FWAM Session B: Function Approximation and Differential Equations

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Wednesday afternoon, 10/30/19

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LECTURE 1

interpolation, integration, differentiation, spectral methods

Goals and plan

Overall: graph of $f(x)$ needs ∞ number of points to describe, so how handle f to user-specified accuracy in computer w/ least cost? (bytes/flops)

- Interpolation: also key to numerical ODE/PDEs...
  task: given exact $f(x_j)$ at some x_j, model $f(x)$ at other points x?

  App: cheap but accurate "look-up table" for possibly expensive func.

  Contrast: fit noisy data = learning (pdf for) params in model, via likelihood/prior
- Numerical integration:

  App: computing expectation values, given a pdf or quantum wavefunc.

  App: integral equation methods for PDEs (Jun Wang's talk)
- Numerical differentiation:

  App: build a matrix (linear system) to approximate an ODE/PDE (Lecture II)

  App: get gradient ∇f, eg for optimization (cf adjoint methods)

Key concepts:
convergence rate, degree of smoothness of f, global vs local,
spectral methods, adaptivity, rounding error & catastrophic cancellation

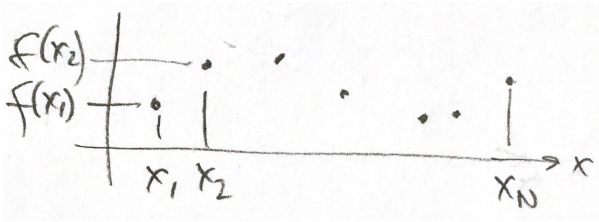
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

Interpolation in 1D ($d = 1$)

Say $y_j = f(x_j)$ known at nodes $\{x_j\}$ N-pt "grid"

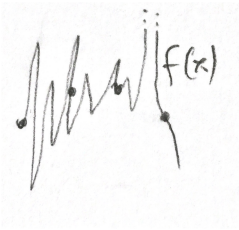
note: exact data, not noisy

want interpolant $\tilde{f}(x)$, s.t. $\tilde{f}(x_j) = y_j$



hopeless w/o assumptions on f, eg smoothness, otherwise...

- extra info helps, eg f periodic, or $f(x) = \text{smooth} \cdot |x|^{-1/2}$

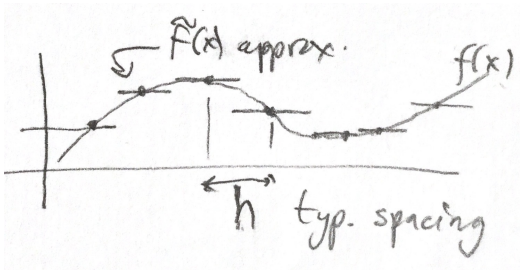


Simplest: use value at x_j nearest to x

"snap to grid"

Error $\max_x |\tilde{f}(x) - f(x)| = \mathcal{O}(h)$ as $h \to 0$

holds if f' bounded; ie f can be nonsmooth but not crazy

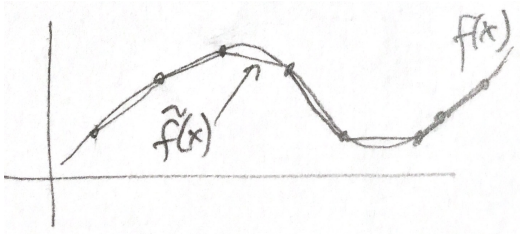


Recap notation "$\mathcal{O}(h)$": exists C, h_0 s.t. error $\leq Ch$ for all $0 < h < h_0$

Piecewise linear: "connect the dots"

max error $= \mathcal{O}(h^2)$ as $h \to 0$

needs f'' bounded, ie smoother than before



Message: a higher order method is *only* higher order if f smooth enough

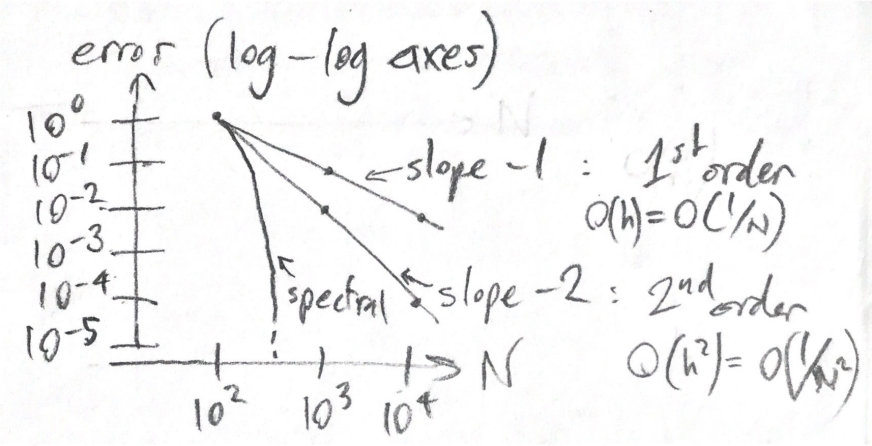
Interlude: convergence rates

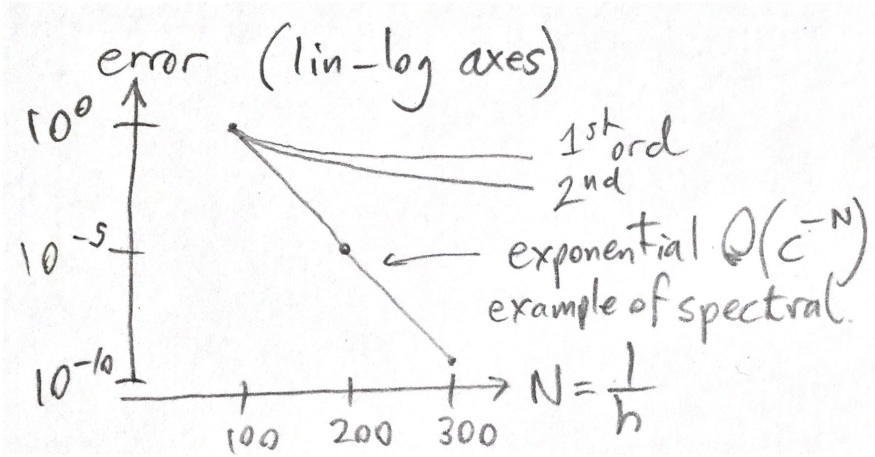
Should know or measure convergence rate of any method you use

- "effort" parameter N eg # grid-points $= 1/h^d$ where h = grid spacing, d = dim

We just saw algebraic conv. error $= \mathcal{O}(N^{-p})$, for order $p = 1, 2$

There's only one graph in numerical analysis: "relative error vs effort"





Note how spectral gets many digits for small N crucial for eg 3D prob.

