ESQC 2026

Mathematical Methods Lecture 5

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Today’s agenda

- We are already familiar with **calculus, vector calculus,** and **linear algebra**
- We will have a look at **some more advanced mathematical tools**
    - Hilbert space
    - Fourier analysis

Introduction to Hilbert space

Motivation

$$\frac{\partial E(\mathbf{x}_*)}{\partial x_i} = 0$$

- Previously, we studied

$$\nabla E(\mathbf{x}_*) = 0 \quad \text{minimization of energy}$$

- What if we want to optimize not a vector but a **function?**

$$E[\psi] = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

- **Can we have something like:**

$$\frac{\delta E[\psi]}{\delta \psi} = 0 \quad ?$$

Calculus of variations

- Yes, indeed: **calculus of variations** gives the language

$$E[\psi] = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$\frac{\delta E[\psi]}{\delta \psi} = 0 \qquad \Longleftrightarrow \quad \hat{H}\psi = E\psi$$

Eigenvalue equation in Hilbert space

- Now, we will look at the language for the last part: **infinite dimenional vector spaces**

Functions as vectors

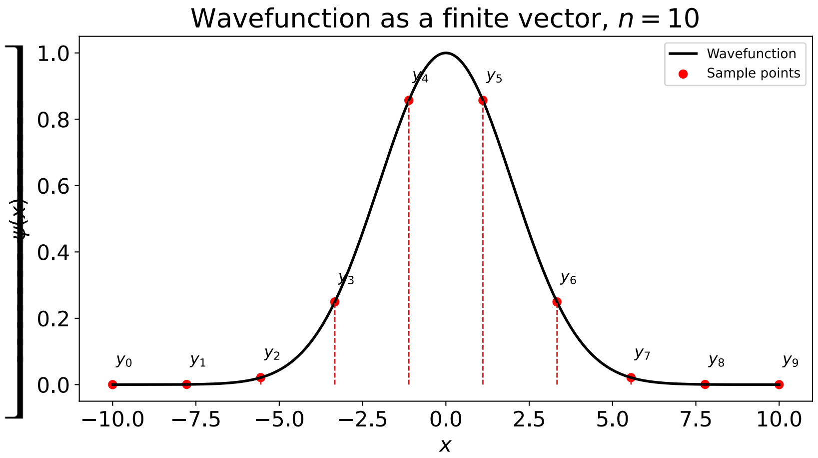
- A **function** can be viewed as a **vector,** since we can take **linear combinations:**

$$u(x) = f(x) + g(x) \quad v(x) = \alpha\, f(x)$$

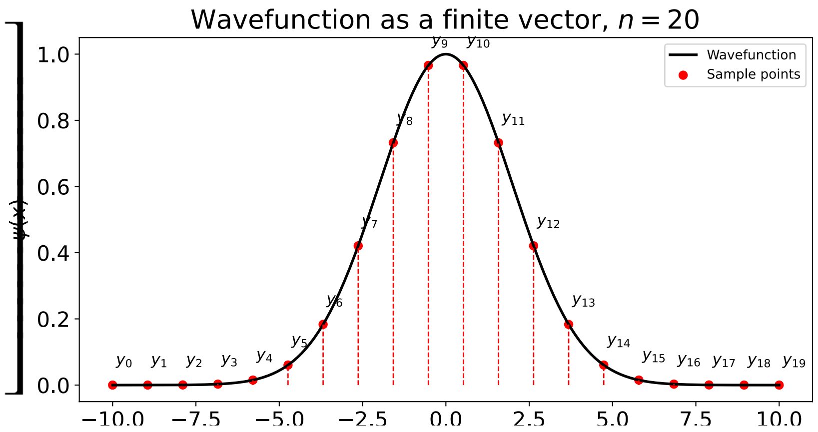
- What is the **dimension** of such a vector space?
- We can try to **approximate** with samples:

