Numerical methods combine many fields of math:

- Approx. theory, representation theory, linear algebra, ODEs, PDEs, CS, ...

PDEs are the language of continuum mechanics:

- Solid mechanics & fluid dynamics across fields

Broad opportunities for collaboration on the math-science spectrum.

Review of basic numerical methods

Poisson eqn

$$-\Delta u(x) = f(x), \qquad x \in \mathbb{R}^D$$

$$+ \text{BCs}$$

Here Δ is the "Laplacian"

$$\underset{\substack{\uparrow \\ \text{math} \\ \text{notation}}}{\Delta f} = \underset{\substack{\uparrow \\ \text{physics} \\ \text{notation}}}{\nabla^2 f} = \nabla \cdot \nabla f = (\partial_x \partial_x + \partial_y \partial_y + \partial_z \partial_z) f$$

Many applications:

1) Gauss' law for gravity

$$\vec{g} = -\nabla \phi$$

$$\nabla \cdot \vec{g} = -\nabla^2 \phi = -4\pi G \underset{\substack{\uparrow \\ \text{density} \\ \text{field}}}{\rho} (x)$$

2) Fluid dynamics

Incompressible Navier-Stokes

$$\begin{cases} \partial_t \vec{u} + \vec{u}\cdot\nabla\vec{u} = -\nabla p + \nu\nabla^2\vec{u} + \vec{f} \\ \nabla\cdot\vec{u} = 0 \end{cases}$$

$$\rightarrow \quad -\nabla^2 p = \nabla\cdot\left(\vec{u}\cdot\nabla\vec{u} - \vec{f}\right)$$

3) Steady-state heat/diffusion:

$$\partial_t T = \kappa\nabla^2 T + S(x)$$

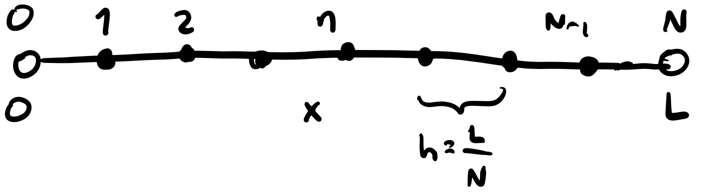
$$\partial_t = 0 \rightarrow -\nabla^2 T = \kappa^{-1} S(x)$$

Consider 1D problem, $x \in [0,L]$

"Dirichlet" boundary conditions: $u(0) = a$

$u(L) = b$

Standard approach: discretize onto grid



$$x_n = \frac{nL}{N} = nh$$

Want to solve for $u_n = u(x_n)$ on the grid.

This discretization turns the differential equation into a linear algebra problem (solve a matrix).

Approximate derivatives using finite differences/Taylor series

$$u'(x) = \frac{u(x+h) - u(x)}{h} + \mathcal{O}(h)$$

$$= \frac{u(x) - u(x-h)}{h} + \mathcal{O}(h)$$

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + \mathcal{O}(h^2)$$

$$\rightarrow u_n'' = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \mathcal{O}(h^2)$$

$$\frac{1}{h^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 + a/h^2 \\ f_2 \\ \vdots \\ \\ f_{N-1} + b/h^2 \end{bmatrix}$$

Matrix system: $D^2 \cdot \vec{u} = \vec{f}_{pert}$, $\quad \vec{u} \in \mathbb{R}^N$

- Banded matrix
- Bandwidth based on stencil size: $B = k+1$
- Solve in $\mathcal{O}(NB^2)$ time, error $\mathcal{O}(N^{-k})$

⌈ Fast solver: linear in N

Algebraic accuracy: polynomial in N ⌋

Spectral function approximation

Let's go back to accuracy. Increasing k makes the matrix slower to solve. Also encounter Runge phenomenon as $k \to N$. This is the limit of "global interpolation": use whole function to understand local behavior. Good idea, but proper way is to use expansions in orthogonal global basis functions rather than Taylor series.

