

FWAM Session B: Function Approximation and Differential Equations

Alex Barnett¹ and Keaton Burns²

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)

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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)

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Key concepts:

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

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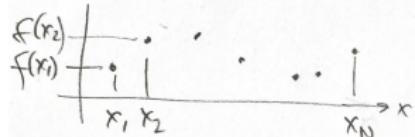
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

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. $\tilde{f}(x_j) = y_j$

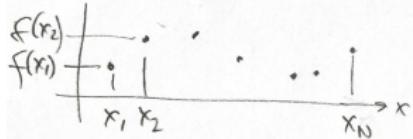


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hopeless w/o assumptions on f , eg smoothness, otherwise...

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

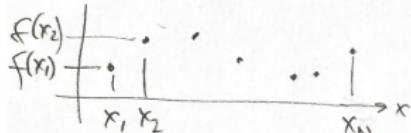


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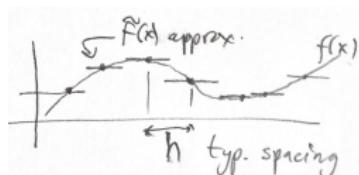
Simplest: use value at x_j nearest to x

"snap to grid"

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

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 $0 < h < h_0$

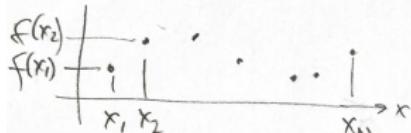


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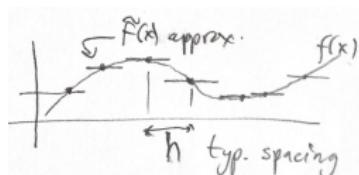
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Piecewise linear:

"connect the dots"

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

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 $p = 1, 2$

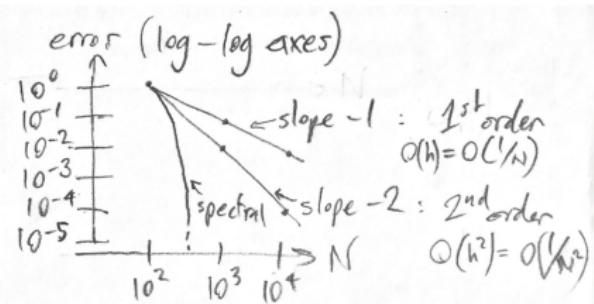
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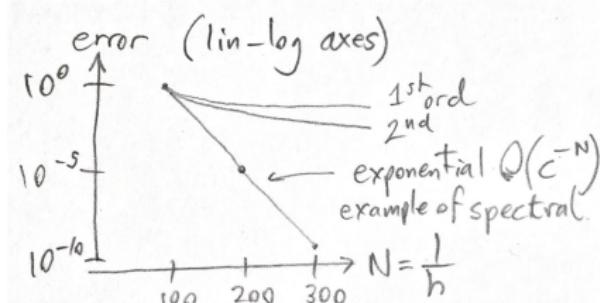
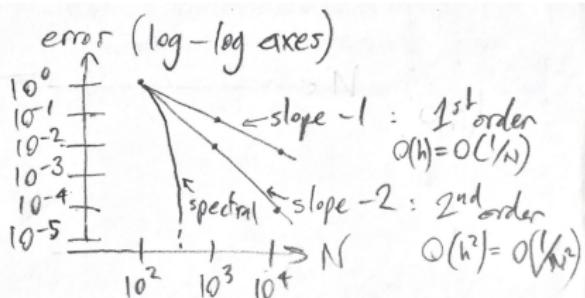
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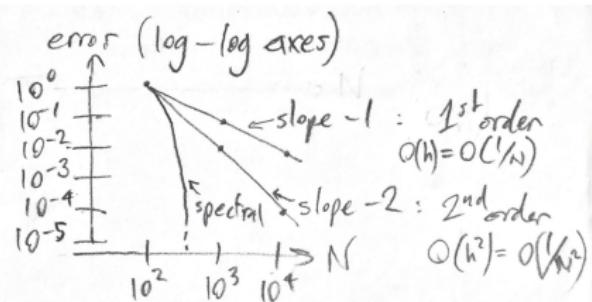
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Note how spectral gets many digits for small N

crucial for eg 3D prob.