$$\text{dimension} = \infty$$

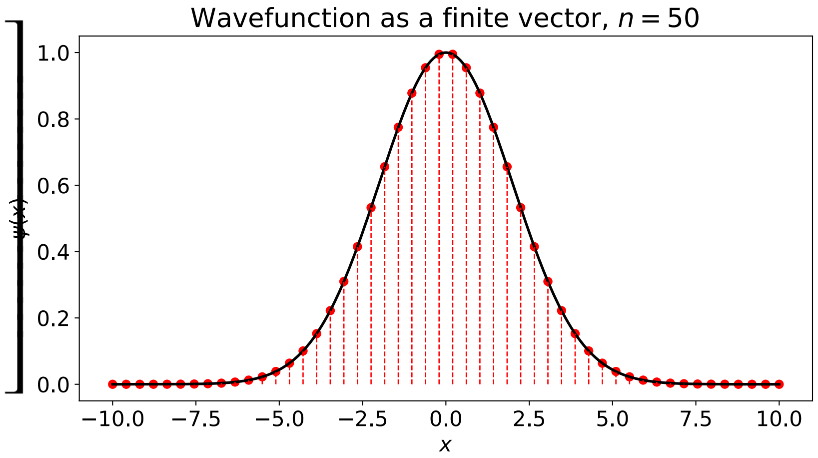
$$f \approx \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{10} \end{bmatrix}$$



$$f \approx \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{20} \end{bmatrix}$$



$$f \approx \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{50} \end{bmatrix}$$



Inner product between functions

- Compare **inner product** between vectors and **Riemann sum**

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^{n} x_i y_i \qquad \int_a^b f(x)g(x)\,dx \approx \Delta x \sum_{i=1}^{n} f(x_i)g(x_i)$$

- Indicates that the **inner product between functions** could be:

$$\langle f, g \rangle = \int_a^b f(x)g(x)\,dx$$

Hilbert space

- In quantum mechanics **Hilbert space** is (typically) a **vector space of functions**
- It has an **inner product** given by integrating functions against each other
- Example: Hilbert space of **orbitals** $L^2(\mathbb{R}^3)$

«Square-integrable» functions over R^3

$$\psi : \mathbb{R}^3 \to \mathbb{R} \quad \text{with some technical conditions}$$

$$||\psi||^2 = \int |\psi(\mathbf{r})|^2 \, d\mathbf{r} < +\infty \qquad \leftarrow \text{norm}$$

$$\langle \psi, \varphi \rangle = \int \psi(\mathbf{r})\varphi(\mathbf{r}) \, d\mathbf{r} < +\infty \qquad \leftarrow \text{inner product}$$

NB!

- Point of possible confusion:

$$\psi(\mathbf{r}) \qquad \text{vs.} \qquad \mathbf{r}$$

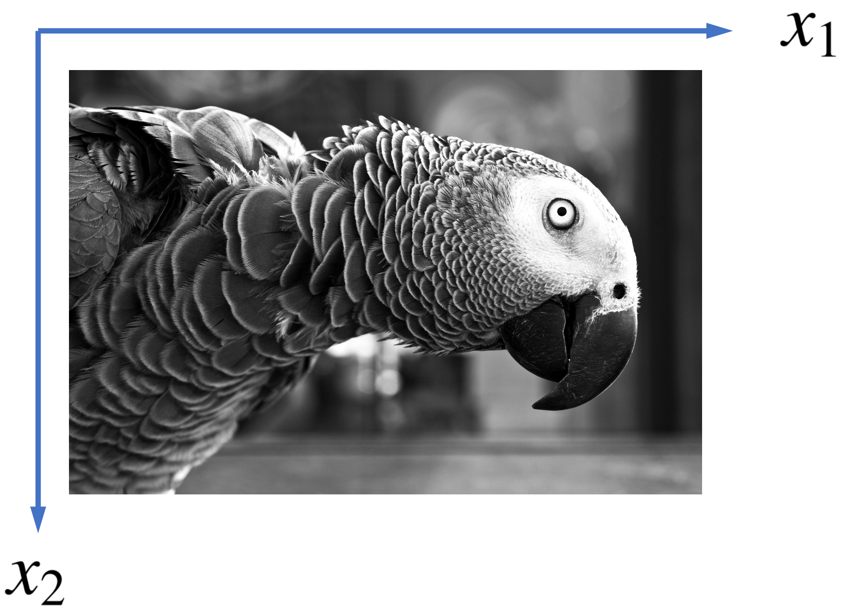
New vector
= function of
a vector

A 3D vector

Demo

- (There is nothing special about $\mathbf{r} = (r_1, r_2, r_3)$)