Pick global functions $\{\phi_n(x)\}$ that are orthogonal under some inner product:

$$\langle \phi_n | \phi_m \rangle = \int \phi_n^*(x)\, \phi_m(x)\, w(x)\, dx = \delta_{n,m}$$

Spectral representation of $u(x)$ are the expansion coeffs $\{\hat{u}_n\}$:

$$u(x) = \sum_{n=0}^{\infty} \hat{u}_n \phi_n(x), \qquad \hat{u}_n = \langle \phi_n | u \rangle$$

We want basis functions that give quickly converging expansions for smooth functions.

Fundamental example: Fourier series for functions on the circle.

$$\phi_n = e^{inx}, \quad w(x) = \frac{1}{2\pi}, \quad x \in [0, 2\pi)$$

Theorem: If $f^{(i)}$ is periodic & continuous for $i=0,\dots,k-2$ and $f^{(k)}$ is integrable, then $\exists C$ s.t. $|\hat{f}_n| \le C|n|^{-k}$.

So continuous differentiability gives *algebraic index* of convergence. If $f \in C^\infty$, then Fourier series converges *exponentially*, faster than any polynomial in n.

Spectral numerical methods are an alternative to finite differences. Instead of finding $u(x)$ on a discrete grid, try to find the first N series coefficients:

$$u_N(x) = \sum_{n=0}^{N-1} \hat{u}_n \phi_n(x) \approx u(x)$$

The *truncation error* of this discretization is the error from neglecting terms with $n \ge N$.

$$E_T(N) = |u(x) - u_N(x)| = \Big|\sum_{n\ge N} \hat{f}_n \phi_n(x)\Big|$$

$$\le \sum_{n \ge N} |\hat{f}_n|$$

If u has algebraic convergence: $|\hat{u}_n| \sim \mathcal{O}(n^{-k})$

$$E_T(N) \sim \mathcal{O}(N^{-k+1}) \sim \mathcal{O}(N|\hat{f}_N|)$$

If u has exponential convergence: $|\hat{u}_n| \sim \mathcal{O}(e^{-\mu n})$

$$E_T(N) \sim \mathcal{O}(e^{-\mu N}) \sim \mathcal{O}(|\hat{f}_N|).$$

The last retained coefficient scales with the error (built-in error estimate), and this converges exponentially in N for PDEs with smooth solutions.

Spectral PDEs

We discretize a PDE by inserting the spectral solution and project the PDE against the basis functions:

$$\langle \phi_m | -\kappa \nabla^2 \sum_n \hat{u}_n \phi_n \rangle = \langle \phi_m | \sum_n \hat{f}_n \phi_n \rangle$$

$$-\kappa \sum_n \hat{u}_n \underbrace{\langle \phi_m | \nabla^2 \phi_n \rangle}_{\hat{D}^2_{mn}} = \sum_n \hat{f}_n \underbrace{\langle \phi_m | \phi_n \rangle}_{\delta_{mn}}$$

$$-\kappa \sum_n \hat{D}^2_{mn} \hat{u}_n = \hat{f}_m$$

$$-\kappa \hat{D}^2 \cdot \hat{u} = \hat{f}$$

Same as before, but now $\vec{u} \to \hat{u}$, $D^2 \to \hat{D}^2$.

What is $\hat{D}^2$?

$$\hat{D}^2_{mn} = \langle \phi_m | \nabla^2 \phi_n \rangle$$

$$= \frac{1}{2\pi} \int_0^{2\pi} e^{-imx} \partial_x^2 e^{inx} dx = -n^2 \delta_{m,n}.$$

Fourier modes are eigenfunctions of the derivative

$\Rightarrow$ constant coeff. linear diff ops have diagonal representation in Fourier series.

Faster & exponentially accurate!

These methods generalize to multiple dimensions & systems of equations. Fourier spectral methods like this are the basis for the largest turbulence simulations in the world.

