ESQC 2024

Mathematical Methods Lecture 5

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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

Complex analysis

Why complex analysis?

Wavefunction is complex !

Complex notation simplifies (!)

- Time-dependent Schrödinger equation

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

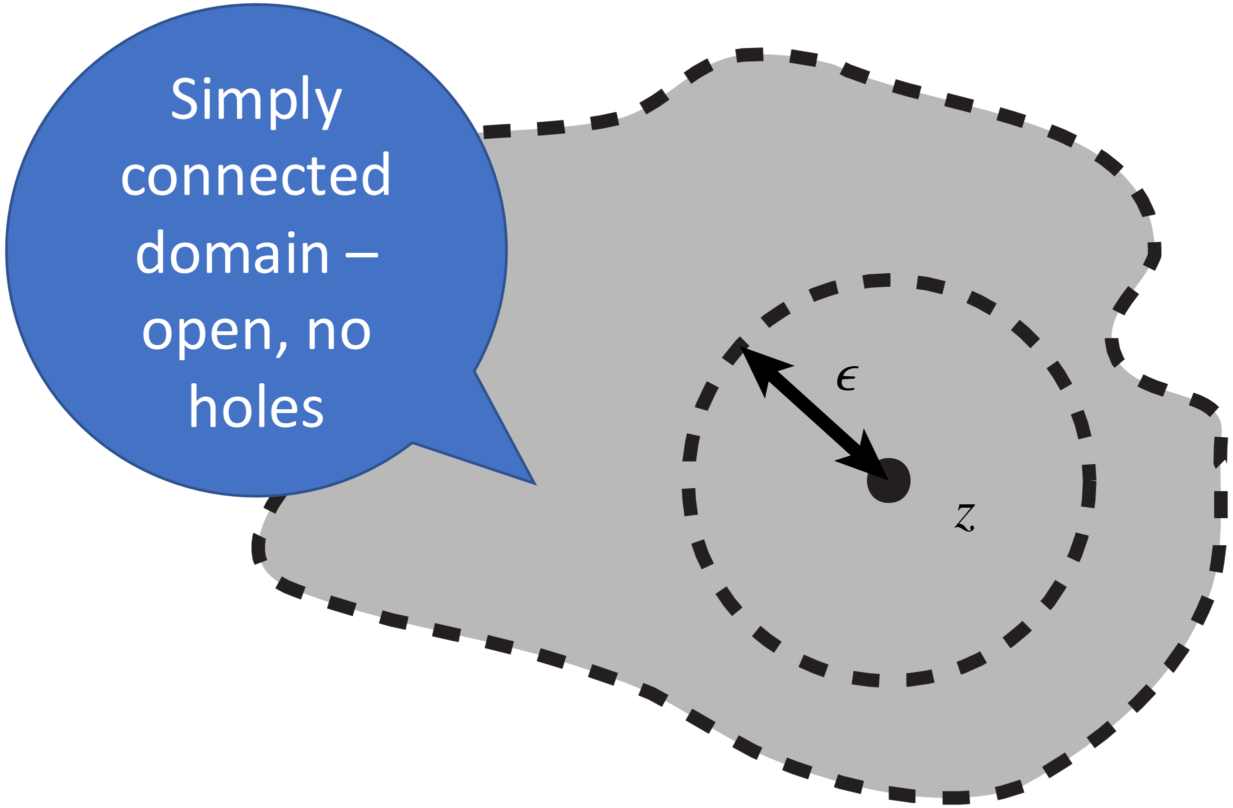
- Wave phenomena

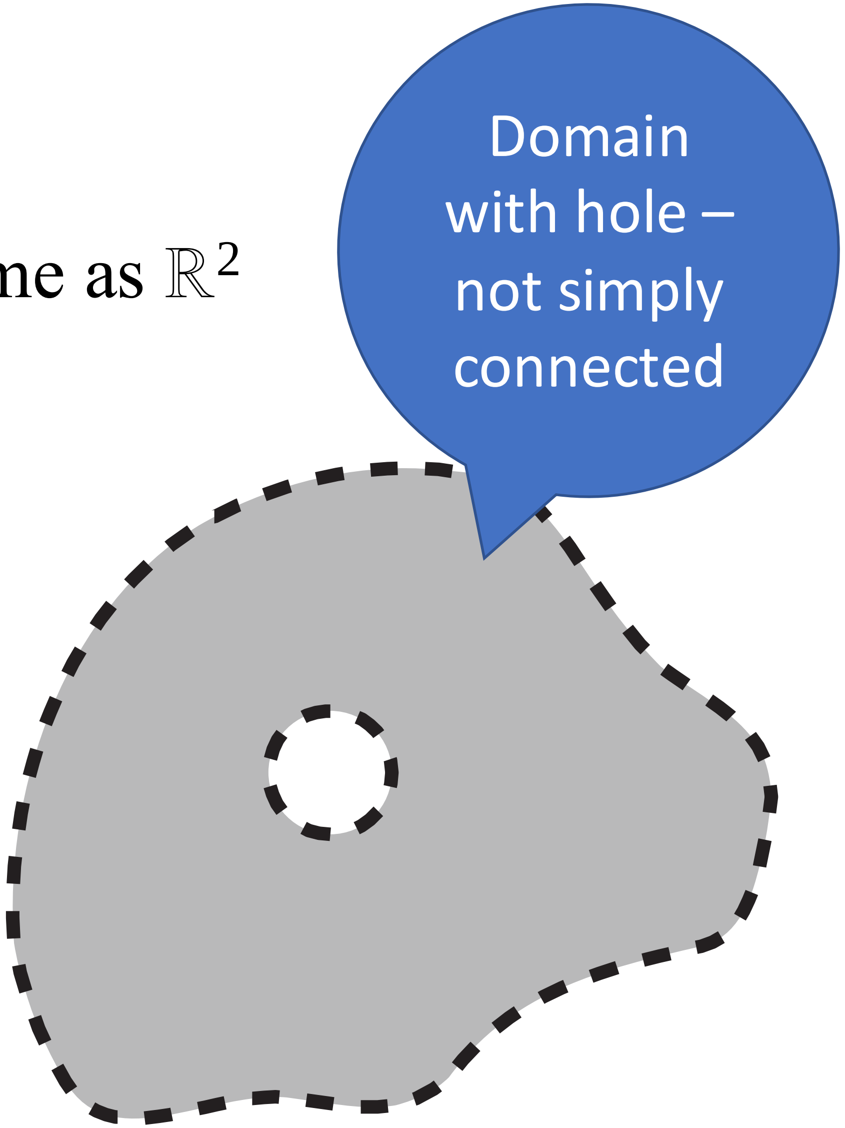
$$\cos(kx - \omega t) = \mathrm{Re}\,\exp[\mathrm{i}(kx - \omega t)]$$

- Response theory: *poles* of response function
- Evaluation of integrals – analytic continuation
- Perturbation theory of eigenvalues
- Application to analysis of *real* functions

