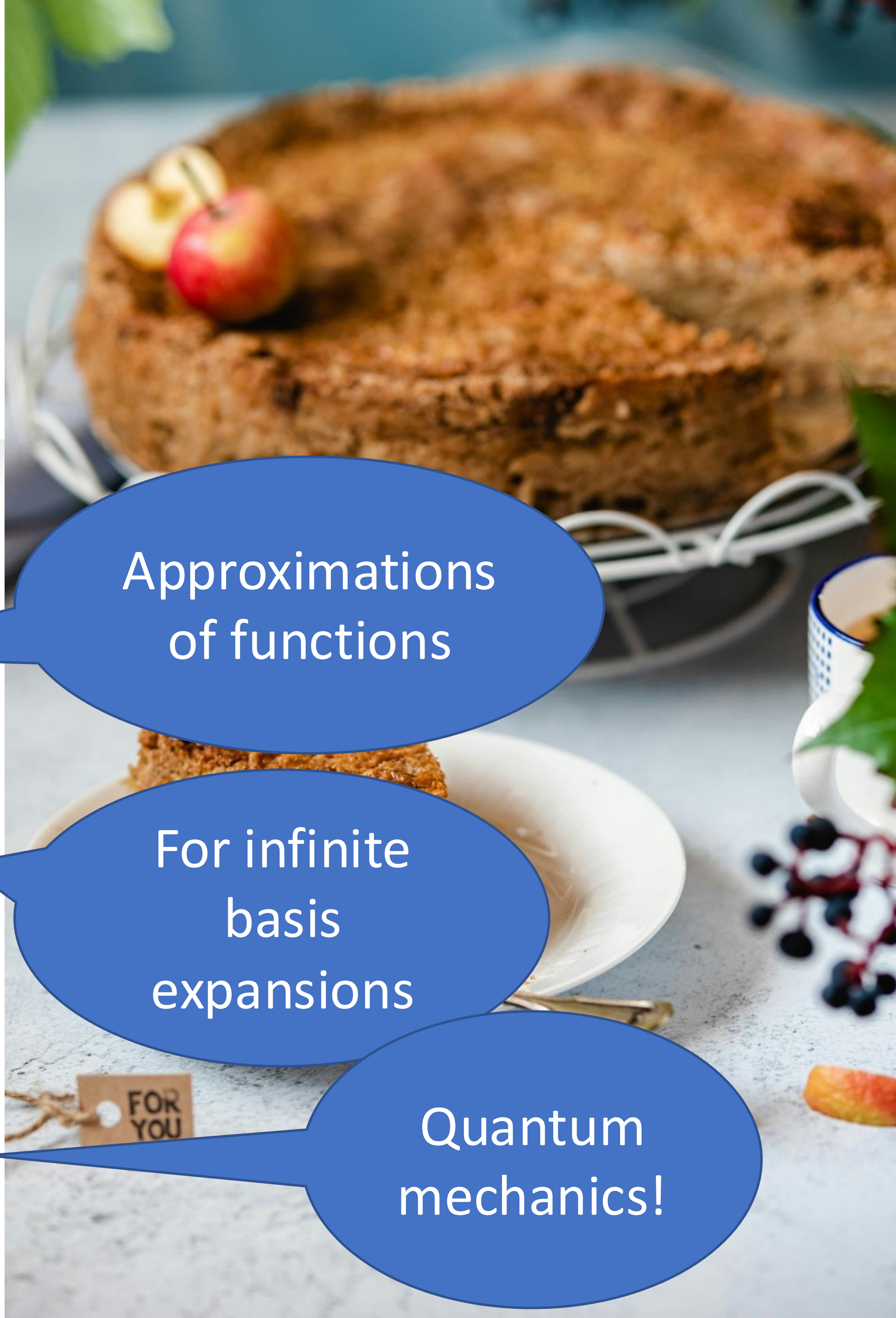
Examples of infinite dimensions

- The space of cake recipe ingredients list (from yesterday)
- The space of *all* polynomials, unlimited degree
- A space of sequences

$$\text{seq} = \{c : \mathbb{N} \to \mathbb{F}\}\,, \qquad c = (c_0, c_1, c_2, \cdots)$$

- The space of *square integrable functions*

$$L^2(\mathbb{R}^N) = \left\{ f : \mathbb{R}^N \to \mathbb{C} \;\middle|\; \int_{\mathbb{R}^N} |f(x)|^2 \, \mathrm{d}^N x < +\infty \right\}$$