"spectral" = "superalgebraic", beats $\mathcal{O}(N^{-p})$ for any p

- how many digits to you want? for 1-digit (10% error), low order ok, easier to code

<rant> test your code w/ *known exact soln* to check error conv. <\rant>

How big is prefactor C in error $\leq Ch^p$? Has asymp. rate even kicked in yet? :)

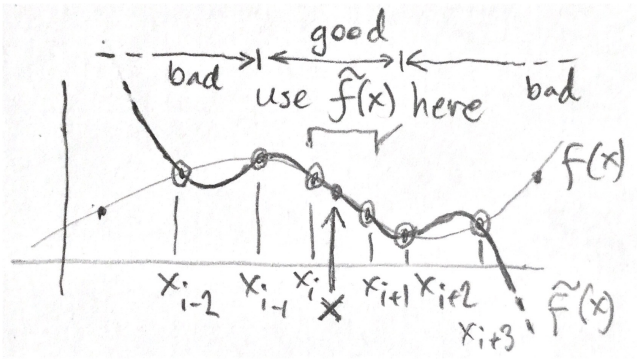
Higher-order interpolation for smooth f: the local idea

Pick a p, eg 6. For any target x, use only the nearest p nodes:

Exists unique degree-$(p-1)$ poly, $\sum_{k=0}^{p-1} c_k x^k$
which matches local data $(x_j, y_j)_{j=1}^{p}$

generalizes piecewise lin. idea

do not eval poly outside its central region!



- error $\mathcal{O}(h^p)$, ie high order, but $\tilde{f}$ *not* continuous ($\tilde{f} \notin C$) has small jumps

  if must have cont, recommend splines, eg cubic $p = 3$: $\tilde{f} \in C^2$, meaning $\tilde{f}''$ is cont.

How to find this degree-$(p-1)$ poly?

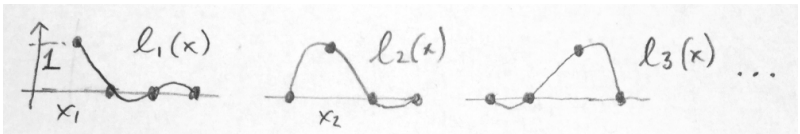
1) crafty: solve square lin sys for coeffs $\sum_{k<p} x_j^k c_k = y_j \qquad j = 1, \ldots, p$

   ie, $V\mathbf{c} = \mathbf{y}$ V="Vandermonde" matrix, is ill-cond. but works

2) traditional: barycentric formula $\tilde{f}(x) = \dfrac{\sum_{j=1}^{p} \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^{p} \frac{1}{x-x_j} w_j}$ $\qquad w_j = \frac{1}{\prod_{i \neq j}(x_j - x_i)}$

   [Tre13, Ch. 5]

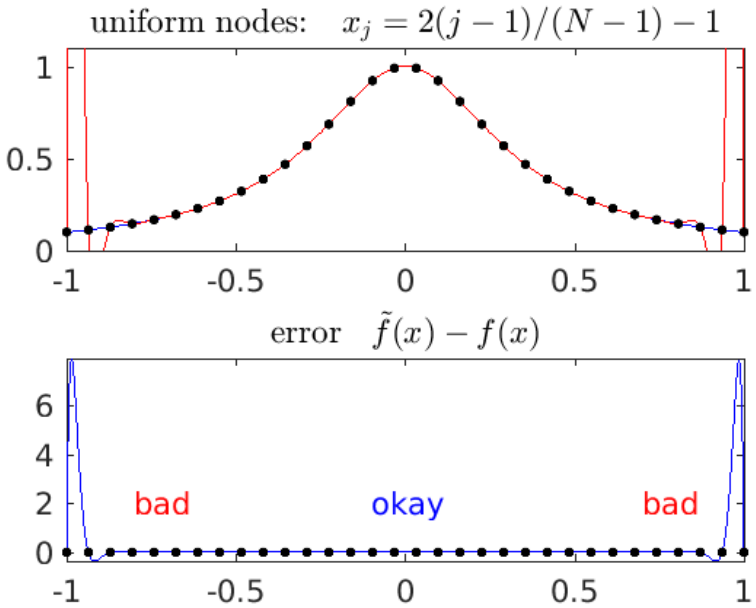
Either way, $\tilde{f}(x) = \sum_{j=1}^{p} y_j \ell_j(x)$ where $\ell_j(x)$ is jth Lagrange basis func:

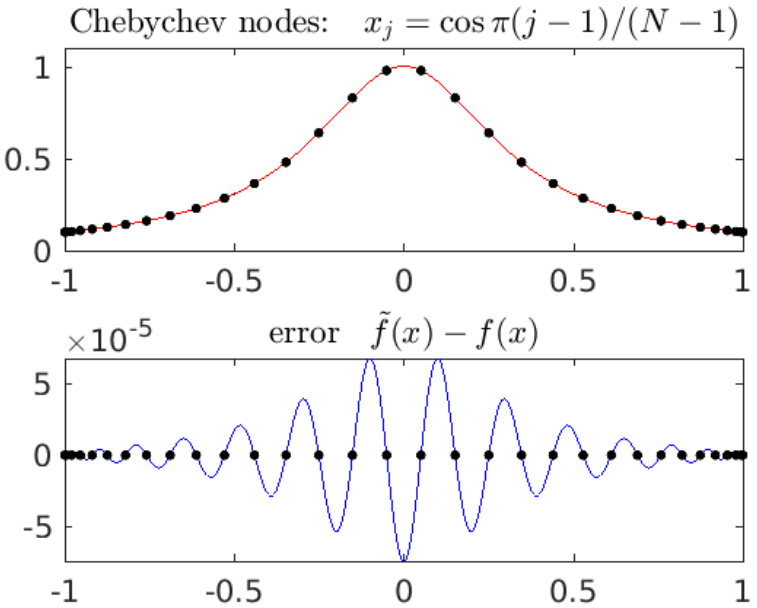


Global polynomial (Lagrange) interpolation?

Want increase order p. Use *all* data, get single $\tilde{f}(x)$, so $p = N$? "global"

$p = N = 32$, smooth (analytic) $f(x) = \frac{1}{1+9x^2}$ on $[-1, 1]$: (Runge 1901)





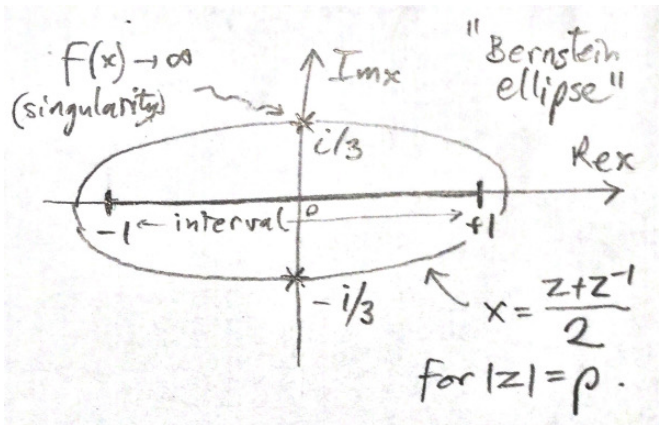
- warning: unif. grid, global interp. fails → only use locally in central region

But exists good choice of nodes...