Complex plane topology

- The complex plane is topologically the same as $\mathbb{R}^2$





$$B_\epsilon(z) = \{\, w \in \mathbb{C} \mid |w - z| < \epsilon \,\}$$

Definition : Complex number operations

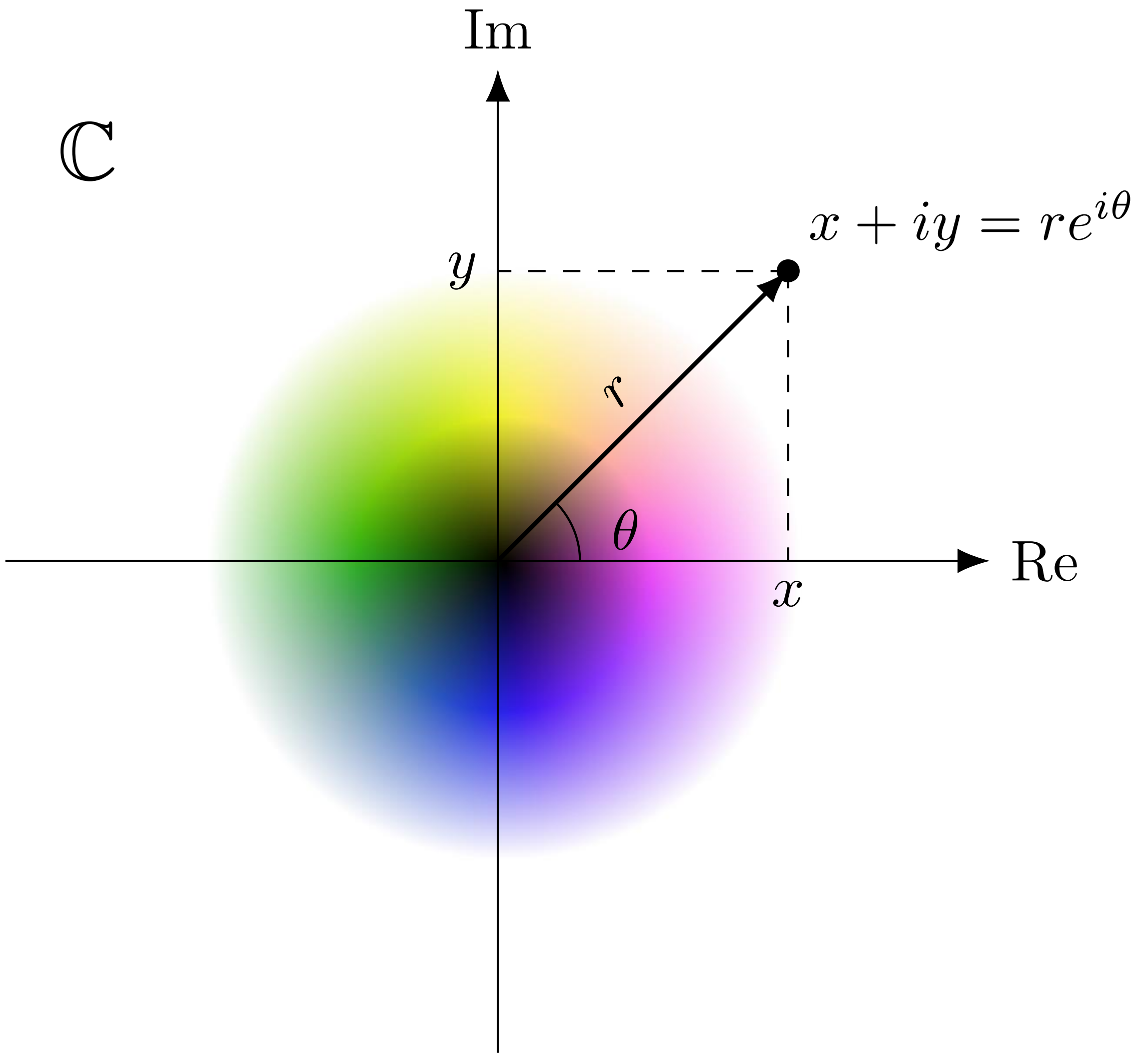
Let $z = x + \mathrm{i}y \in \mathbb{C}$.

- $\operatorname{Re} z = x$, $\operatorname{Im} z = y$ ***real and imaginary part***
- $\bar{z} = z^* = x - \mathrm{i}y$ ***complex conjugate***
- $z = re^{i\theta}$, ***polar form***
  where $e^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$ ***Euler's formula***
- $\operatorname{Arg} z = \theta$ ***argument/angle/phase***
- $|z|^2 = \bar{z}z = \operatorname{Re} z^2 + \operatorname{Im} z^2 = r^2$ ***squared***
  modulus/norm

Visualization using color wheel

- Color the complex numbers according to angle and modulus

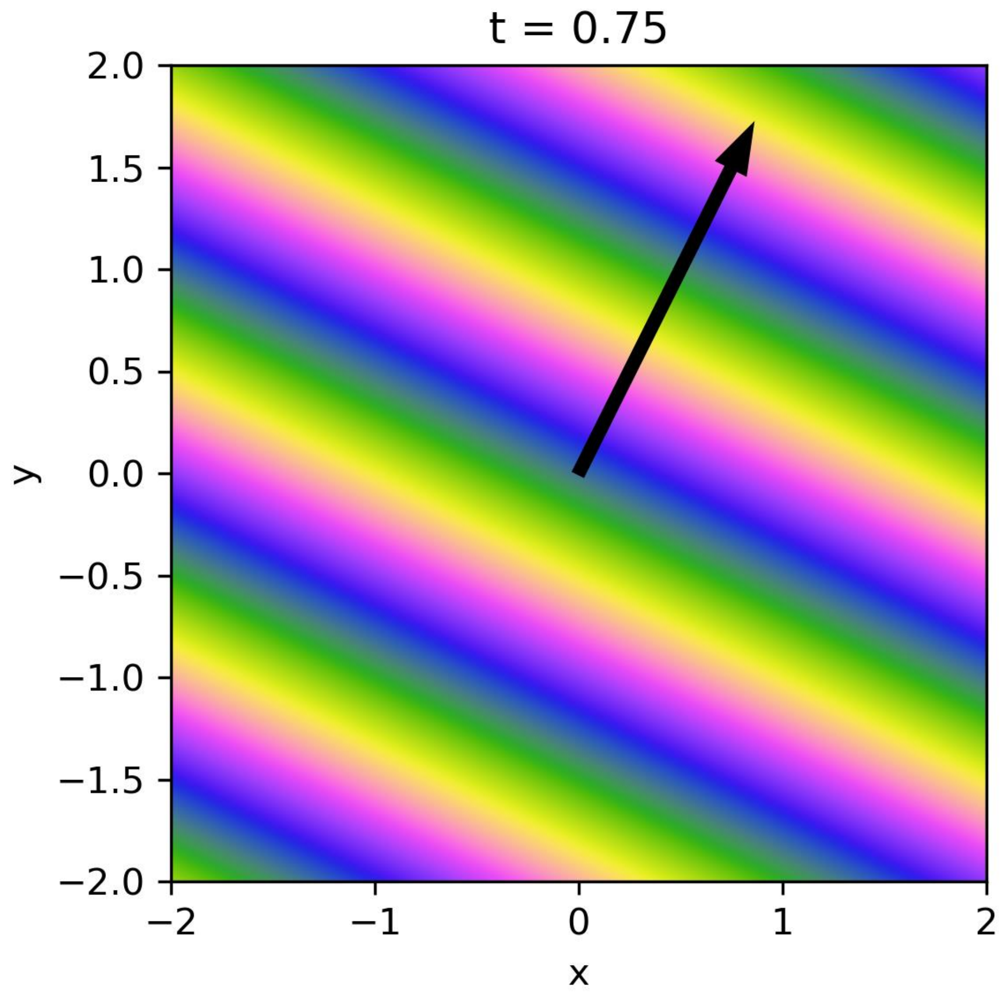
$$r = |x + iy|, \quad \theta = \mathrm{Arg}(x + iy)$$