Approximations of functions

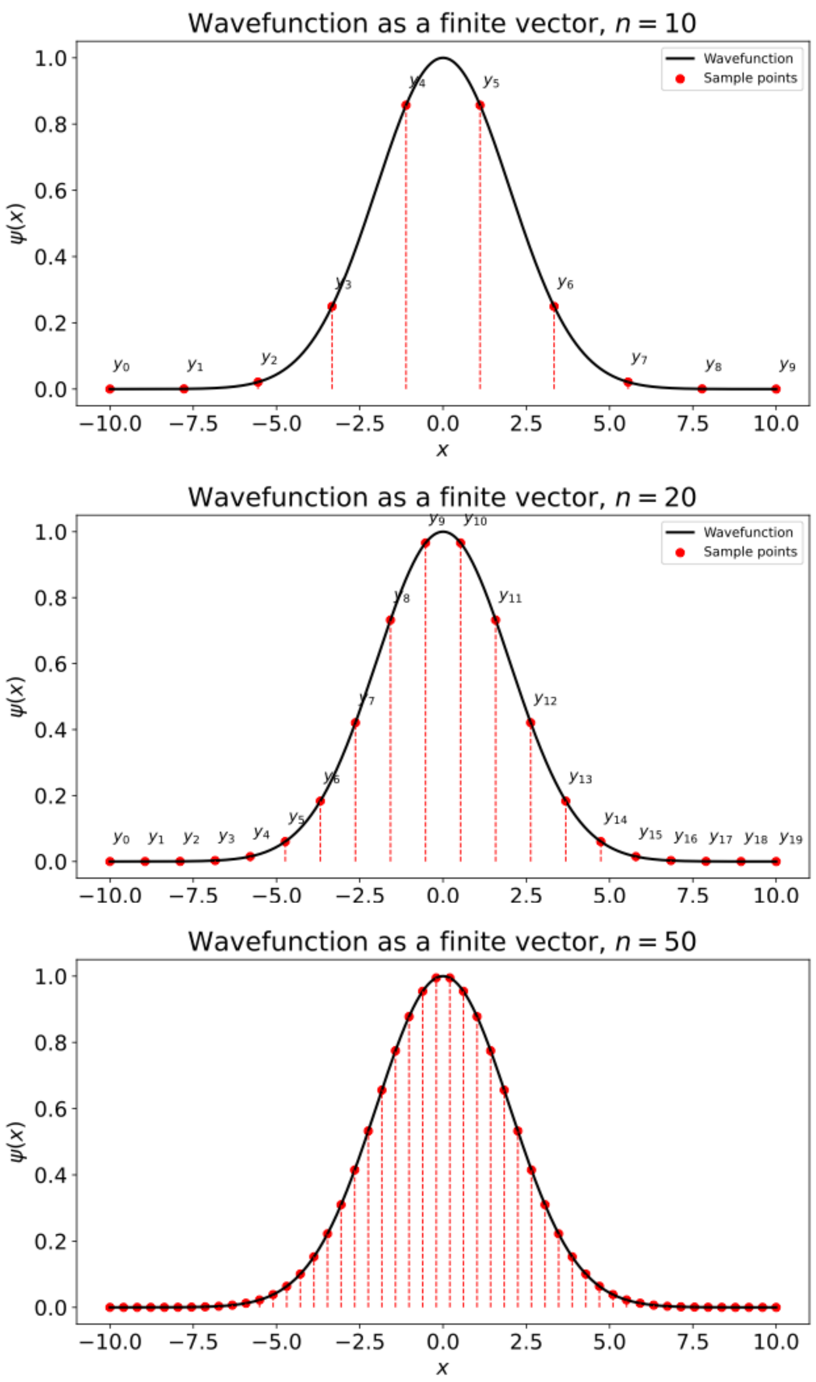
For infinite basis expansions

Quantum mechanics!

How to think about something like $L^2(\mathbb{R})$

- A function over $\mathbb{R}$ – infinite number of values!
- We can imagine an increasingly long finite vector of samples
- In quant chem: *a finite basis set of functions*

$$\psi(x) = \sum_{i=1}^{n} \psi_n \phi_n(x) \qquad |\psi\rangle = \sum_{i=1}^{n} \psi_n |\phi_n\rangle$$



What distinguishes the examples?

- Consider the question:
  - Which functions are close to each other?
- Use for different notions of ”closeness”
- *Extremely valuable!*

Hilbert and Banach spaces

The spaces of partial differential equations

Now it is getting a little more abstract

A metric embodies concept of distance

Definition 22: Metric

Let M be a set. A function $f : S \times S \rightarrow \mathbb{R}$ is a *metric* if it satisfies the following axioms:

1. $d(x, y) = d(y, x)$ ***symmetry***
2. $d(x, y) \geq 0$, and $d(x, y) = 0$ if and only if $x = y$ ***positivity and nondegeneracy***
3. $d(x, y) \leq d(x, z) + d(z, y)$ ***triangle inequality***

The pair (M, d) is a *metric space*.