$$\psi(x_1, x_2) =$$



- **Demo:** `lecture-5-functions-as-vectors.ipynb`

Matrices become operators

- In Hilbert space, a linear transformation can **act on every point**
- It can be thought of as **an infinite matrix**
- Can contain **partial differential operators**

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)$$

$$\hat{V} = V(\mathbf{r})$$

Demo

- We revisig lecture-5-functions-as-vectors.ipynb

- We revisit lecture-2-diagonalization.ipynb

    - We see that operators can be **unbounded**

Finite dimensional linear algebra

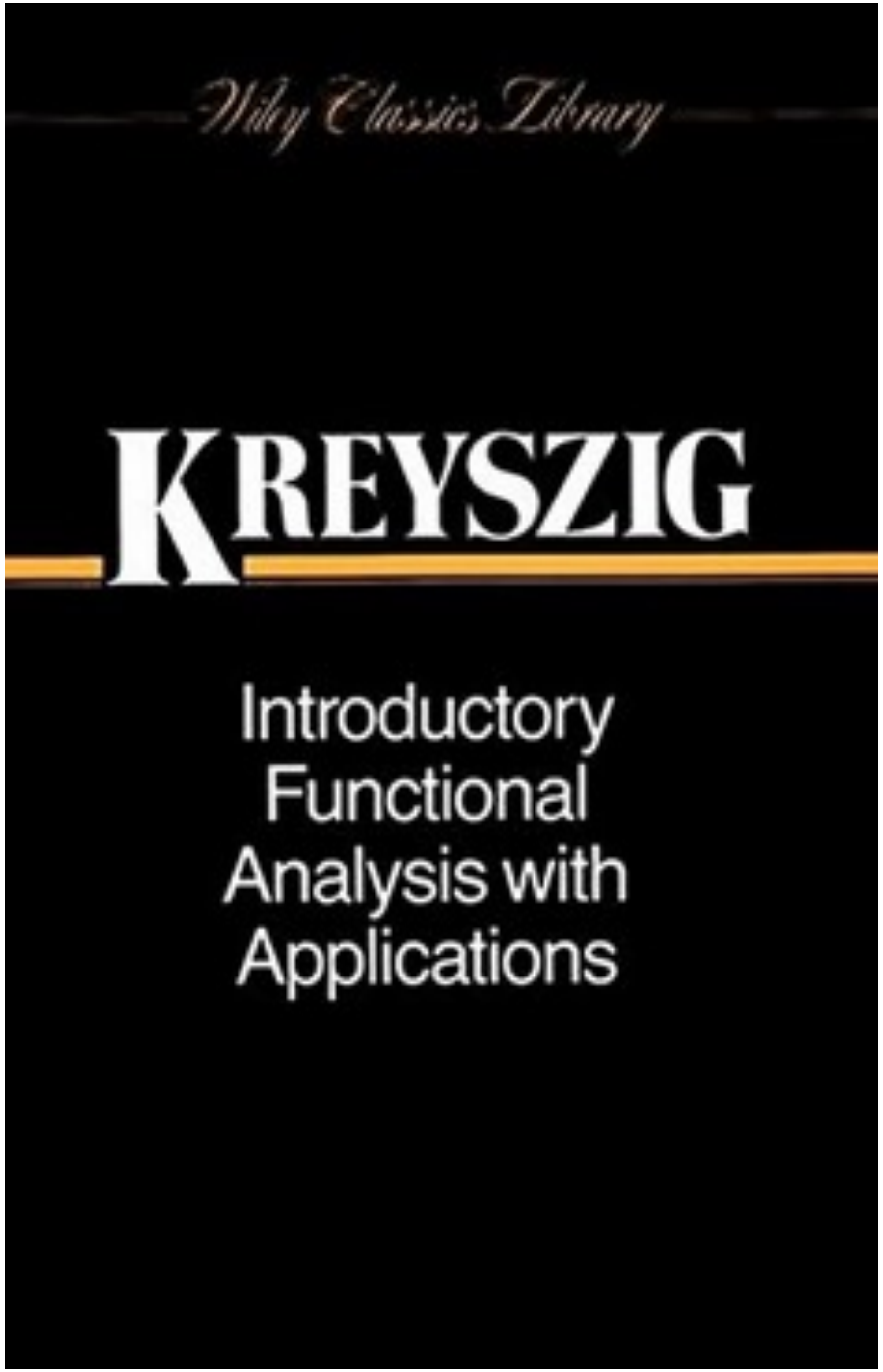
- Vector $\mathbf{x}$
- Vector space $\mathbb{C}^n$
- Inner product $\mathbf{x}^H\mathbf{y}$
- Norm $\sqrt{\mathbf{x}^H\mathbf{x}}$
- Orthogonality $\mathbf{x}^H\mathbf{y} = 0$
- Basis vectors $\mathbf{e}_i$
- Matrix A
- Eigenvector $H\mathbf{x}_k = \lambda_k\mathbf{x}_k$