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

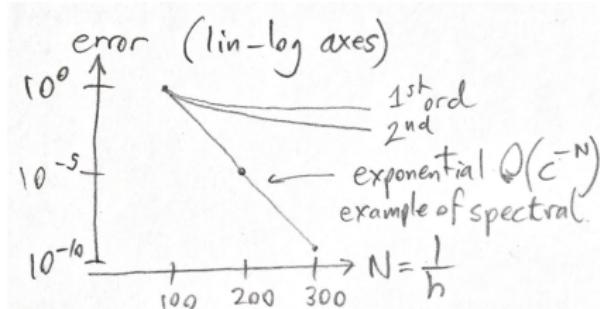
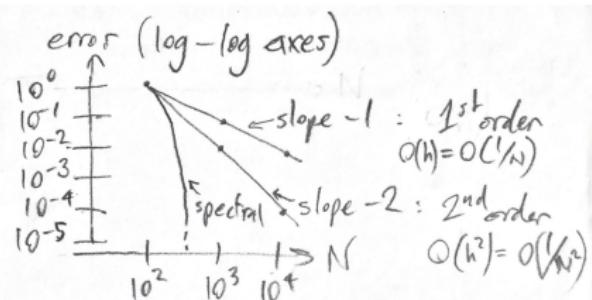
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<rant> test your code w/ known exact soln to check error conv. <\rant>

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

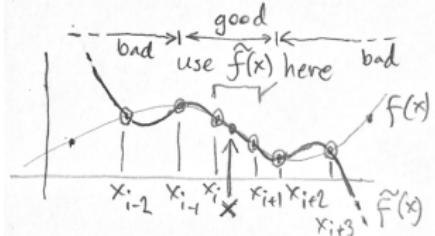
Higher-order interpolation for smooth f : the local idea

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!



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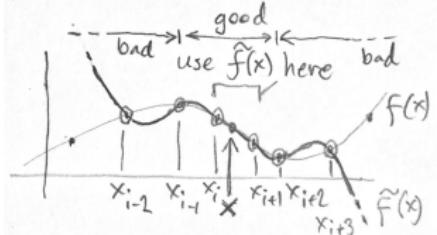
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if must have cont, recommend splines, eg cubic $p = 3$: $\tilde{f} \in C^2$, meaning \tilde{f}'' is cont.



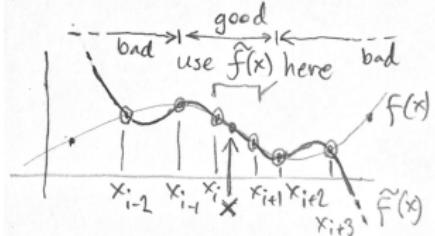
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How to find this degree- $(p-1)$ poly?

- 1) crafty: solve square lin sys for coeffs $\sum_{k < p} x_j^k c_k = y_j \quad j = 1, \dots, p$
ie, $V\mathbf{c} = \mathbf{y}$ V ="Vandermonde" matrix, is ill-cond. but works

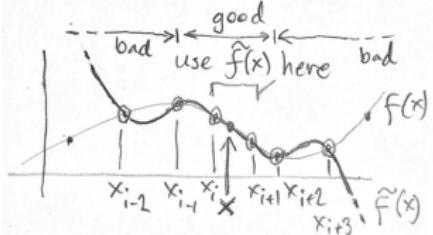
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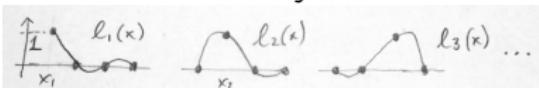
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2) traditional: barycentric formula $\tilde{f}(x) = \frac{\sum_{j=1}^p \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^p \frac{1}{x-x_j} w_j} \quad w_j = \frac{1}{\prod_{i \neq j} (x_j - x_i)}$ [Tre13, Ch. 5]