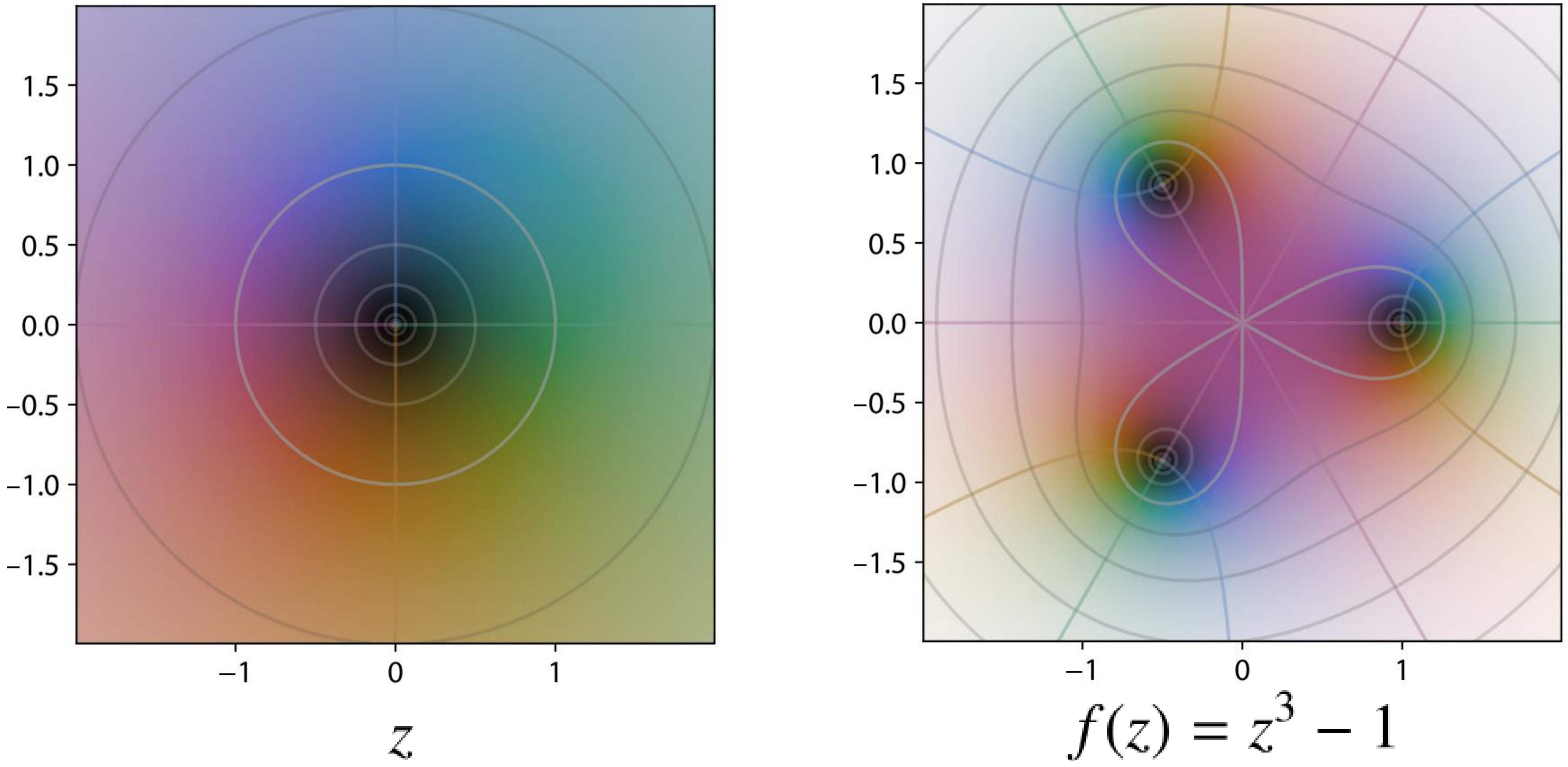
Example: Plane wave in 2d

$$\psi(\mathbf{r}, t) = \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$$

$$\omega = \pi, \quad \mathbf{k} = (0.75\pi, 1.5\pi)$$



Example from https://en.wikipedia.org/wiki/Domain_coloring



The idea of a pure function

- Which functions $f(z)$ are "pure functions of complex z"?

$$f(z) = z \qquad f(z) = a_0 + a_1 z + a_2 z^2 + \cdots a_n z^n \qquad f(z) = \frac{1}{z}$$

$$f(z) = \operatorname{Re} z = \frac{1}{2}(z + \bar{z})$$

Not "pure" 🙁

- "Pure" become infinitely differentiable!
- Beautiful and useful theorems on their behavior

Definition : Complex differentiability

The function $f : U \to \mathbb{C}$, $U \subset^{\text{open}} \mathbb{C}$, is (complex) differentiable at $z \in U$ if the limit

$$\lim_{h \to 0} \frac{f(z+h) - f(z)}{h} = f'(z) = \frac{\mathrm{d}f}{\mathrm{d}z} \tag{1}$$

exists. The expression $h \to 0$ means the same as in the $\mathbb{R}^2$ case.

If D is an open domain in $\mathbb{C}$, and if $f(z)$ is complex differentiable for all $z \in D$, we say that f is ~~*analytic*~~ *in D*.

holomorphic

The definition is *the same* as
in one-variable calculus,
BUT *h* can approach 0 in more ways!

Cauchy—Riemann equations

- A complex function $f : \mathbb{C} \to \mathbb{C}$ can be viewed as a function $f : \mathbb{R}^2 \to \mathbb{R}^2$

$$f(z) = u(x, y) + \mathrm{i}v(x, y)$$

- Consequence of complex differentiability:

Strongly restricts complex differentiable functions!

$$\frac{\partial u(x, y)}{\partial x} = \frac{\partial v(x, y)}{\partial y} \qquad \frac{\partial u(x, y)}{\partial y} = -\frac{\partial v(x, y)}{\partial x}$$

Example : Derivative of monomial

Let us apply the definition of the derivative to $f(z) = z^n$.

$$f(z+h) = (z+h)^n = z^n + hnz^{n-1} + \text{higher order terms.}$$

Thus

$$\frac{f(z+h) - f(z)}{h} = \frac{hnz^{n-1} + \text{h.o.t.}}{h} = nz^{n-1} + \text{h.o.t.},$$

so that the limit becomes

$$\frac{\mathrm{d}}{\mathrm{d}z} z^n = nz^{n-1} \tag{3}$$

We were able to perform the limit just by doing complex algebra. Notably, $z \in \mathbb{C}$ was completely arbitrary, so the derivative exists everywhere.