"Chebychev": means non-unif. grid density $\sim \frac{1}{\sqrt{1-x^2}}$

- our first spectral method
  max err $= \mathcal{O}(\rho^{-N})$ exponential conv!

  $\rho > 1$ "radius" of largest ellipse in which f analytic



Node choice and adaptivity

Recap: poly approx. $f(x)$ on $[a,b]$: exist good & bad node sets $\{x_j\}_{j=1}^N$

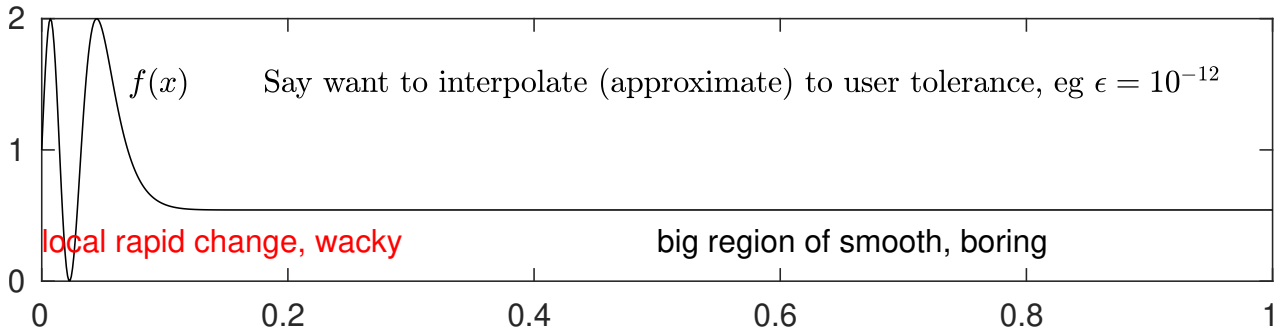
Question: Do *you* get to choose the set of nodes at which f known?

- data fitting applications: No (or noisy variants: kriging, Gaussian processes, etc)

  use local poly (central region only!), or something stable (eg splines) [GC12]
- almost all else, interp., quadrature, PDE solvers: Yes so pick good nodes!

Adaptivity idea

global is inefficient if f smooth in most places, but not everywhere



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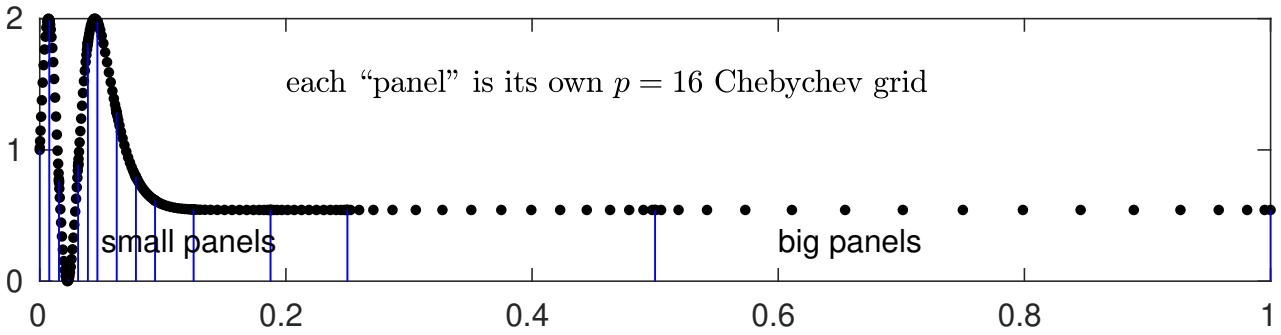


automatically split (recursively) panels until max err $\leq \epsilon$

via test for local error

1D adaptive interpolator codes to try:

- `github:dbstein/function_generator` py+numba, fast (Stein '19)
- `chebfun` for MATLAB big-N Cheb. grids done via FFTs! (Trefethen et al.)

App.: replace nasty expensive $f(x)$ by cheap one! optimal "look-up table"

Global interpolation of periodic functions I

Just did f on intervals $[a,b]$. global interp. (& integr., etc.) of smooth *periodic* f differs!

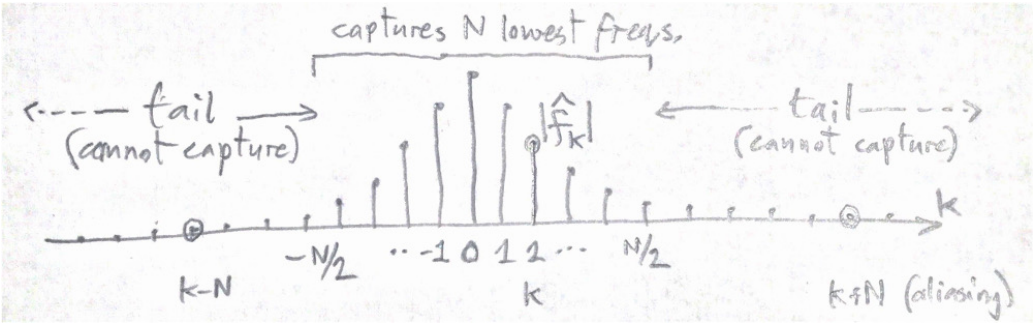
Periodic: $f(x+2\pi) = f(x)$ for all x, $\quad f(x) = \sum_{n\in\mathbb{Z}} \hat{f}_k e^{ikx}$ Fourier series

Instead of poly's, use truncated series $\quad \tilde{f}(x) = \sum_{|k|<N/2} c_k e^{ikx}$ "trig. poly"

What's best you can do?

get N coeffs right $c_k = \hat{f}_k$

error $\sim$ size of tail $\{\hat{f}_k\}_{|k|\geq N/2}$



How read off c_k from *samples* of f on a grid?

uniform grid best (unlike for poly's!); non-uniform needs linear solve, slow $\mathcal{O}(N^3)$ effort

Uniform grid $x_j = \frac{2\pi j}{N}$, $\quad$ set $c_k = \frac{1}{N}\sum_{j=1}^{N} e^{ikx_j} f(x_j)$ simply $\mathbf{c} = FFT[\mathbf{f}]$

easy to show $c_k = \cdots + \hat{f}_{k-N} + \hat{f}_k + \hat{f}_{k+N} + \hat{f}_{k+2N} + \ldots$

$= \hat{f}_k$ desired $+ \sum_{m\neq 0} \hat{f}_{k+mN}$ aliasing error, small if tail small

Summary: given N samples $f(x_j)$, interp. error = truncation + aliasing

a crude bound is $\max_{x\in[0,2\pi)} |\tilde{f}(x) - f(x)| \leq 2 \sum_{|k|\geq N/2} |\hat{f}_k|$

ie error controlled by sum of tail

Global interpolation of periodic functions II

As grow grid N, how accurate is it? just derived err $\sim$ sum of $|\hat{f}_k|$ in tail $|k| \geq N/2$

Now $\hat{f}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-ikx}dx = \frac{1}{2\pi}\int_0^{2\pi} f^{(p)}(x)\frac{e^{-ikx}}{(ik)^p}dx$ integr. by parts p times

So for a periodic $f \in C^p$, recall first p derivs of f bounded
$\hat{f}_k = \mathcal{O}(k^{-p})$, tail sum $\mathcal{O}(N^{1-p})$ $(p-1)$th order acc. (better: [Tre00])

Example of: f smoother $\leftrightarrow$ faster $\hat{f}_k$ tail decay $\leftrightarrow$ faster convergence

Even smoother case: f analytic, so $f(x)$ analytic in some complex strip $|\operatorname{Im} x| \leq \alpha$
then $\hat{f}_k = \mathcal{O}(e^{-\alpha|k|})$, exp. conv. $\mathcal{O}(e^{-\alpha N/2})$ (fun proof: shift the contour)
as with Bernstein ellipse, to get exp. conv. *rate* need understand f *off its real axis* (wild!)