Norms embody concept of length

Definition 57: Norm

A *norm* $||\cdot|| : V \to \mathbb{R}_+ = [0, +\infty[$ is a function that satisfies the following axioms:

1. $||x|| \geq 0$, and $||x|| = 0$ if and only if $x = 0$. ***positivity***
2. $||\alpha x|| = |\alpha|||x||$ ***absolute homogeneity***
3. $||x + y|| \leq ||x|| + ||y||$ ***triangle inequality***

$$d(x, y) = ||x - y||$$

Norms define metrics

Inner products give concept of angles

Definition 58: Inner product

An *inner product* $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ is a map which satisfies the following axioms:

1. $\langle x, x \rangle \geq 0, \quad \langle x, x \rangle = 0$ if and only if $x = 0$ — ***non-negative***
2. $\langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle$ — ***linearity***
3. $\langle \alpha y + \beta z, x \rangle = \bar{\alpha} \langle y, x \rangle + \bar{\beta} \langle z, x \rangle$ — ***conjugate linearity***
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$ — ***hermiticity***

$$d(x, y) = \|x - y\| = \langle x - y, x - y \rangle^{1/2}$$

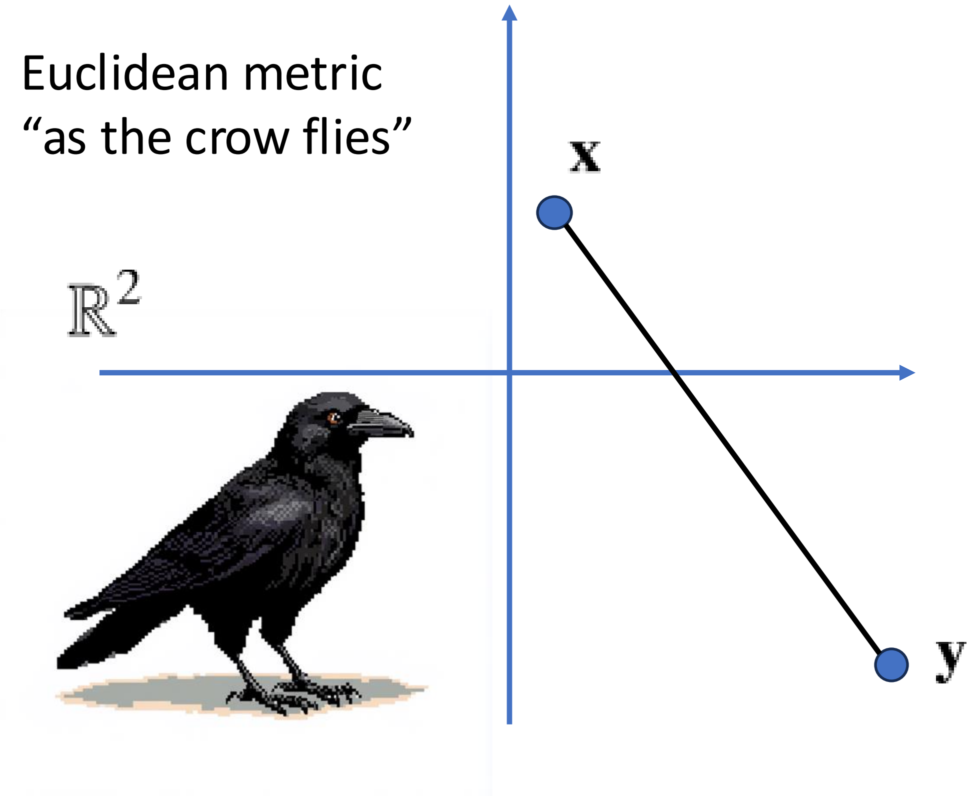
Inner products give metrics, too

Two metrics in the plane (from norms)