Notice how algebra is used, no limits needed

Example : Derivative of $\bar{z}$ does not exist

Let us try to see if $f(z) = \bar{z}$ is differentiable. Let us consider the limit $h = \delta x \to 0$ in $\mathbb{R}$.

$$\lim_{\delta x \to 0} \frac{f(x + \delta x + \mathrm{i}y) - f(x + \mathrm{i}y)}{\delta x} = \frac{\delta x}{\delta x} = 1. \tag{1}$$

However, if we allow $h = \mathrm{i}\delta y \to 0$ instad, with $\delta y \in \mathbb{R}$, then

$$\lim_{\delta y \to 0} \frac{f(x + \mathrm{i}(\delta y + y)) - f(x + \mathrm{i}y)}{\delta y} = \frac{-\mathrm{i}\delta y}{\delta y} = -\mathrm{i}. \tag{2}$$

Since the two limits are not the same, the complex limit cannot exist, since limits are unique.

This is in fact a very simple example of a continuous function from $\mathbb{C} \to \mathbb{C}$ which is not differentiable anywhere! Such an exampe is much harder to find for functions $\mathbb{R}^2 \to \mathbb{R}^2$.

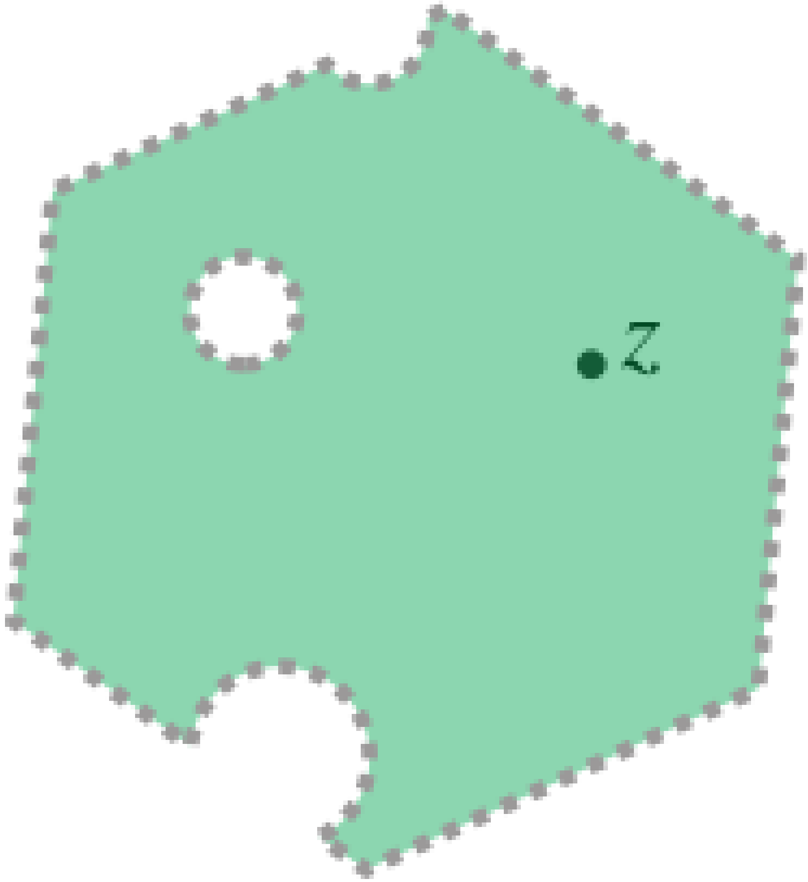
Re z is not complex differentiable either

Holomorphic functions

- Given $f : U \to \mathbb{C}$
- If f is complex differentiable at all $z \in U$
- We say that f is <u>holomorphic</u>
- *Cauchy-Riemann implies:*
  - *f is infinitely many times differentiable*

Etymology:
• **Holo-**: from the Greek word *holos*, meaning "whole" or "entire."
• **-morphic**: from the Greek word *morphē*, meaning "form" or "shape."

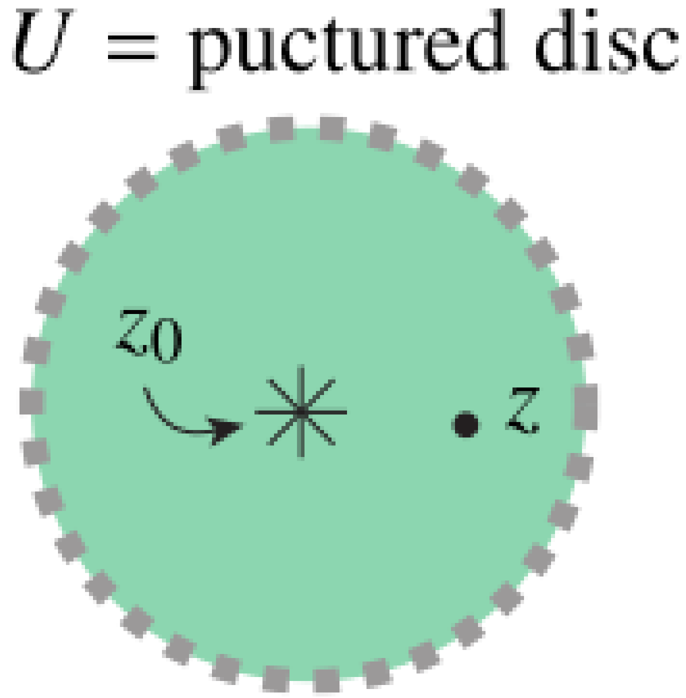
U = open subset of $\mathbb{C}$



Isolated singularities

- Suppose *f* is holomorphic in a punctured disc (z_0 not in set)
- We say that *f* has an <u>isolated singularity</u>
- Three options:

1. *Removable singularity:*
    - *f* can be extended to the hole
2. *Pole of order p:*
    - *f* cannot be extended, $f(z) \sim \dfrac{C}{(z - z_0)^p}$
3. *Essential singularity:*
    - *f* cannot be extended, does not behave like a pole



Holomorphic functions are analytic

- Recall that if *f* is differentiable

$$f(z+h) = f(z) + hf'(z) + O(h^2)$$

Small error

- But holomorphic means infinitely differentiable
- Remarkably, we have a convergent *power series*

$$f(z+h) = f(z) + hf'(z) + \frac{1}{2}h^2 f''(z) + \cdots$$

Infinite series, no error!

- *There is always a (possible infinitely large) disc where the series converges*

Example : Geometric series

The geometric series,

$$f(z) = \frac{1}{1-z} = 1 + z + z^2 + \cdots \qquad \text{for } |z| < 1. \tag{1}$$

The function $f(z)$ is complex differentiable at any $z \neq 1$:

$$f(z+h) = \frac{1}{1-z-h} = \frac{1}{1-z}\frac{1}{1-h/(1-z)} = \frac{1}{1-z}\left(1 + \frac{h}{1-z} + \text{h.o.t.}\right), \tag{2}$$

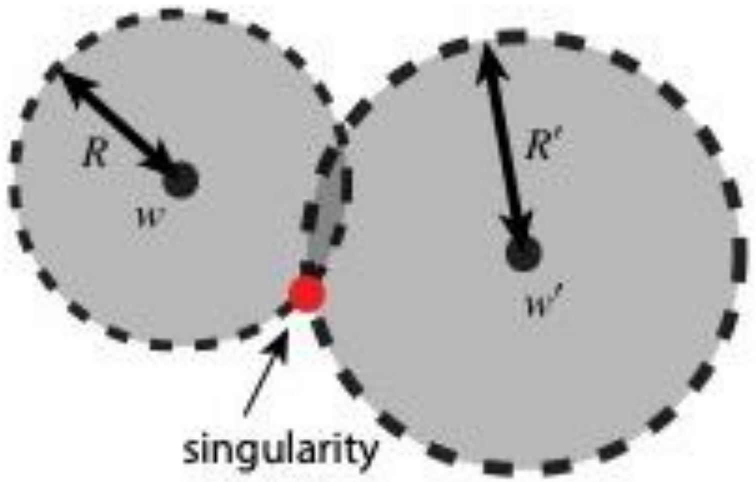
so that $f'(z) = \frac{1}{(1-z)^2}$.