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

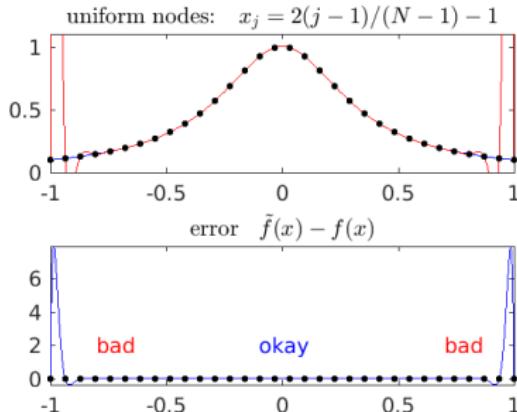


Global polynomial (Lagrange) interpolation?

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

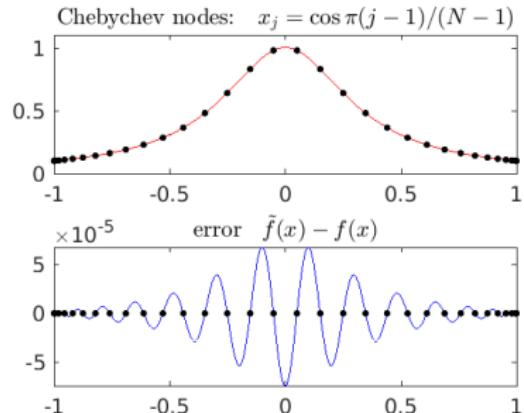
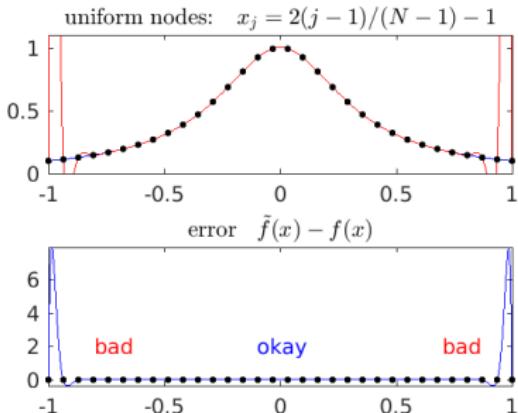
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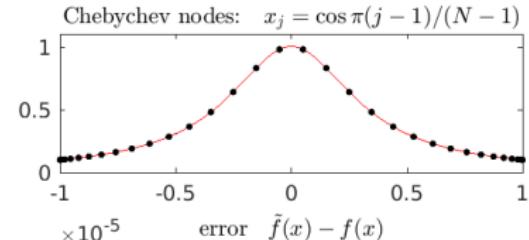
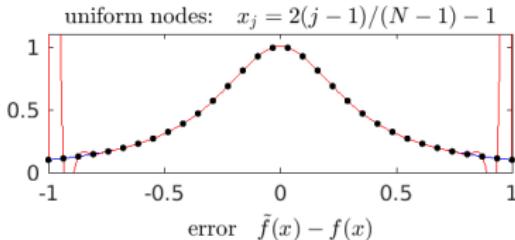
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But exists good choice of nodes...

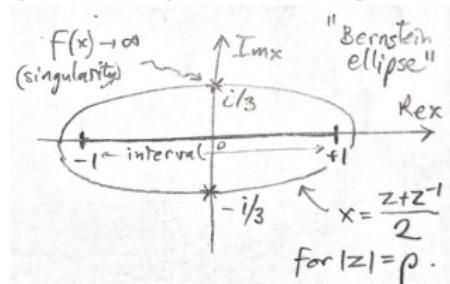
"Chebychev": means non-unif. grid density $\sim \frac{1}{\sqrt{1-x^2}}$

- our first spectral method

$$\max \text{err} = \mathcal{O}(\rho^{-N})$$

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!