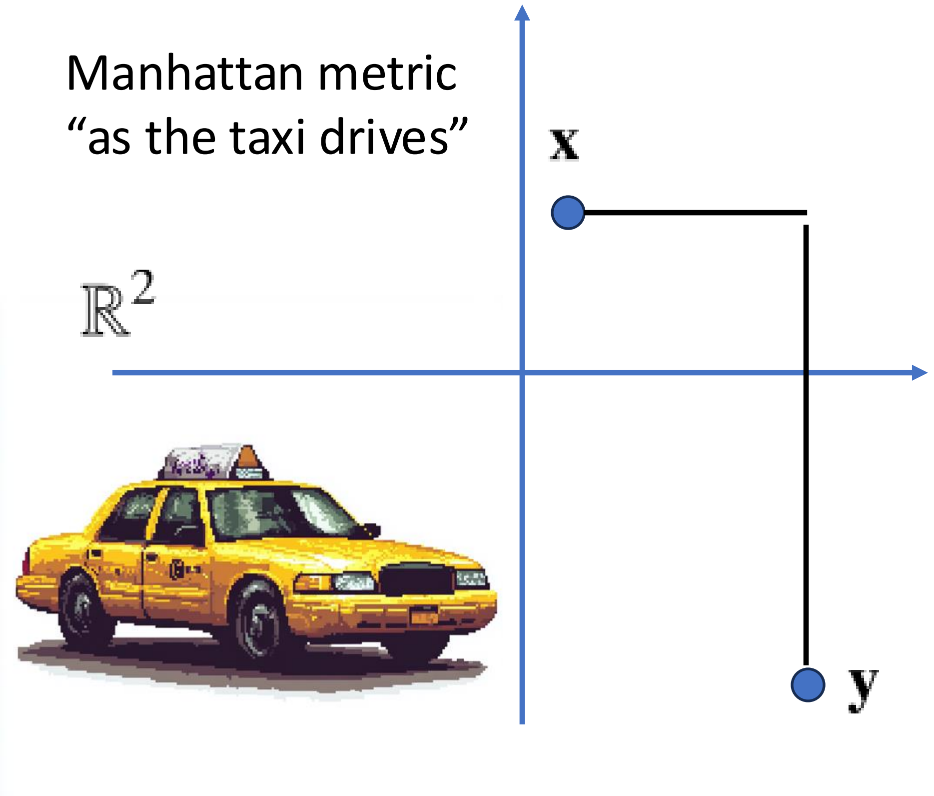
$$d(\mathbf{x},\mathbf{y}) = \sqrt{|x_1 - y_1|^2 + |x_2 - y_2|^2}$$

$$d(\mathbf{x},\mathbf{y}) = |x_1 - y_1| + |x_2 - y_2|$$

Euclidean metric
“as the crow flies”



Manhattan metric
“as the taxi drives”



Definition 53: Banach and Hilbert space

A *Banach space* is a complete normed vector space. A *Hilbert space* is a complete inner product space.

- In all cases, *metric spaces*
- The spaces of quantum mechanics, DFT, coupled-cluster theory ...
- Infinite dimensional (separable) Hilbert space: *infinite orthonormal basis*

$$\psi(x) = \sum_{i=1}^{\infty} \psi_n \phi_n(x)$$

What can we do with a Banach space?

1. From norm to *open sets*
   - "A topology"
2. From open sets to *convergence of sequences*, *completeness*
3. From completeness to *continuity of functions*
4. *Differentiability of functions*

The metric/norm is the foundation for calculus, vector calculus, calculus of variations …