Hilbert space

- Function – state $\psi(\mathbf{r})$
- Hilbert space $L^2(\mathbb{R}^3)$
- Inner product $\int \psi^*\varphi$
- Norm $\sqrt{\int |\psi|^2}$
- Orthogonality $\int \psi^*\varphi = 0$
- Basis functions ϕ_i
- Linear operator $\hat{A}$
- Eigenfunction $\hat{H}\psi_k = E_k\psi_k$

Functional analysis

- The study of **infinite dimensional vector** spaces
- The **operators** acting on these
- Typically: Spaces of functions
- Extremely important topic for the study of **partial differential equations**

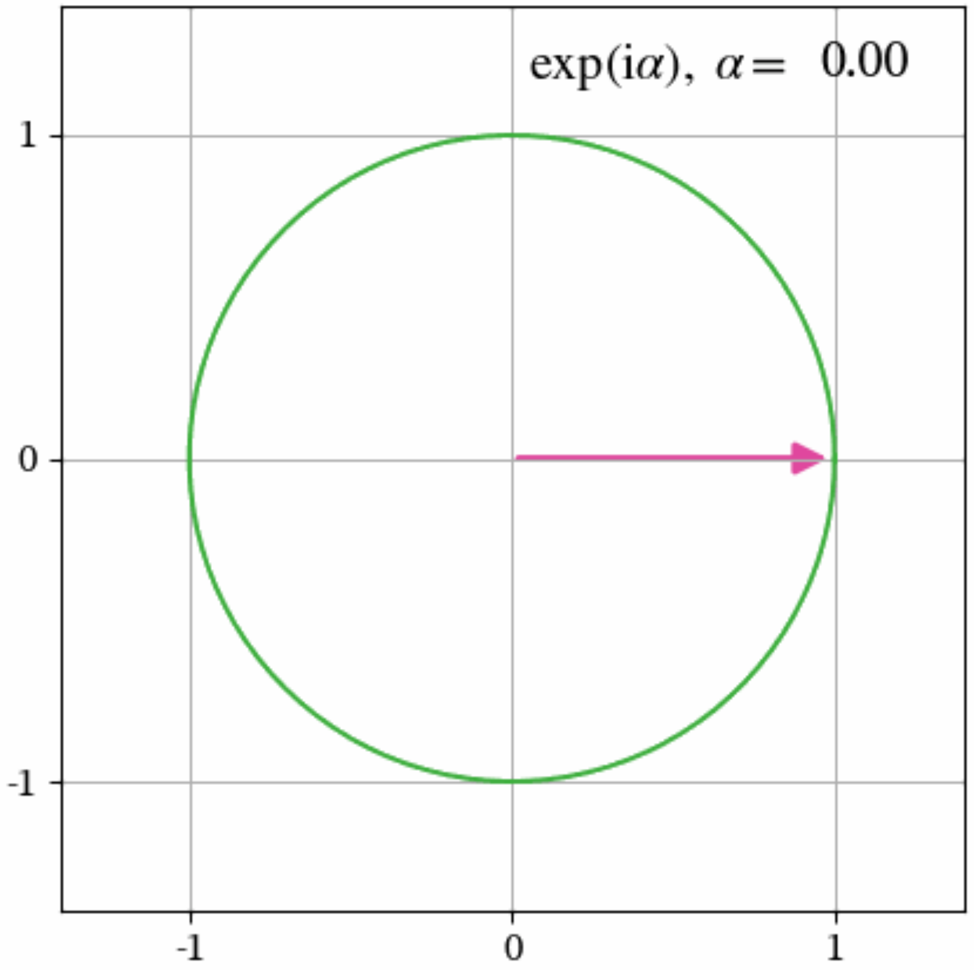


Fourier analysis

Coplex phase factors

- We recall **Euler's formula**

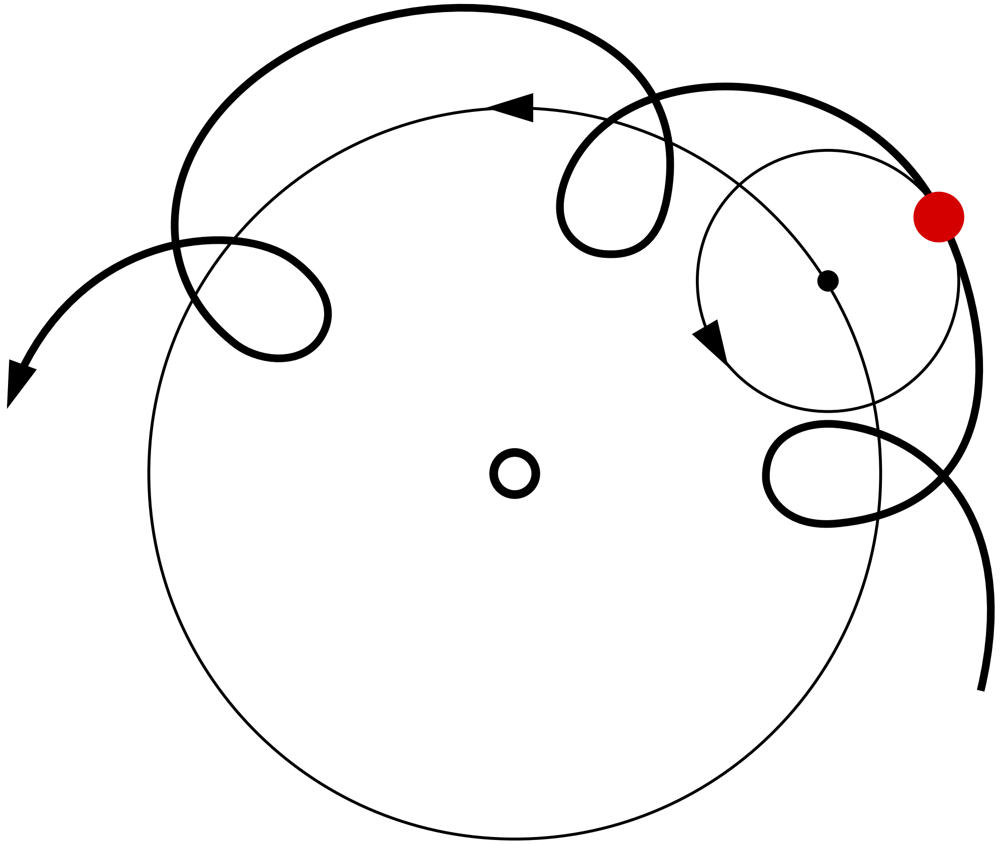
$$e^{i\alpha} = \underbrace{\cos\alpha}_{x\text{-axis}} + \underbrace{i\sin\alpha}_{y\text{ axis}}$$