We note that f is *divergent* as $z \to 1$, this is an example of a *pole* of f.

So functions can be defined as power series!

Convergence radius when starting from different points

- In general, one can develop power series around different points, converging to the *same function*
- *But the convergence radius can be different*
- Radius is determined by *closest singularity*, e.g., pole



Laurent series

No error!

- We can develop power series near a pole!

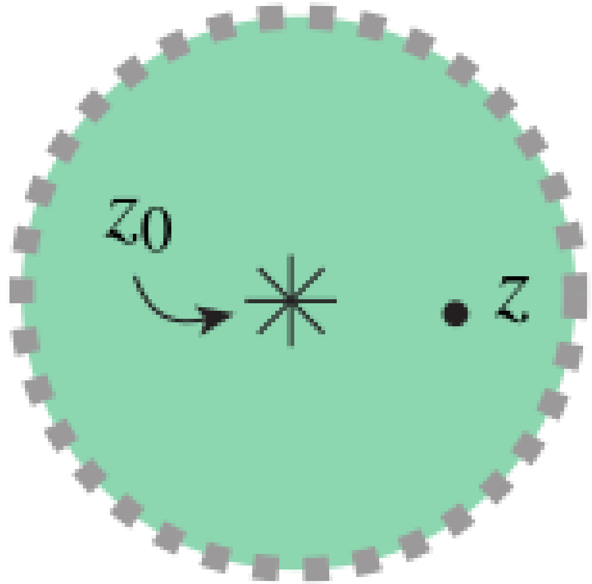
$$f(z) = \sum_{n=-p}^{\infty} c_n (z - z_0)^n$$

- Example:

$$\frac{1}{z(1-z)} = z^{-1} + 1 + z + z^2 + \cdots$$

Laurent expansion around pole at z=0

U = puctured disc



Removable singularity

- This function is defined everywhere except $z = 0$:

$$f(z) = \frac{e^z - 1}{z}$$

- By the usual rules for differentiation, it is holomorphic
- We Taylor expand around the origin and find:

$$f(z) = \frac{1 + z + z^2/2 - 1 + O(z^3)}{z} = 1 + \frac{1}{2}z + O(z^2)$$

- So we can define $f(0) = 1$ and we remove the singularity!

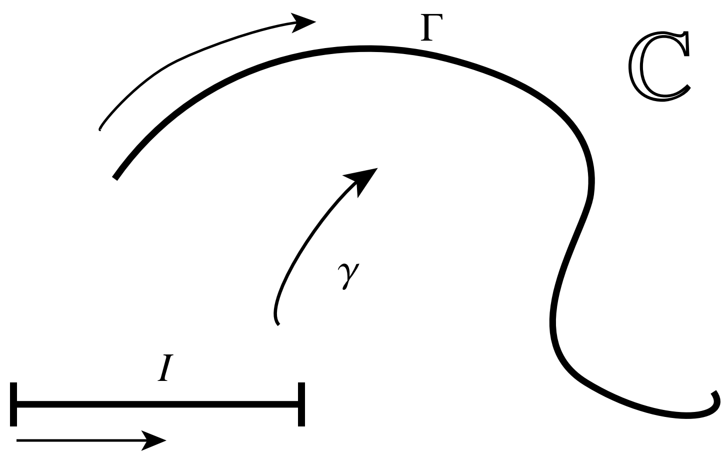
Complex line integrals

Definition : Complex line integral

Let $f : D \to \mathbb{C}$ be continuous, and let Γ be a (piecewise) smooth oriented curve parameterized by $\gamma : I \to \mathbb{C}$. The complex line integral of f along Γ is now defined as

$$\int_\Gamma f(z)\,\mathrm{d}z = \int_I f(\gamma(t))\gamma'(t)\,\mathrm{d}t, \tag{1}$$

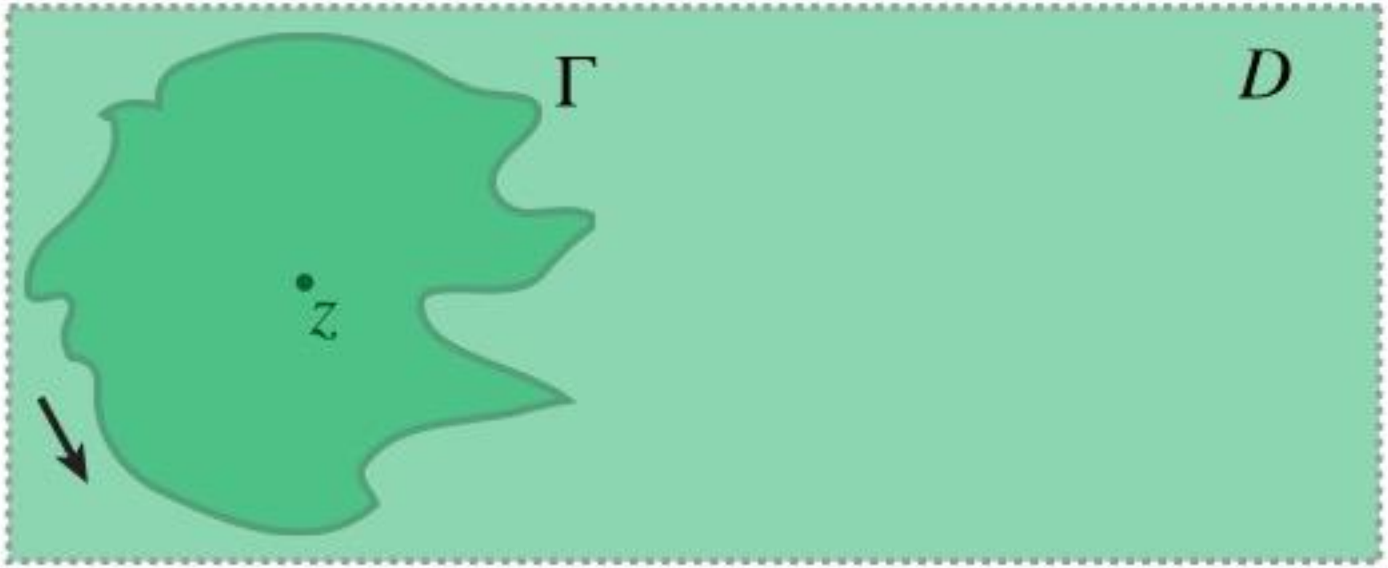
which is independent of parameterization. Note that $\mathrm{d}z = \gamma'(t)\mathrm{d}t$, an infinitesimally small piece of the curve.