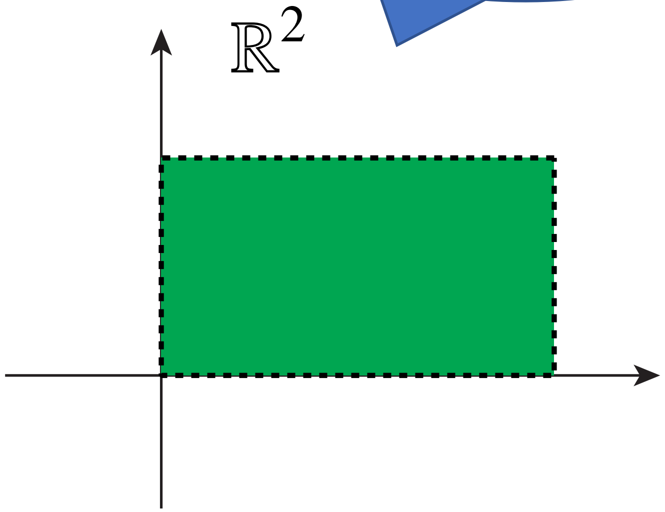
Spaces of functions

$$f : \Omega \rightarrow \mathbb{F}$$

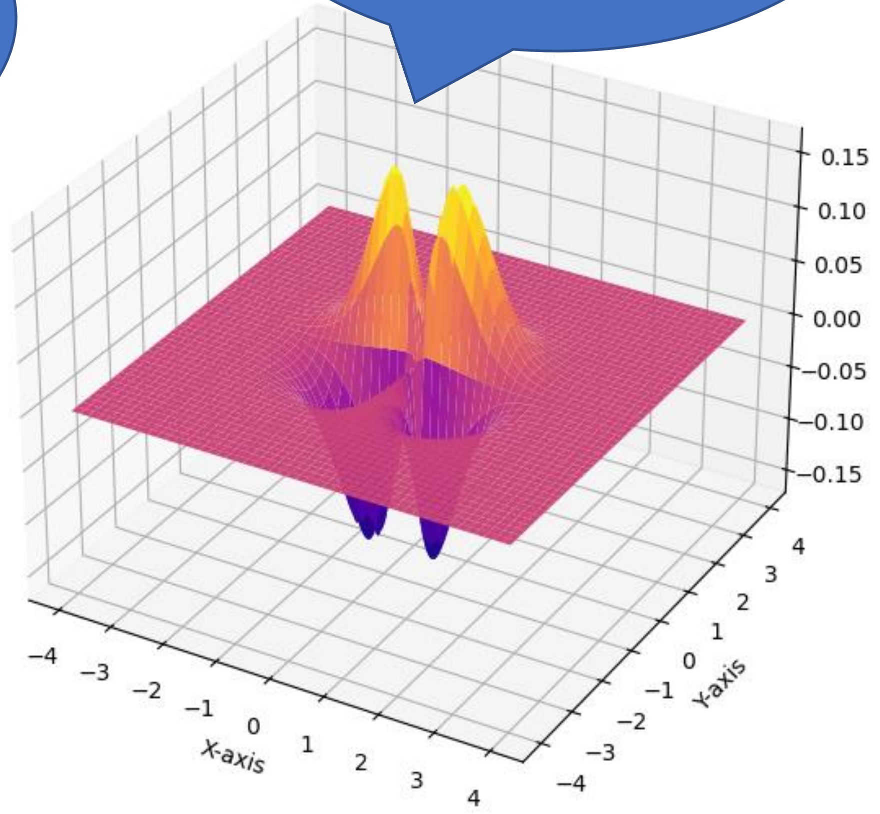
Intervals are typical

$[a, b] \subset \mathbb{R}$

Boxes in *n* dimensions



Here is an example function



L^p spaces

- For $1 \leq p < \infty$

$$f : \Omega \to \mathbb{F} \qquad \|f\|_p = \left(\int_\Omega |f(x)|^p \, dx \right)^{1/p}$$

- This is a Banach space:

$$L^p(\Omega; \mathbb{F}) = \left\{ f : \Omega \to \mathbb{F} \mid \|f\|_p < +\infty \right\}$$

A notebook example

- How different norms measure closeness of functions.
- This shows us that different norms can be useful

More examples

- **Banach space**:
  - Example:

$$C^0[0,1] = \{f : [0,1] \to \mathbb{R} \mid f \text{ continuous}\},$$

$$\|f\| = \max_{x\in[0,1]} |f(x)|$$

- **Hilbert space**:
  - Example:

$$L^2(\Omega;\mathbb{C}) = \left\{ f : \Omega \to \mathbb{C} \;\middle|\; \int_\Omega |f(x)|^2 \,\mathrm{d}x < +\infty \right\}$$

$$\langle f, g\rangle = \int_\Omega \overline{f(x)} g(x) \,\mathrm{d}x$$

ℓ_p *spaces*

- Discrete versions of L^p

$$u : \mathbb{N} \to \mathbb{F} \qquad\qquad ||u||_p = \left(\sum_{i=0}^{\infty} |u_i|^p \right)^{1/p}$$

$$\ell_p(\mathbb{N}; \mathbb{F}) = \left\{ u : \mathbb{N} \to \mathbb{F} \mid ||u||_p < +\infty \right\}$$

- *A Hilbert space:*

$$\ell_2(\mathbb{N}; \mathbb{F}), \quad \langle u, v \rangle_2 = \sum_{i=1}^{\infty} \overline{u}_i v_i$$

The archetypal (separable) Hilbert space

- Recall that in finite dimensions, $\mathbb{F}^n$ was the archetypal Hilbert space
- In infinite dimensions:

$$\ell_2 = \mathbb{F}^\infty, \quad u = [u_1, u_2, \cdots], \quad \sum_{i=1}^{\infty} |u_i|^2 < +\infty$$

$$\langle u, v \rangle_{\ell_2} = \sum_{i=1}^{\infty} \overline{u_i} v_i$$

- *All Hilbert spaces are isomorphic to this space, when an (infinite) orthonormal basis is chosen*

Linear transformations over Banach space

- In finite dimensions: all operators associated with *matrices*
- No longer true!
- Bounded vs. unbounded transformations
- Key feature:
  - Bounded transformations are *continuous*
  - Unbounded transformations are *discontinuous*
  - Unbounded transformations *usually not defined for all vectors*

Definition 61: Bounded linear transformations

Let V and W be Banach spaces over $\mathbb{F}$, and let $D(T) \subset V$ be a linear subspace.Let $T : V \to W$ be a linear transformation, i.e., for all $u, v \in D(T)$ and all $\alpha \in \mathbb{F}$,

$$T(\alpha u) = \alpha T u,$$

and

$$T(u + v) = Tu + Tv.$$

The linear space $D(T)$ is called the *domain of* T, and it may or may not be all of T. Let $\|T\|_{L(V,W)}$ be the norm ("operator norm") defined by

$$\|T\|_{L(V,W)} = \sup \left\{ \frac{\|Tu\|_W}{\|u\|_V} \mid 0 \neq u \in D(T) \right\}. \tag{5.29}$$

If $\|T\|_{L(V,W)} < +\infty$ and $D(T) = V$, then T is a *bounded, or countinuous, linear transformation from* V *to* W.