Epicycles of planetary motion

- Ptolemaic and Copernican system of astronomy was *geocentric*
- But observations required ***epicycles***
- An early form of ***Fourier series***

$$z(t) = a_0 e^{ik_0 t} + a_1 e^{ik_1 t}$$



Epicycles of planetary motion

- Ptolemaic and Copernican system of astronomy was *geocentric*
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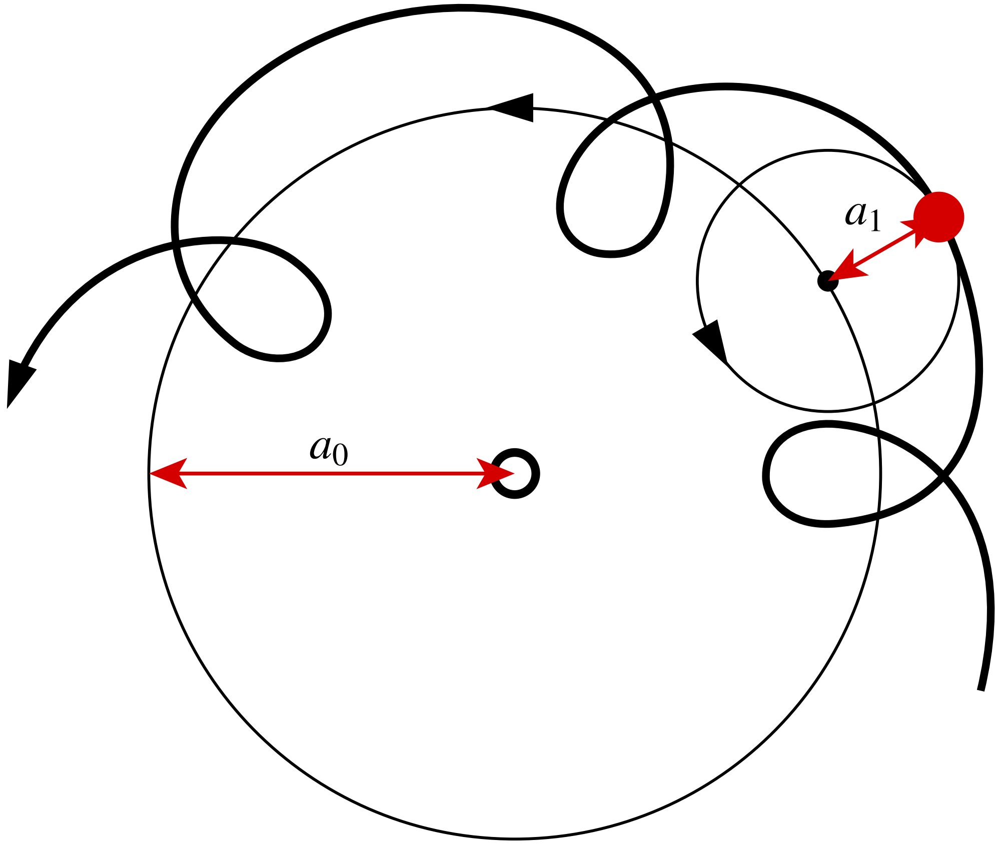
$$z(t) = a_0 e^{ik_0 t} + a_1 e^{ik_1 t}$$

- (The ancient Greeks did not use complex numbers)