Smoothest case: "band-limited" f with $\hat{f}_k = 0$, $|k| > k_{\max}$,
then interpolant *exact* once $N > 2k_{\max}$

That's theory. In real life you always measure your conv. order/rate!

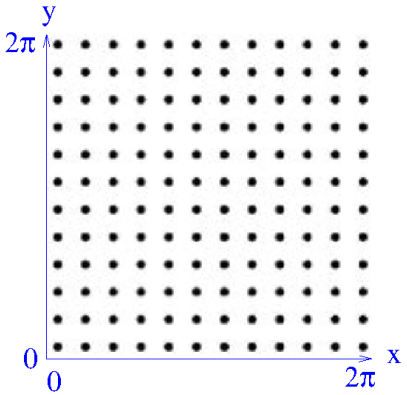
Messages:

- f smooth, periodic, global interpolation w/ uniform grid: spectral acc.
- key to spectral methods. FFT cost $\mathcal{O}(N \log N)$ swaps from $f(x_j)$ grid to $\hat{f}_k$

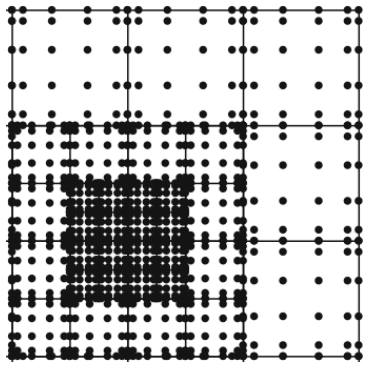
Flavor of interpolation in higher dims $d > 1$

If you *can* choose the nodes:

tensor product of 1D grids
either global
or adaptively refined boxes

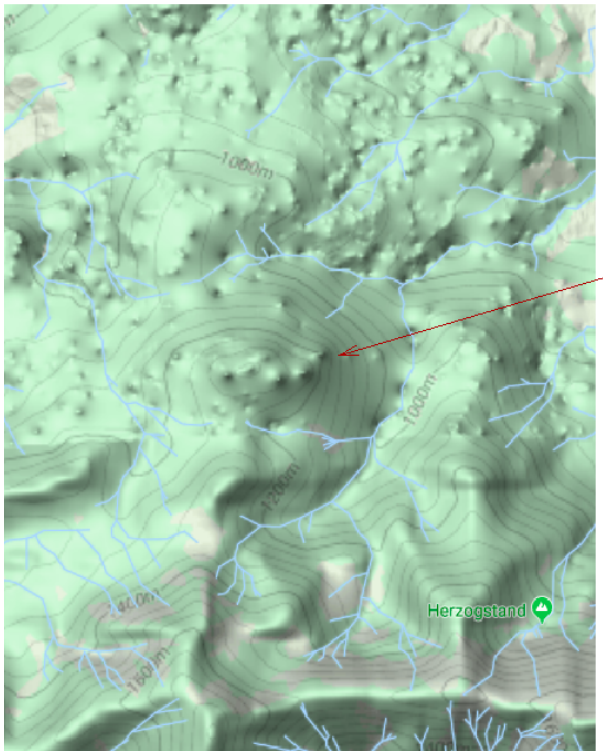


periodic, global


adaptive $p = 6 \times 6$ Cheby

If *cannot* choose the nodes: interp. $f(\mathbf{x})$ from scattered data $\{\mathbf{x}_i\}$ is hard

eg google terrain: $f(\mathbf{x})$ rough $\rightarrow$ garbage:



height f(x) interp from unstructured points in 2D, kernel method

pock−marks!

interp from Cartesian grid, more accurate

But if know f smooth:

locally fit multivariate polynomials

If also data noisy, many methods:

kriging (Gauss. proc.), NUFFT, RBF...

If also high dim $d \gg 1$:

tensor train, neural networks...

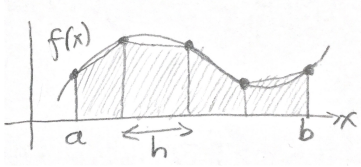
Numerical integration (back to $d = 1$)

Task: eval. $\int_a^b f(x)dx$ accurately w/ least number of func. evals, N

"quadrature": nodes $\{x_j\}$, weights $\{w_j\}$, s.t. $\int_a^b f(x)dx \approx \sum_{j=1}^N w_j f(x_j)$

Idea: get interpolant $\tilde{f}$ thru data $f(x_j) \to$ *integrate that exactly*

Examples: "intepolatory quadrature"



- local piecewise linear $\to$ composite trapezoid rule

  $w_j = h$ except $h/2$ at ends. low-order, err $\mathcal{O}(N^{-2})$, avoid!

- N-node global poly $\to$ gives $\{w_j\}$ integrating degree $N-1$ exactly

  f analytic: err $\mathcal{O}(\rho^{-N})$ solve lin sys $V^T\mathbf{w} = \{\int_a^b x^k dx\}_{k=0}^{N-1}$ (Newton–Cotes)

- better: "Gaussian" $\{x_j, w_j\}$ integrates deg. $2N-1$ exactly! err $\mathcal{O}(\rho^{-2N})$

Adaptive quadrature (Gauss in each panel) excellent: codes `quadgk`, `scipy`, etc

- periodic case: $x_j = \frac{2\pi j}{N}$, $w_j = \frac{2\pi}{N}$ excellent "periodic trap. rule"

  easy to check integrates e^{ikx} exactly for $|k| < N$, "Gaussian"

  f analytic in $|\operatorname{Im} x| < \alpha$ gives exp. conv. $\mathcal{O}(e^{-\alpha N})$, twice as good as interp!

demo:
```
N=14; sum(exp(cos(2*pi*(1:N)/N)))/N - besseli(0,1)
ans = 1.3e-15
```

Advanced integration

- custom quadr. for singularity eg $f(x) = \text{smooth} \cdot |x|^{-1/2}$ (Rokhlin school)
  or for arb. set of funcs. "generalized Gaussian quad." (CCM: Manas Rachh)
- high-order end-corrections to uniform trap. rule (Alpert '99)
- oscillatory functions: deform contour to $\mathbb{C}$ "numerical steepest descent"

...