Example 26: Example of unbounded linear transformation

Let $\ell_2(\mathbb{N}, \mathbb{R})$ be the space of square summable sequences of real numbers, i.e., $u = (u_n) \subset \mathbb{R}$ with

$$\sum_{n=1}^{\infty} u_n^2 < +\infty.$$

Let A be the operator that is defined by

$$(Au)_n = nu_n,$$

i.e., each element in the sequence is multiplied by n. Let $(e_m)_n = \delta_{m,n}$ be the sequence which is zero everywhere except for the m'th position, where we have a 1. Then $Ae_m = (0, 0, 0, \cdots, m, \cdots)$ where the m is in the m'th position. We have $||Ae_m|| = m$, which grows to infinity as $m \to +\infty$. Therefore A is not bounded.

Furthermore, the sequence given by $u_n = n^{-1}$ is square summable, that is,

$$||u||^2 = \sum_n n^{-2} < +\infty.$$

However, $Au = (1, 1, 1, 1, \dots)$ which is clearly not square summable. So A cannot be defined on all of $\ell_2(\mathbb{N}, \mathbb{R})$.

Example 27: Unbounded operator

Let $u_\alpha \in L^2(\mathbb{R})$ be given by

$$u_\alpha(x) = N(\alpha)\exp(-\alpha x^2/2). \tag{5.30}$$

Here, $N(\alpha) = (\alpha/\pi)^{1/4}$ is such that $\|u_\alpha\| = 1$. Let $\hat{D} = \partial_x$, and compute

$$\partial_x u_\alpha(x) = -\alpha x u_\alpha(x). \tag{5.31}$$

We obtain

$$\frac{\|\partial_x u_\alpha\|}{\|u_\alpha\|} = \sqrt{2}\alpha \tag{5.32}$$

This goes to infinity as $\alpha \to +\infty$. Thus, ∂_x is unbounded. Similarly, it is easy to show that the kinetic energy operator $-\nabla^2/2$ for a single particle is unbounded.

Eigenvalues may not exist

- In finite dimensions: Any matrix has an eigenvalue!
- (We did not mention this earlier, but true!)

Example 28: Shift operator

Let $V = \ell_2(\mathbb{N};\mathbb{C})$, the space of square summable sequencess $u = (u_i) \subset \mathbb{C}$ with complex coefficients. Let T be the *shift operator*:

$$T(u_0, u_1, \cdots) = (0, u_0, u_1, \cdots).$$

This operator has no eigenvalues, and it is an instructive exercise to show this. (See the exercises.)

Yesterday …

… : Spectral theorem for Hermitian operators

Suppose $A \in \mathbb{F}^{n\times n}$ is Hermitian, i.e., $A^H = A$. Then, there exists an orthonormal basis $\{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$, and real numbers $\{\lambda_1, \cdots, \lambda_n\}$, such that

$$A\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

Equivalently,

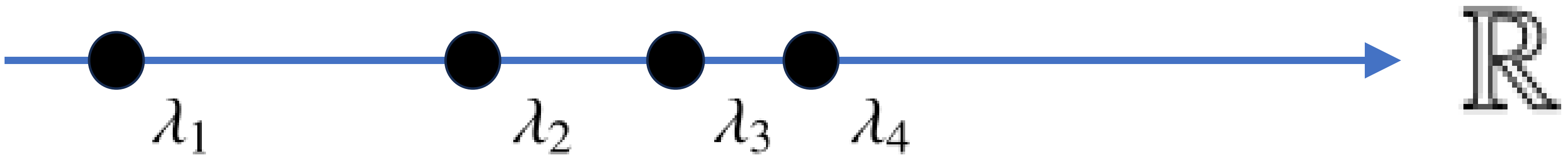
$$A = \sum_{i=1}^{n} \mathbf{u}_i \lambda_i \mathbf{u}_i^H = U\Lambda U^H$$

where $\mathbf{u}_i$ is the ith column of U, and where Λ is a diagonal matrix with elements $\Lambda_{ij} = \lambda_i \delta_{ij}$.