Theorem : Cauchy theorem

Let $f : D \to \mathbb{C}$, where D is a simply connected open domain. Let Γ be a piecewise smooth simple closed curve in D. Then,

$$\oint_{\Gamma} f(z)\,\mathrm{d}z = 0. \tag{1}$$

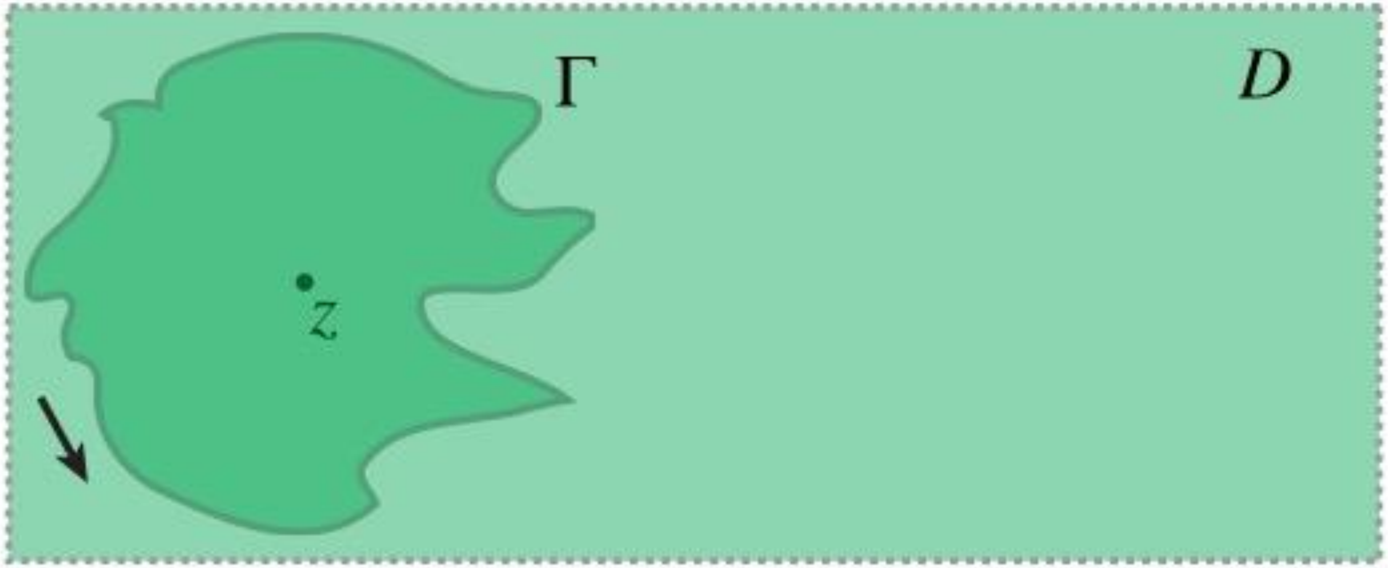


Theorem : Cauchy integral formula

Let the function $f : D \to \mathbb{C}$ be complex differentiable, and let Γ be a simple closed curve in D. Then,

$$f(z_0) = \frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z - z_0} \, dz. \quad (1)$$

The value of the function depends only on the value on the curve!



Theorem

Let D be simply connected, and let $f : D \to \mathbb{C}$ be complex analytic in D. Then f is *infinitely* many times differentiable, and we have the power series representation

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n, \quad \text{where} \quad a_n = \frac{f^{(n)}(z)}{n!} \tag{1}$$

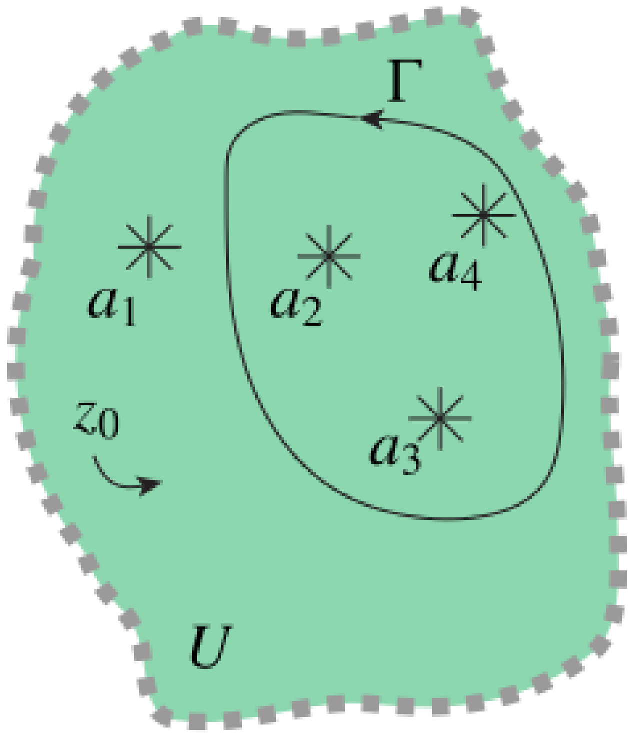
The derivatives are given by the formula

$$f^{(n)}(z) = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma \frac{f(w)}{(w - z)^{n+1}} \, \mathrm{d}w. \tag{2}$$

Cauchy residue theorem

$$U_0 = U \setminus \{a_1, a_2, \cdots\}$$

Recall Laurent: $$f(z) = \sum_{n=-p}^{\infty} c_n (z - z_0)^n$$



Definition of residue at singularity:

$$\mathrm{Res}(f, z_0) = c_{-1}$$

Residue theorem: If f holomorphic in U_0

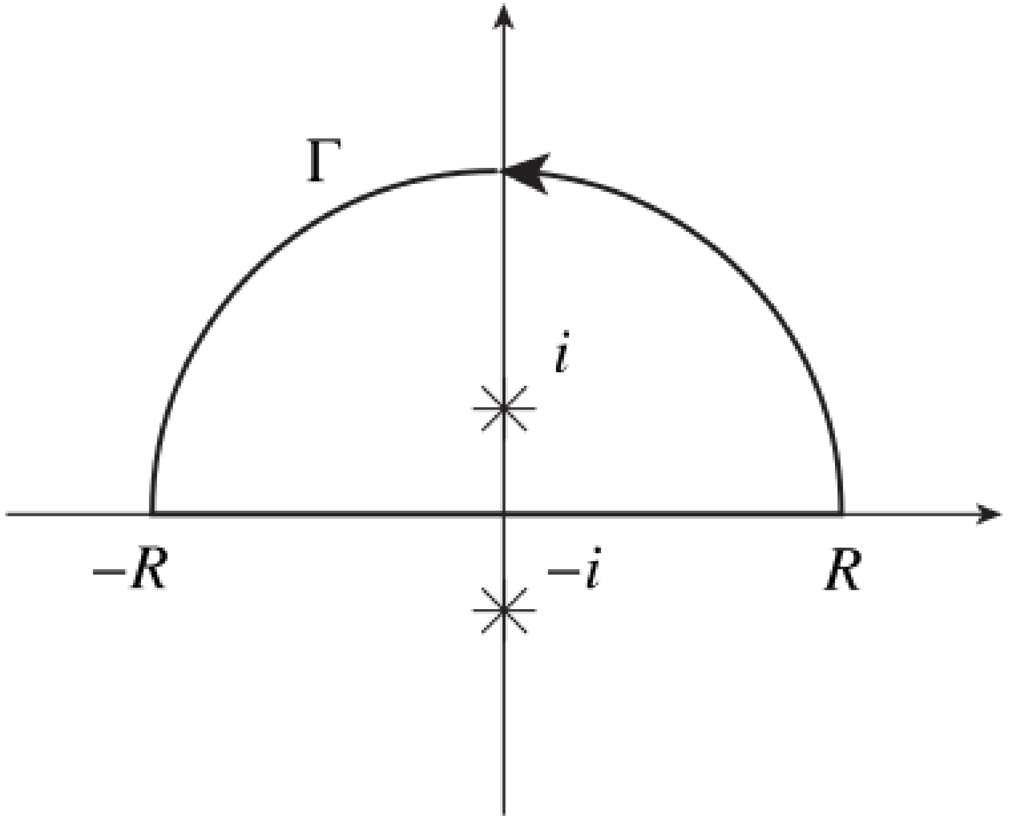
$$\oint_\Gamma f(z)\, dz = 2\pi i \sum \mathrm{Res}(f, a_k)$$