Higher dimensions $d > 1$

code: `integral2`, etc, `quadpy`

For $d \lesssim 5$, tensor product quadr. of 1D n-node grids in each dim

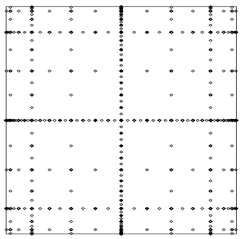
other coord systems: eg sphere can use tensor product in (θ, ϕ). Or: iterate over dims.

adaptivity works: automatically refine boxes but soon enter research territory!

$\int_\Omega f(\mathbf{x}) d\mathbf{x}$ in nasty domain $\Omega \subset \mathbb{R}^d$? FEM meshing, blended conforming grids...

Much higher $d \gg 1$

tensor prod: exp. # f evals. $N = n^d$ kills you :("curse of dim."



- "sparse grids" scale better as $N \sim n(\log n)^d$ (Smolyak '63)
- (quasi-)Monte Carlo: $\sum_{j=1}^N f(\mathbf{x}_j)$, for random $\mathbf{x}_j$ err $\mathcal{O}(N^{-1/2})$, slow conv!

importance sampling (Thurs am session), custom transformations...

Numerical differentiation

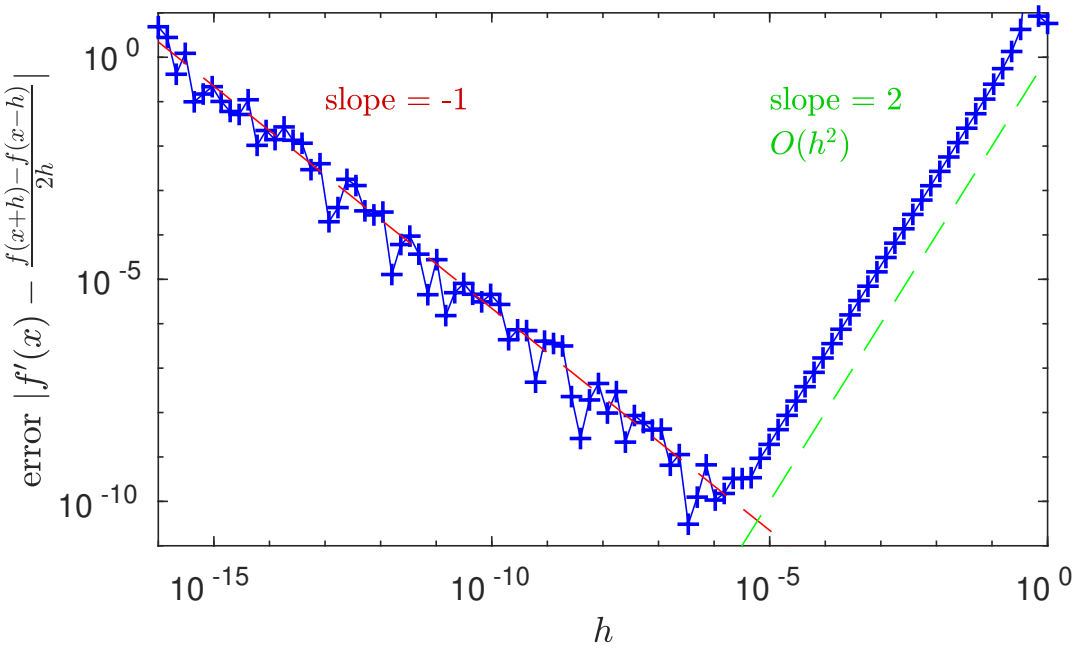
Task: given ability to eval. $f(\mathbf{x})$ anywhere, how get $\nabla f(\mathbf{x})$? assume smooth

Finite differencing idea, 1D: $f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \mathcal{O}(h^2)$ Taylor's thm

"centered difference" formula

Want smallest error:
suggests taking $h \to 0$?

Let's see how that goes...



- shrinking $\mathcal{O}(h^2)$ error gets swamped by a new growing error... what?
- CPU arithmetic done only to relative "rounding error" $\epsilon_{\text{mach}} \sim 10^{-16}$
- subtracting v. close $f(x+h)$ and $f(x-h)$: "catastrophic cancellation"
- balance two error types: $h_{\text{best}} \sim \epsilon_{\text{mach}}^{1/3} \sim 10^{-5}$

Essential reading: floating point, backward stability [GC12, Ch. 5–6] [TBI97, Ch. 12–15]

High-order (better!) differentiation, $d = 1$

As w/ integration: get interpolant $\to$ differentiate it exactly [Tre00, Ch. 6]

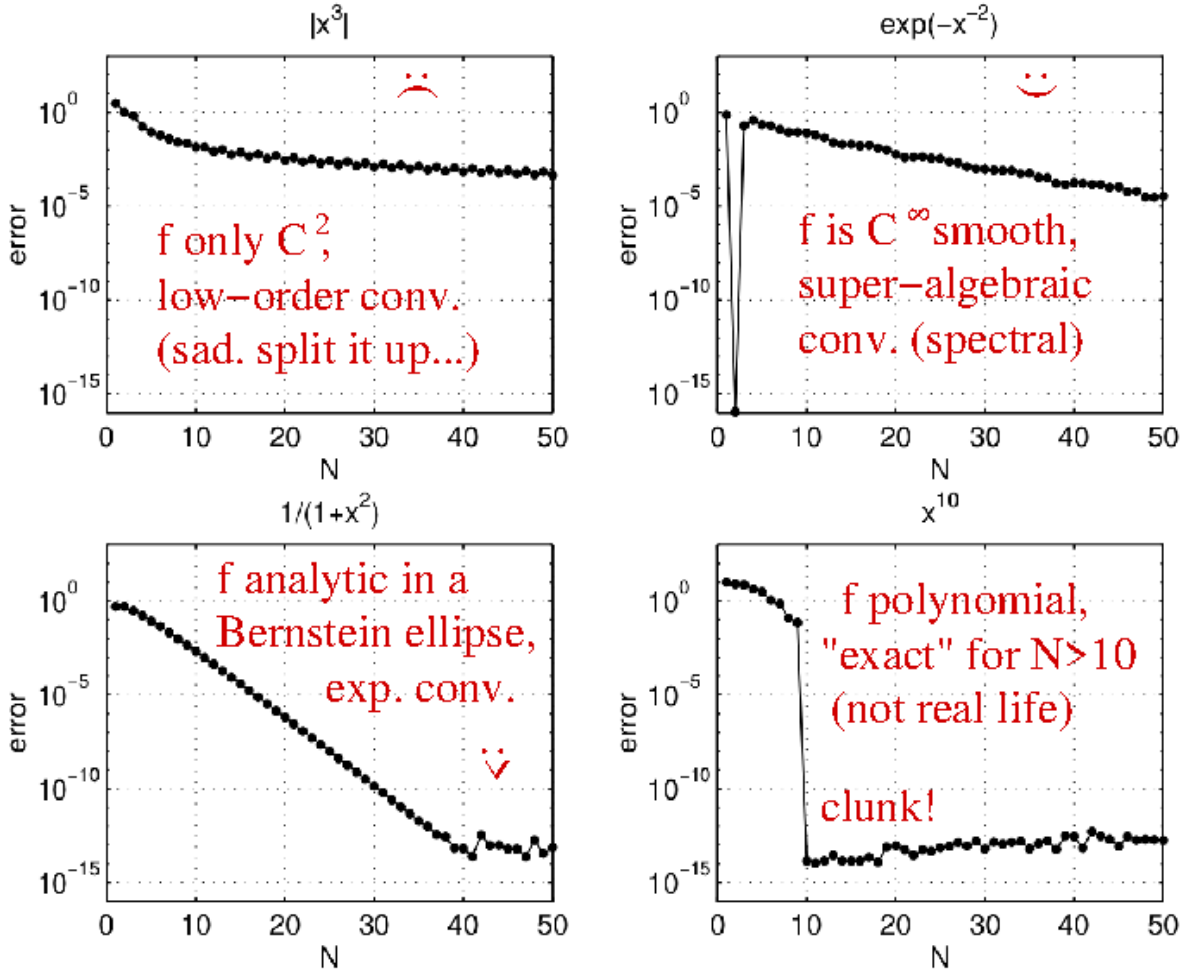
Get $N \times N$ matrix D acting on func. values $\{f(x_j)\}$ to give $\{f'(x_j)\}$. Has simple formula