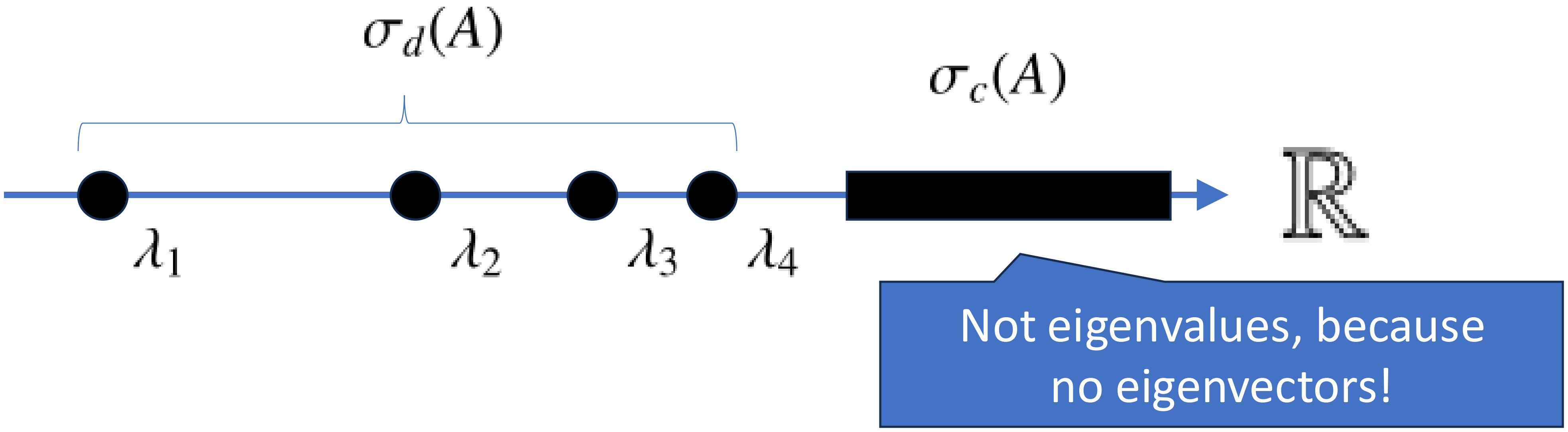
There exists an orthonormal basis such that A is just stretching of axes

Spectrum “=“ eigenvalues

- In finite dimensions spectrum is a discrete set:



- In infinite dimensions, possible with *continua*:



Rough version of spectral theorem

- In finite dimensions:

$$A = \sum_{i=1}^{n} \mathbf{u}_i \lambda_i \mathbf{u}_i^H$$

- Infinite dimensions, using bra-ket notation ...

$$A = \sum_{i=1}^{n} |u_i\rangle \, \lambda_i \, \langle u_i| + \int_{\sigma_c} d\lambda \, |\xi(\lambda)\rangle \, \lambda \, \langle \xi(\lambda)|$$

Sobolev spaces

Useful for analysis of partial differential equations

Kinetic energy example

- Consider a single electron wavefunction:

$$\psi \in L^2(\mathbb{R}^3)$$

- Kinetic energy:

$$\langle \psi, \hat{T}\psi \rangle = \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} \overline{\nabla\psi(\mathbf{r})} \cdot \nabla\psi(\mathbf{r}) \, d^3 r$$

- All allowed states of electrons must have finite kinetic energy

Sobolev spaces

- Function spaces for *partial differential equations*
- Previously we had for example

$$\psi \in L^2([a,b]) \quad \text{means that} \quad \int |\psi(x)|^2 \, dx < +\infty$$

- Can be useful to also require something on derivatives!

$$\partial_x \psi \in L^2([a,b]) \quad \text{means that} \quad \int |\frac{\partial}{\partial x}\psi(x)|^2 \, dx < +\infty$$

- A simple Sobolev norm:

$$||\psi||_{W^{1,2}} = ||\psi||_2 + ||\partial_x \psi||_2$$

Example

Smaller and smaller oscillations

- We consider a function sequence

$$f_n \in L^2([-10, 10]), \quad f_n(x) = e^{-x^2/2}\left(1 + \frac{1}{\sqrt{n}} \sin(nx)\right)$$

- Jupyter notebook: We compute L^2 norms and W^{12} norms

General definition

Definition 58: Sobolev space

Let $\Omega \subset \mathbb{R}^n$ be open. Let $p \in [1, +\infty]$ (including infinite). Let $u \in L^p(\Omega)$, and suppose u has weak derivatives up to order $k \geq 1$ that are *also* in $L^p(\Omega)$. Then we say that $u \in W^{k,p}(\Omega)$, a Sobolev space. The Sobolev space $W^{k,p}(\Omega)$ is a Banach space with norm

$$||u||_{W^{k,p}} = ||u||_p + \sum_{\alpha, |\alpha| \leq k} ||\partial_\alpha u||_p, \tag{5.22}$$

where α denotes a partial derivative of order $\leq k$. [For example, order 1 means $\alpha \in \{1, \cdots, n\}$, order 2 means $\alpha = (\alpha_1, \alpha_2)$ with $\alpha_i \in \{1, \cdots, n\}$, and so on.]