Sum over holes inside curve

Example: Evaluation of integral

- Task: compute: $\int_{-\infty}^{\infty} \frac{1}{x^2+1}\,dx$
- Use residue theorem on Γ
- Find Laurent expansion around *i*
  - *Res(f,i) = 1/(2i)*
- Integral over semicircle is small, only integral on [-*R*,*R*] left
- Take limit as *R* to infinity

$$\lim_{R\to\infty}\int_{-R}^{R} \frac{1}{x^2+1}\,dx = 2\pi i\frac{1}{2i} = \pi$$



$$x^2+1 = (x+i)(x-i)$$

Fourier series and transform

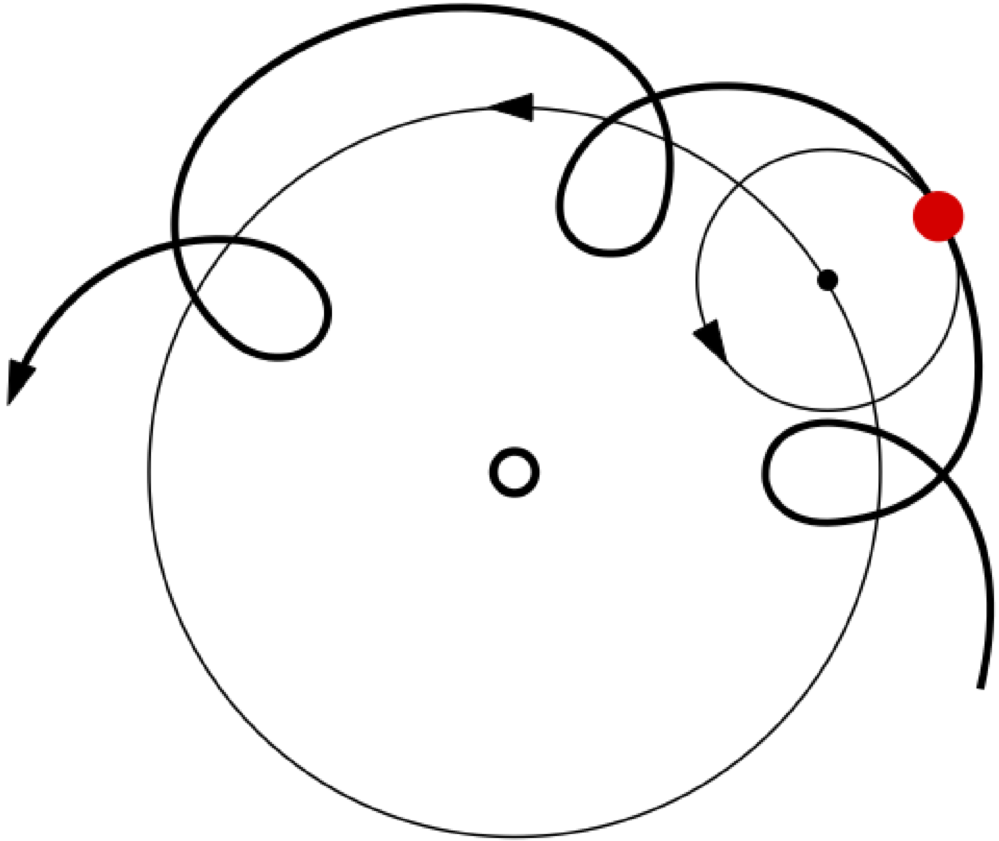
What is Fourier theory good for?

- Some partial differential equations become simpler
  - Poisson equation ...
- Plane-wave basis sets
  - Solid state systems, crystals ...
- Response theory
  - How a quantum system responds to periodic perturbations (e.g., EM waves)
- Signal processing, image analysis