Examples:

N Chebychev nodes

in $[-1, 1]$

shown: max error in f'



- for N large, the dense D is never formed, merely applied via FFT

spectral solvers for ODE/PDEs. codes: `chebfun`, `PseudoPack`, `dedalus`... Lecture II

Summary: we scratched the surface

Can integrate & differentiate smooth funcs given only point values $f(x_j)$

Both follow from building a good (fast-converging) interpolant

For f smooth in 1D, can & should easily get many (10+) digits accuracy

Concepts:

convergence order/rate	how much effort will you have to spend to get more digits?
smoothness	smooth $\Leftrightarrow$ fast convergence; nonsmooth needs custom methods
global	(one interpolation formula/basis for the whole domain)
vs local	(distinct formulae for x in different regions)
spectral method	global, converge v. fast, even non-per. can exploit FFT
adaptivity	auto split boxes to put nodes only where they need to be
rounding error & catastrophic cancellation	how not shoot self in the foot
tensor products for 2D, 3D	for higher dims: randomized/NN/TN (Th/Fr sessions)

See recommended books at end, and come discuss stuff!

FLATIRON INSTITUTE
Center for Computational Mathematics

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

Basic overview of how different methods work.
Understand error properties and suitability for different equations.

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general
  - Finite Volume Methods Fluids
  - "Traditional" Finite Elements Mechanics
  - "Modern" Finite Elements Higher order
  - Spectral Methods Best accuracy for smooth solutions
- Boundary Integral Methods Linear problems w/ boundary data

Reminder of types and applications of diff. eq.

- ODEs: eg pendulum $u''(t) + \sin(u(t)) = 0$
  Task: solve $u(t)$ given initial conditions e.g. $u(0) = 1$, $u'(0) = 0$
  Others: local chemical/nuclear reactions ($\mathbf{u}(t)$ is vector of multiple components)
- Time-independent PDEs: eg Poisson eqn $\Delta u(\mathbf{x}) = g(\mathbf{x})$
  Task: solve $u(\mathbf{x})$ given forcing, boundary conditions
  Steady state of heat/diffusion, Gauss's law for conservative forces
  $u(\mathbf{x})$ is chemical concentration, gravitational/electric potential
  Δu means Laplacian $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \cdots =$ curvature of u
  $g(\mathbf{x}) =$ volume source of chemical, mass or charge density
  Others: Stokes eqn for velocity field $\mathbf{u}$ in viscous fluid
  Others: t-indep. Schrödinger eqn for quantum systems: $\Delta\psi = (V - E)\psi$
- Time-dependent PDEs: eg advection-diffusion $\partial_t c + \nabla \cdot (\mathbf{u}c) = \Delta c$
  Task: solve $c(\mathbf{x}, t)$ given initial & boundary conditions
  Others: Navier-Stokes, magnetohydrodynamics, ...

Choose method based on solution behavior (Mike's talk next)
Or boundary conditions: simple (periodic box) vs complicated domain

Typical solution strategies

Time-independent PDEs:

1. Discretize variables (grid points, cells, basis functions)
2. Discretize operators/equations (derivatives)
3. Solve resulting algebraic system

Time-dependent PDEs: "method of lines"

1. Discretize variables (grid points, cells, basis functions)
2. Discretize operators/equations (derivatives)
3. Solve resulting coupled ODEs for evolution of coefficients

ODEs:

- Treat spatial problems as time-indep. PDEs "boundary value problems"
- Evolve temporal problems with finite differences "initial value problems"

Finite difference methods

Basic viewpoint:

- Discretize variables on a discrete grid
- Construct Taylor-series approximations to values at neighboring points
- Using N points, expand to N terms (error $\mathcal{O}(h^N)$)
- Eliminate to get approximation to d-th derivative (error $\mathcal{O}(h^{N-d})$)

E.g. Centered differences on 3 points: $x-h$, x, $x+h$

$$u(x+h) = u(x) + u'(x)h + u''(x)h^2/2 + \mathcal{O}(h^3)$$
$$u(x-h) = u(x) - u'(x)h + u''(x)h^2/2 + \mathcal{O}(h^3)$$

To approximate $u'(x)$, subtract to eliminate $u''(x)$:

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

To approximate $u''(x)$, add to eliminate $u'(x)$:

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

Extra order here due to symmetry

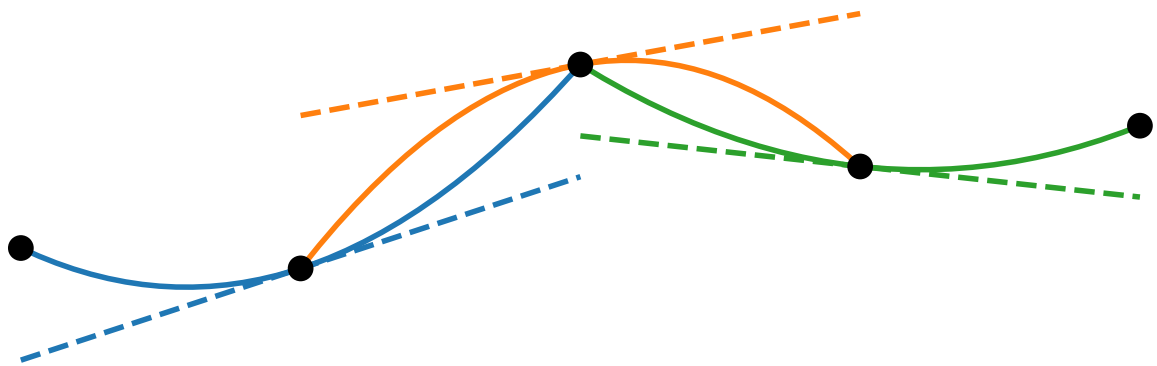
Finite difference methods

Alternate viewpoint:

- Discretize variables on a discrete grid
- Construct interpolating polynomial on N nearest points.