Beyond periodic boxes

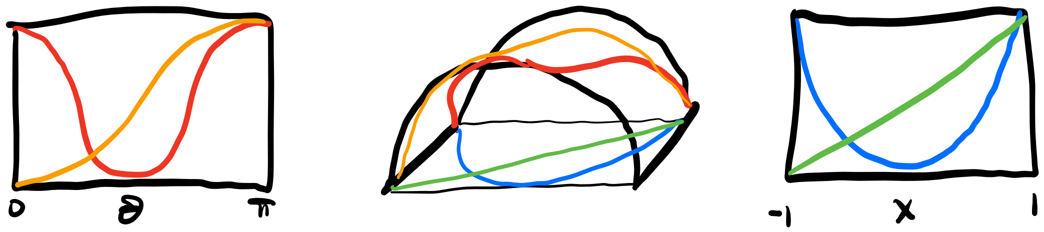
Fourier series work for periodic dimensions. For others, use orthogonal polynomials. In particular, the Chebyshev polys:

$$T_n(x) = \cos(n\theta), \quad \theta = \cos^{-1}(x), \quad x \in [-1,1].$$

Can show (pset) that these are orthogonal with weight $w(x) = \frac{1}{\sqrt{1-x^2}}$.

and $\deg(T_n) = n$.

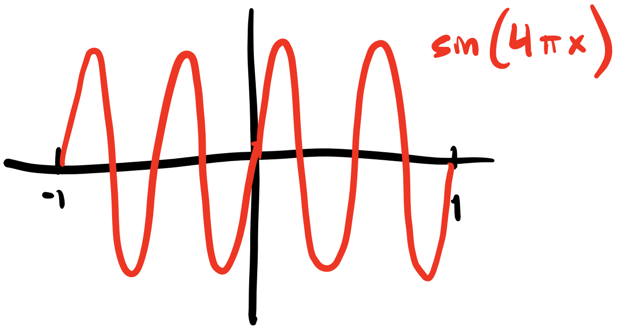
Geometrically these are the projections of cosine modes on the cylinder onto the plane:

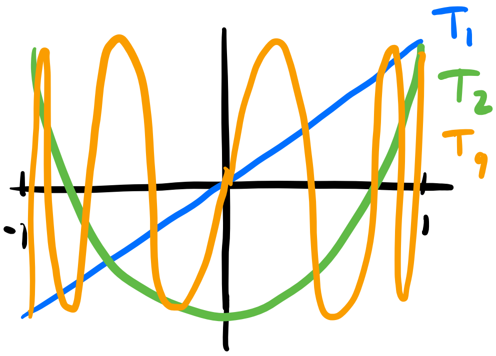


Great things follow from this connection:

- Same convergence theory, but now for general functions on [-1,1] (periodicity of f and $f^{(k)}$ no longer required).

Example: Chebyshev expansion of $\sin(k\pi x)$

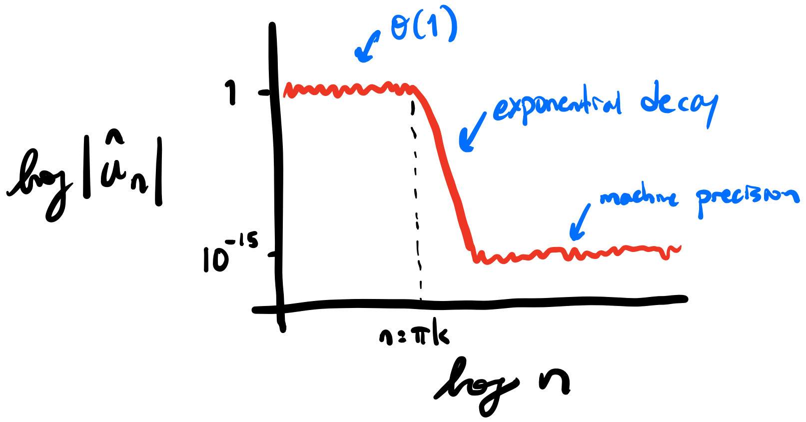




Chebyshev poly's oscillate faster near endpoints.

Need $N \approx \pi \cdot k$ to resolve same lengthscale near $x=0$.

$\Rightarrow$ Numerical spectrum



Differential operators are no longer diagonal (can't be), but can be made banded with some tricks.

Current research in "modern spectral methods": find bases and solvers for more geometries maintaining:

1) Fast runtimes (quasi-linear in N)
2) Spectral (exponential) accuracy
3) Equation flexibility