Rayleigh-Ritz variational principle

- Recall unbounded operator only defined on *domain* $D(\hat{H})$
- *We need finite kinetic energy*

$$E_{\text{ground state}} = \inf \left\{ \frac{\langle \psi, \hat{H}\psi \rangle}{\langle \psi, \psi \rangle} \;\middle|\; \psi \in D(\hat{H}) \right\}$$

- Domain is a Sobolev spce!
- *Errors are best measured in Sobolev norms.*

The axioms of quantum mechanics

Using what we have seen so far

Classical configuration space

Electron spin associated with 2 copies of space!

- A single electron can be at any

$$x = (\mathbf{r}, \sigma) \in \mathbb{R}^3 \times \{\uparrow, \downarrow\}$$

- N electrons can be configured as

$$(x_1, \cdots, x_N) \in [\mathbb{R}^3 \times \{\uparrow, \downarrow\}]^N = X^N$$

$$X = \mathbb{R}^3 \times \{\uparrow, \downarrow\}$$

Axiom 1: State space

- The states of a quantum system are (up to a global phase factor) *normalized elements in a separable Hilbert space* $\mathcal{H}$
- For a single electron:

$$\mathcal{H} = L^2(X;\mathbb{C}) \implies \psi = (\psi_\uparrow, \psi_\downarrow) \in [L^2(\mathbb{R}^3)]^2$$

A more general L2
space than
previously seen ...

Axiom 2: Observables

- Observables are represented by *self-adjoint operators over* $\mathcal{H}$
- Examples:

Position: $\hat{x},\ \hat{y},\ \hat{z}$

Momentum: $-i\hbar\partial_x,\ -i\hbar\partial_y,\ -i\hbar\partial_x$

Kinetic energy: $-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_z^2)$

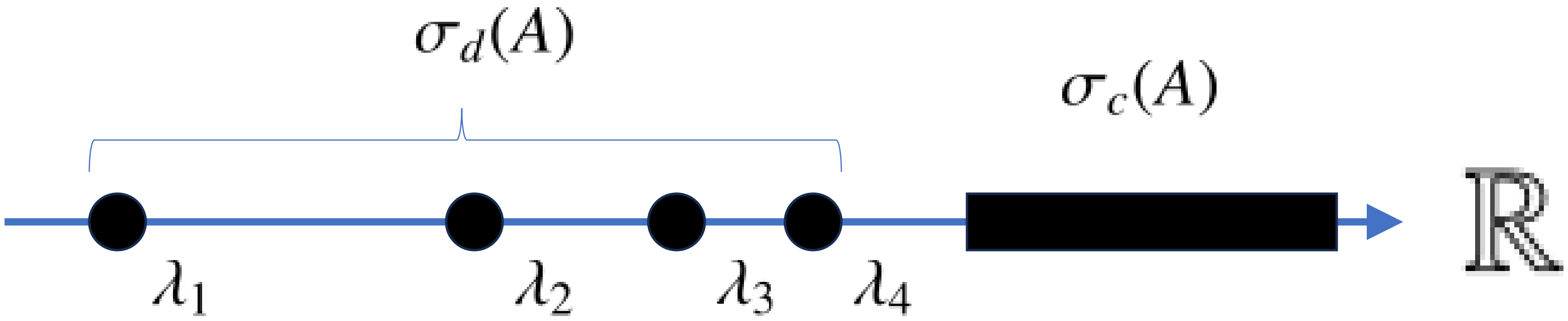
Total energy: $\hat{H} = \hat{T} + \hat{V}$

Kinetic energy: $\hat{T} = -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2 + \partial_z^2)$

All these are unbounded operators ...

Axiom 3: Outcomes of measurements

- The outcomes of measurements of an observable $\hat{A}$ are the *spectral points* of the observable



- Immediately after the measurement, the wavefunction is *projected onto the corresponding eigenfunction* (wavefunction collapse)

Axiom 4: Born interpretation

- Recall the spectral decomposition:

$$A = \sum_{i=1}^{n} |u_i\rangle\, \lambda_i\, \langle u_i| + \int_{\sigma_c} d\lambda\, |\xi(\lambda)\rangle\, \lambda\, \langle \xi(\lambda)|$$

- The probability of obtaining an outcome in, e.g., $I = [\lambda, \lambda + d\lambda]$

$$P(I) = \sum_{\lambda_i \in I} |\langle u_i, \psi\rangle|^2 + \int_I d\lambda |\langle \xi(\lambda), \psi\rangle|^2$$

Axiom 5: Time evolution

- Between measurements, the state evolves according to the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi(t) = \hat{H}\psi(t)$$

- This is not rigorous!
- Stone's Theorem fixes this: Propagator is always well-defined:

$$\psi(t) = \exp(-it\hat{H}/\hbar)\psi(0)$$

- TDSE satisfied in a generalized sense