  Unique, degree N-1.
- Differentiate this local interpolant to approximate derivatives.

E.g. Centered differences using 3 points:



$$\Delta u(x) = f(x) \quad \rightarrow \quad D_2 \cdot \mathbf{u} = \mathbf{f}$$

$$\partial_t u(x) = \Delta u(x) + f(x) \quad \rightarrow \quad \partial_t \mathbf{u} = D_2 \cdot \mathbf{u} + \mathbf{f}$$

Implicit & Explicit Timestepping

Consider temporal ODE $u'(t) = f(u(t))$.
Timesteppers solve using finite differences to advance $u_n \to u_{n+1}$

- Explicit schemes: just need $f(u_n)$. Simple but unstable for large steps
  E.g. forward Euler: use 1st-order forward difference k = timestep; $u_n := u(kn)$

$$u'(t) = -\lambda u(t) \quad \lambda > 0$$
$$u_{n+1} - u_n = -k\lambda u_n$$
$$u_{n+1} = (1 - k\lambda)u_n$$

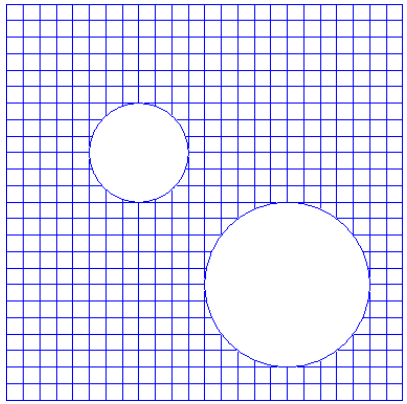
$k\lambda < 2$ for stability

- Implicit schemes: require inverting $f(u^{n+1})$ Stable but expensive
  E.g. backward Euler: use 1st-order backward difference

$$u'(t) = -\lambda u(t) \quad \lambda > 0$$
$$u_{n+1} - u_n = -k\lambda u_{n+1}$$
$$u_{n+1} = (1 + k\lambda)^{-1} u_n$$

Finite difference methods

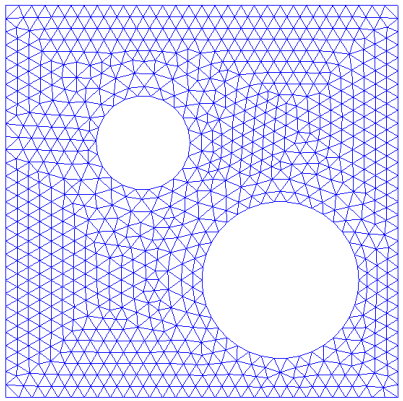
- Simple to adjust order of accuracy / directionality
- Extends to multiple dimensions with regular grids
- Some more advanced techniques:
  - Conservative schemes
  - Select stencils term by term "upwinding"
  - Adaptive stencil selection for jumps "WENO"
- Restricted to simple geometries / well-structured grids



Resources: LeVeque "Finite Difference Methods for ODE/PDE" [LeV07]
Codes: e.g. Pencil code (magnetohydrodynamics)

Finite element methods

- Partition domain into elements. Unstructured
- Represent variables with basis functions on elements:



$$u(\mathbf{x}) = \sum_{n=1}^{N} u_n \phi_n(\mathbf{x})$$

"Trial functions" ϕ_n usually polynomials on each element

- Solve equations using Galerkin/weighted-residual method:

$$\partial_t u(\mathbf{x}) + Lu(\mathbf{x}) = f(\mathbf{x})$$

$$\int \psi_m(\mathbf{x}) \left[\partial_t u(\mathbf{x}) + Lu(\mathbf{x}) - f(\mathbf{x})\right] \, d\mathbf{x} = 0$$

For all "test functions" ψ_m

- Solve resulting algebraic system:

$$M \cdot \partial_t \mathbf{u} + S \cdot \mathbf{u} = M \cdot \mathbf{f}$$

"Mass matrix" M, "stiffness matrix" S

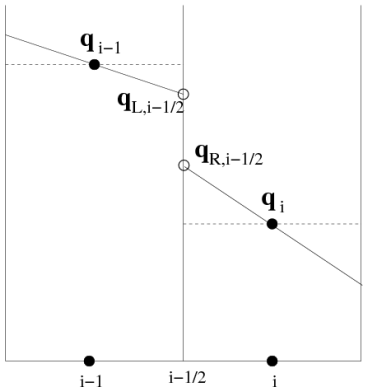
Finite volume methods

- Piecewise constants inside elements

  $M = I$, easy explicit formulation

- Integrate flux terms by parts:

$$\int \psi_m \nabla \cdot \mathbf{j}\, d\mathbf{x} = \int_{\Omega_i} \nabla \cdot \mathbf{j}\, d\mathbf{x} = \int_{\delta\Omega_i} \mathbf{n} \cdot \mathbf{j}\, dS$$



- Requires integrating fluxes at cell interfaces (usually 2nd order)

  Many methods for Riemann solvers/flux reconstruction: TVD, ENO, WENO, ...

- Exactly conservative: good for hyperbolic PDEs. Widely used in CFD.
- Similar to finite differences on structured meshes.
- Hard to build high-order schemes on unstructured meshes.

Codes: Arepo, Athena, OpenFOAM

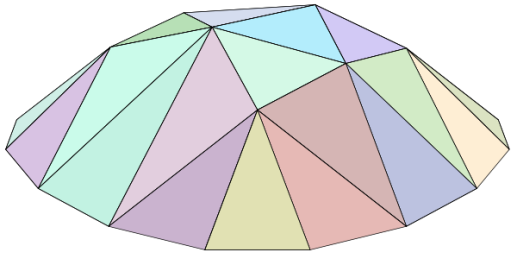
Many local experts in CCA!

Finite element methods

Traditional FEM

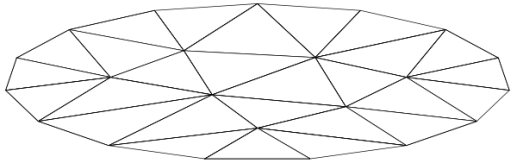
- Use piecewise linear "tent" functions.