Epicycles of planetary motion

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

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



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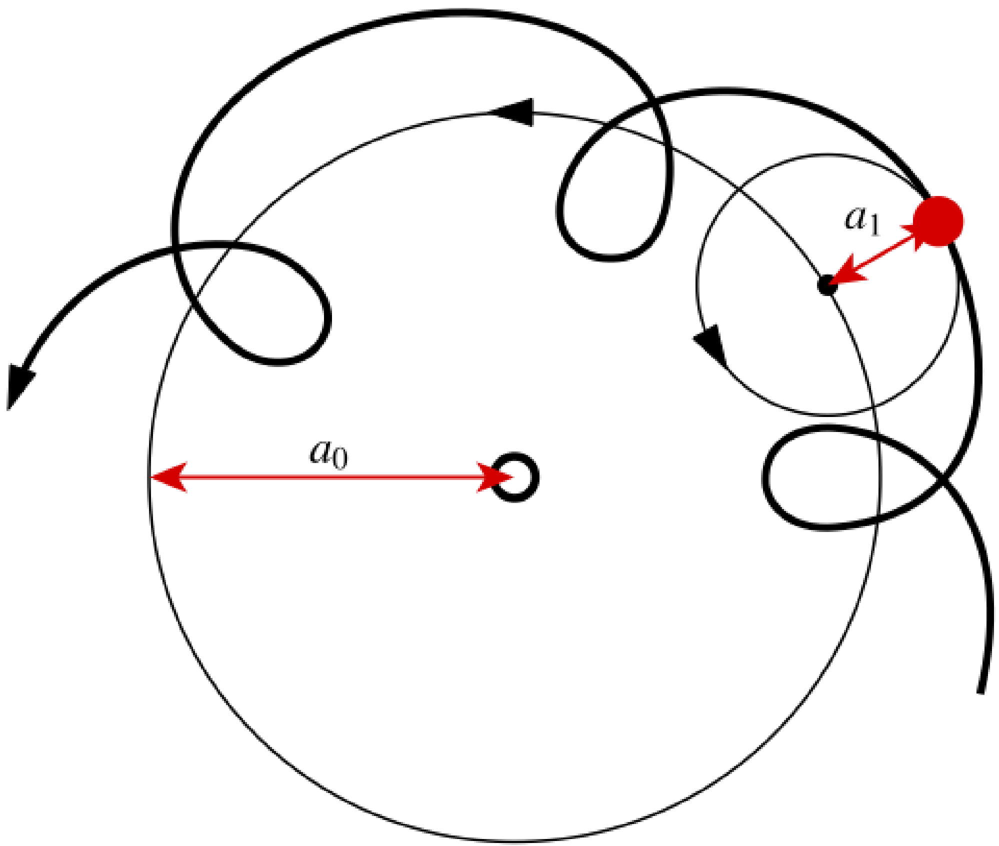
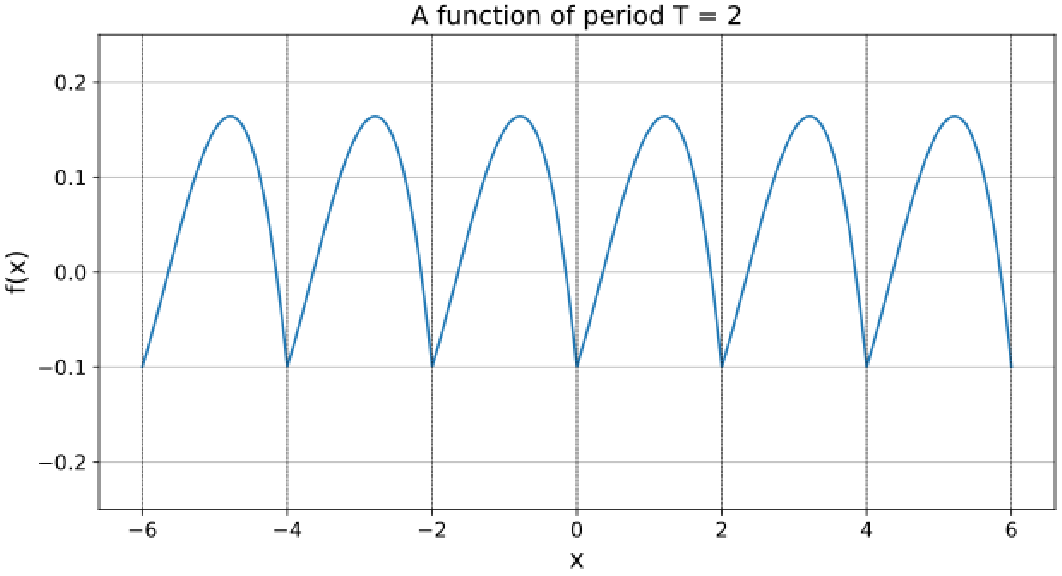
- (The ancient Greeks did not use complex numbers)



Joseph Fourier (1768-1830)

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



Complex Fourier series

- Let $f : \mathbb{R} \to \mathbb{C}$
- The function is *periodic with period T if*

$$f(t + T) = f(t)$$

- Consider now a *Fourier series*

$$\tilde{f}(t) = \sum_{n \in \mathbb{Z}} c_n e^{2\pi i n t/T}, \quad c_n \in \mathbb{C}$$

- Assuming convergence of series, clearly a periodic function

The exponential functions are periodic, shorter and shorter period

Can we find a series such that

$$\tilde{f}(t) = f(t)$$

?

Theorem: Complex Fourier series

- Let $f : \mathbb{R} \to \mathbb{C}$
- Periodic with period T
- Square integrable in $[0,T]$: $$\int_0^T |f(t)|^2 \, dt < +\infty$$

- *Let* $c_n = \frac{1}{T} \int_0^T e^{-2\pi i n t/T} f(t) \, dt$ *and* $\tilde{f}(t) = \sum_{n \in \mathbb{Z}} c_n e^{2\pi i n t/T}, \quad c_n \in \mathbb{C}$

- *Then* $\tilde{f}(t) = f(t)$ *"almost everywhere"*

In terms of infinite dimensional Hilbert

- The exponential functions are orthonormal basis functions for $L^2[0,T]$

$$\phi_n(t) = \frac{1}{\sqrt{T}} e^{2\pi int/T} \qquad \langle \phi_n, \phi_m \rangle = \frac{1}{T} \int_0^T e^{2\pi i(m-n)t/T} \, dt = \delta_{n,m}$$

- Fourier series ”just” a basis expansion!
- But an L^2 function only defined up to “sets of zero length”, so convergence not necessarily everywhere

Examples

- We watch a Jupyter notebook with Fourier series of
  - Square wave
  - Sawtooth wave
  - ...

Dirichlet conditions

Conditions on *f* such that Fourier series converges *everywhere*

1. Must be periodic
2. A finite number of maxima and minima in one period
3. A finite number of discontinuities

- Under these conditions, the series converges everywhere
- Except at discontinuities, where it converges to average of ”jump”
  - See, e.g., square wave example

Sine/cosine series

- Using Euler's formula: $$e^{2\pi int/T} = \cos\left(\frac{2\pi nt}{T}\right) + i\sin\left(\frac{2\pi nt}{T}\right)$$

- We rewrite the Fourier series:

$$\tilde{f}(t) = \sum_{n\in\mathbb{Z}} c_n e^{2\pi int/T}, \quad c_n \in \mathbb{C}$$

$$\tilde{f}(t) = \frac{b_0}{2} + \sum_{n=1}^{\infty} b_n \cos\left(\frac{2\pi nt}{T}\right) + a_n \sin\left(\frac{2\pi nt}{T}\right)$$

$$b_n = c_n + c_{-n}, \quad a_n = i(c_n - c_{-n})$$

Equivalent series, but sine/cosine can be more useful sometimes

Fourier transform

- For functions that are *not periodic:*

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

- The (normalized) Fourier transform is defined as:

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

- Fact: The transform is a *unitary transformation on* $f \in L^2(\mathbb{R};\mathbb{C})$

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

Inverse Fourier transform

- Since transform is unitary, it must have an inverse:

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

Sign in exponent only difference

- What a beautiful symmetry!

Examples

- Jupyter notebook

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

Duality of differentiation and multiplication

- Consider the very informal manipulation:

$$\begin{aligned}\frac{\partial}{\partial x} f(x) &= \frac{1}{\sqrt{2\pi}} \frac{\partial}{\partial x} \int_{\mathbb{R}} e^{ikx} \hat{f}(k)\, dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \left[\frac{\partial}{\partial x} e^{ikx} \right] \hat{f}(k)\, dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} [ik\hat{f}(k)]\, dk\end{aligned}$$

True in Sobolev space

$H^1 = W^{1,2}$

- Suggests, and indeed so: $\left[\frac{\partial f}{\partial x}\right]^{\wedge} = ik\hat{f}$

Duality of smoothness and falloff

- Suppose we can differentiate f a number of times:

$$\frac{\partial^m f}{\partial x^m} \in L^2(\mathbb{R};\mathbb{C})$$

- Since Fourier transform is unitary we must have

$$k^m \hat{f}(k) \in L^2(\mathbb{R};\mathbb{C})$$

$$\hat{f}(k) \sim k^{-m-1/2} \text{ as } |k| \to +\infty, \text{ worst case scenario}$$

Not entirely rigorous statement ...

Example: Filtering an image

- A Jupyter notebook showing high-pass and low-pass filtering using Fast Fourier Transform (FFT)

Last slide

- *Thanks for joining the journey!*
- Make sure to check out the maps, literature and YouTube recs:
- https://simenkva.github.io/esqc_material/