Epicycles upon epicycles …

- By adding more epicycles, **virtually any plane curve can be drawn**

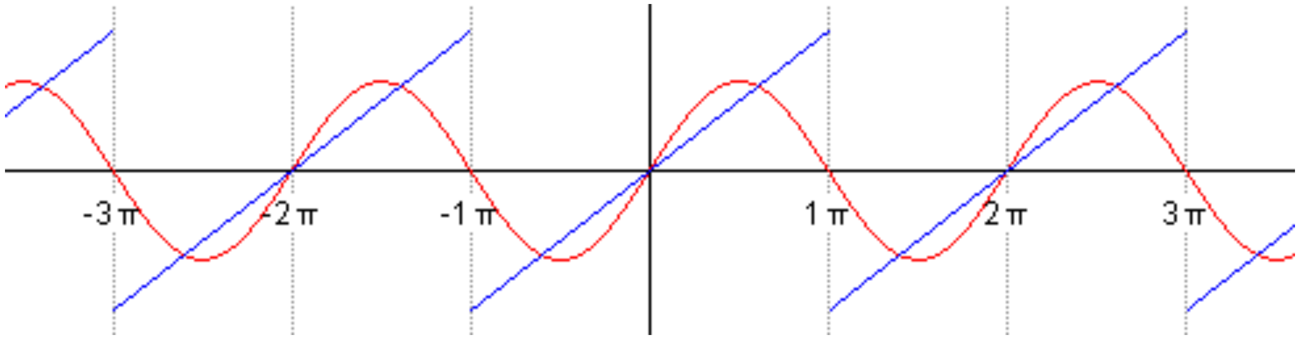
$$f(\theta) \approx \sum_{k=-\infty}^{\infty} a_k e^{\mathrm{i}k\theta} \qquad \leftarrow \text{Fourier series}$$

- In fact alpmost **any complex function** over an interval can be written as a Fourier series

- **Demo:** `lecture-5-epicycles.ipynb`

Joseph Fourier (1768-1830)

- Had the idea that *general* periodic functions could be decomposed into *sinusoidal components*
- A function of period *T*:



Fourier series as Hilbert space basis expansion

- Recall an **orthonormal basis expansion** in finite dimensions:

$$\mathbf{x} = \sum_{i=1}^{n} x_k \mathbf{b}_k, \quad ||\mathbf{b}_1|| = ||\mathbf{b}_2|| = \ldots = 1, \quad \langle \mathbf{b}_1, \mathbf{b}_2 \rangle = \ldots = 0$$

- For a function

$$f : [0, 2\pi] \to \mathbb{C} \qquad \varphi_k(\theta) = \frac{1}{\sqrt{2\pi}} e^{ik\theta}$$

Orthonormal basis

$$||\varphi_k|| = 1 \qquad \langle \varphi_k, \varphi_\ell \rangle = 0, \quad k \neq \ell$$

$$f(\theta) = \sum_{-\infty}^{\infty} c_k \varphi_k(\theta)$$

Infinite basis expansion!

Plane waves and derivatives

- Consider a **plane wave:**

$$\psi(x) = e^{\mathrm{i}kx}$$

- **Eigenfunction** for differentiation:

$$\frac{d}{dx}e^{\mathrm{i}kx} = \mathrm{i}ke^{\mathrm{i}kx}$$

- Differentiation **becomes multiplication** for the plane wave
- **Duality** of position and momentum in quantum mechanics

Fourier transform

- We can generalize Fourier series to almost **arbitrary functions**:

$$f \in L^2(\mathbb{R};\mathbb{C}), \quad \text{i.e.,} \quad \int_{-\infty}^{\infty} |f(x)|^2 \, dx < +\infty$$

- The (normalized) Fourier transform is defined as:

Plane wave basis function

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) \, dx$$

- Fact: The transform is a **unitary transformation**

$$f, g \in L^2 \implies \hat{f}, \hat{g} \in L^2, \quad \langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle$$

Generalization to higher dimensions

- Normalized Fourier transform and inverse:

$$f \in L^2(\mathbb{R}^n;\mathbb{C}), \quad \hat{f}(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\, d^n x$$

$$g \in L^2(\mathbb{R}^n;\mathbb{C}), \quad \check{g}(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i\mathbf{k}\cdot\mathbf{x}} g(\mathbf{k})\, d^n k$$

- Again, a **unitary transformation**

Example

- **Demo:** `lecture-5-image-fourier.ipynb`

A few reasons why we need Fourier analysis

- Often signals are naturally decomposed into plane waves:
  - Spectroscopy: time vs. frequency
- Quantum mechanics: Duality of position and momentum
- Derivatives become multiplication
- Plane-wave electronic-structure methods (solid state)

- ... and more

End of lecture 5

- Thanks for joining the journey!
- Make sure you check out the maps online
    - Feedback welcome!