  Continuous, 2nd order



- "Weak form" from integrating by parts:

$$\int \psi_m \nabla^2 u \, d\mathbf{x} = -\int \nabla \psi_m \cdot \nabla u \, d\mathbf{x}$$



  Lowers order of derivatives, allows linear basis

- Not conservative and $M \neq I$, need implicit schemes or to invert M
- Easy to adjust order of accuracy. Use higher degree polynomials, "p adaptivity"

Modern research: high-order FEM

- Discontinuous Galerkin (FVM + FEM): high order inside elements, but allow discontinuities. Need Riemann solvers again
- Spectral elements: very high order internal representations

Codes: FEniCS, deal.II

Spectral methods

- Expand variables in global basis functions (FEM with one element)
- Solve Galerkin projection of equations. But don't integrate by parts
- **Exponential** accuracy for smooth solutions

Periodic intervals: Fourier series for test/trial functions. Fast w/ FFT

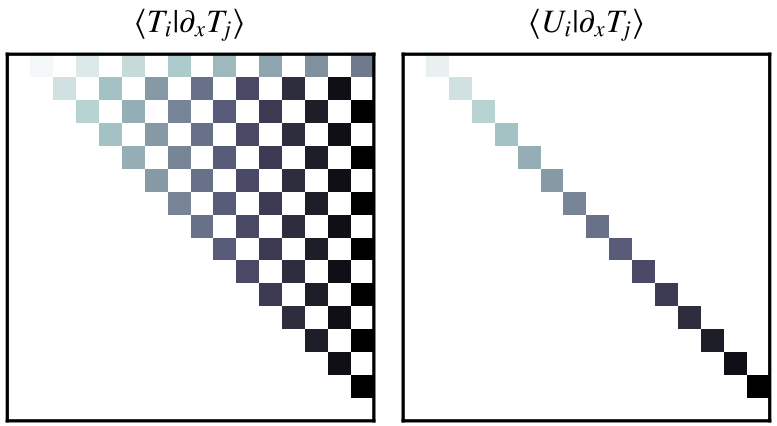
M and *S* matrices typically diagonal, even in multiple dimensions!

$$\nabla^2 \exp(i\mathbf{k}\cdot\mathbf{x}) = -k^2 \exp(i\mathbf{k}\cdot\mathbf{x})$$

Non-periodic intervals: Chebyshev polynomials $T_n(x)$. Fast w/ DCT

Traditional: "collocation" using values at Chebyshev nodes. Dense matrices.

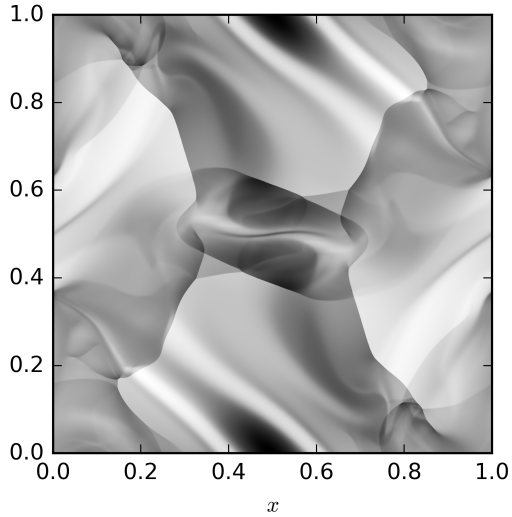
Modern: *M* and *S* banded with right choice of test functions.

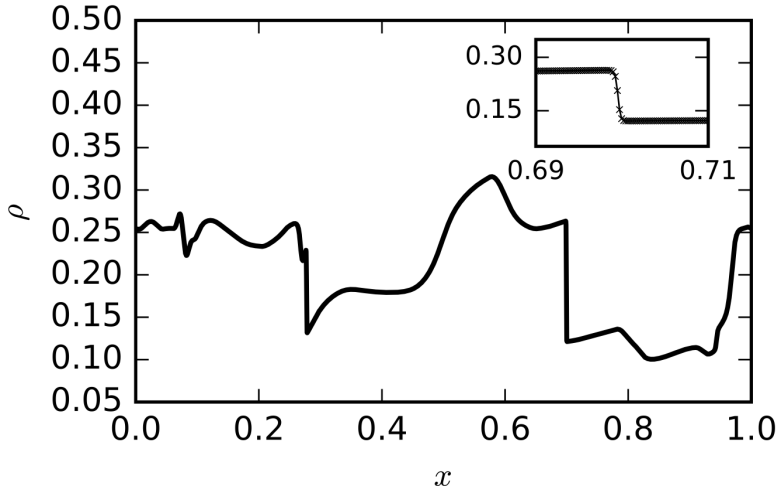


Other geometries: other polynomials, spherical harmonics, ...

Spectral methods

- **Exponential** accuracy for smooth solutions. Need to regularize discontinuities





- Restricted to simple geometries. Boxes, spheres, disks, ...
- Very flexible in terms of equations.
- Not exactly conservative... but very accurate. Use conservation as a diagnostic!

Modern research: sparse methods for arbitrary equations in more geometries.

Resources: Boyd "Chebyshev and Fourier Spectral Methods" [Boy01]
Codes: Chebfun (MATLAB), ApproxFun (julia), Dedalus (Python)

Boundary integral methods

Use knowledge of PDEs in constructing solutions:

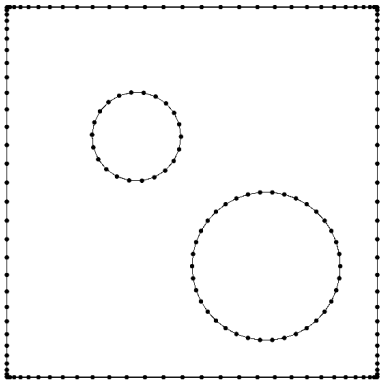
- Linear PDEs dominated by boundary terms
- Solutions involve integrals of fundamental solution (Green's function):

  Reduced dimensionality. Improved conditioning. Low-rank iterations and fast methods.

E.g. for Poisson's equation: $\Delta u(\mathbf{x}) = f(\mathbf{x})$

$$u(\mathbf{x}) = \int G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, d\mathbf{y}$$

$$\Delta G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}), \quad G(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi|\mathbf{x} - \mathbf{y}|}$$



Examples: Stokes flow, Helmholtz equation, Maxwell equations

Usually homogeneous media

Many experts in CCM & CCB. See Jun Wang's talk later today!

Summary

- Finite differences: local polynomial approximations, simple and robust
- Finite elements: local basis functions, complex geometries
- Spectral methods: global basis functions, highly accurate
- Integral methods: reduced dimensionality, linear equations

Best method often depends on multiple factors:

- Problem domain (simple vs complicated)
- Behavior of solutions (Mike's talk next)
- Desired accuracy vs cost
- Code availability
- ...

Many local experts on different methods!

Recommended accessible reading

[Boy01] John P Boyd, *Chebyshev and Fourier spectral methods*, Courier Corporation, 2001.

[GC12] A Greenbaum and T P Chartier, *Numerical methods*, Princeton University Press, 2012.

[LeV07] Randall J LeVeque, *Finite difference methods for ordinary and partial differential equations: steady-state and time-dependent problems*, vol. 98, SIAM, 2007.

[TBI97] L. N. Trefethen and D. Bau III, *Numerical linear algebra*, SIAM, 1997.

[Tre00] Lloyd N. Trefethen, *Spectral methods in MATLAB*, Software, Environments, and Tools, vol. 10, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000.

[Tre13] L. N. Trefethen, *Approximation theory and approximation practice*, SIAM, 2013, `http://www.maths.ox.ac.uk/chebfun/ATAP`.

This document: `https://github.com/ahbarnett/fwam-numpde`

See `code` directory for MATLAB code used to generate figures