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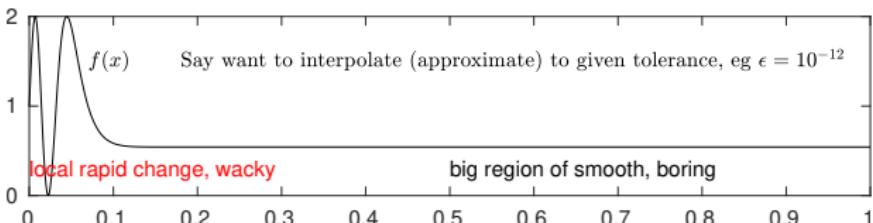
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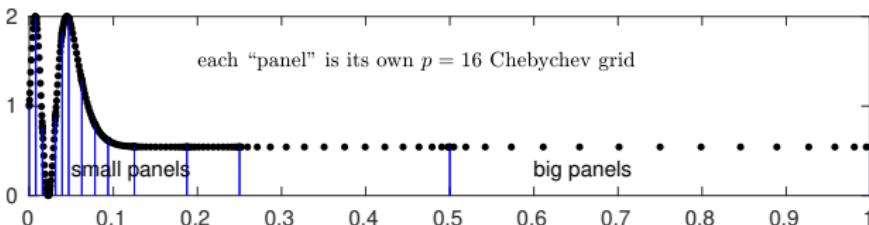
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automatically split
(recursively) panels
until max err $\leq \epsilon$

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 , $f(x) = \sum_{n \in \mathbb{Z}} \hat{f}_k e^{ikx}$ Fourier series

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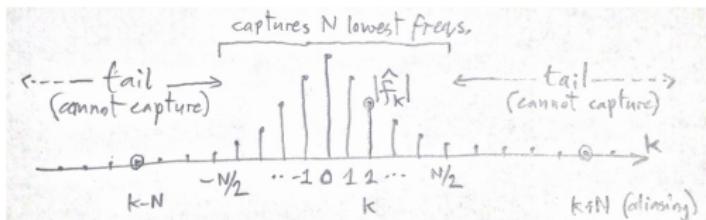
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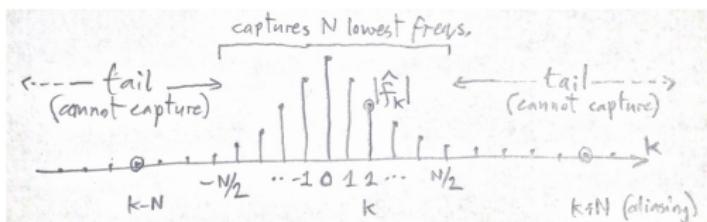
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How read off c_k from *samples* of f on a grid?

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

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

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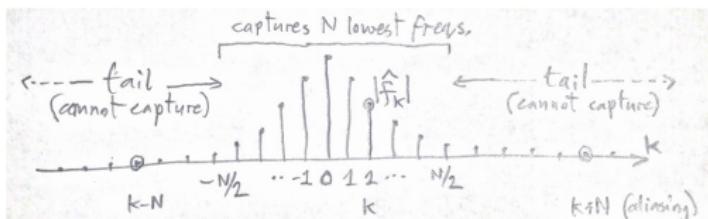
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easy to show $c_k = \dots + \hat{f}_{k-N} + \hat{f}_k + \hat{f}_{k+N} + \hat{f}_{k+2N} + \dots$

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

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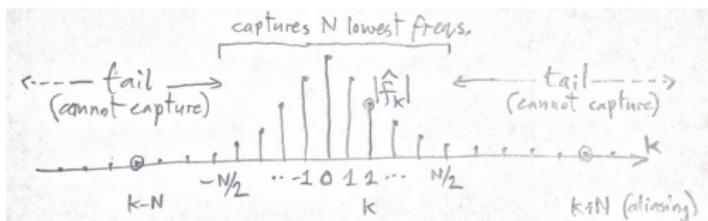
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How read off c_k from *samples* of f on a grid?

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

Uniform grid $x_j = \frac{2\pi j}{N}$, 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 $c_k = \dots + \hat{f}_{k-N} + \hat{f}_k + \hat{f}_{k+N} + \hat{f}_{k+2N} + \dots$

$= \hat{f}_k$ 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 $\text{err} \sim \text{sum of } |\hat{f}_k| \text{ in tail } |k| \geq N/2$

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

$$\hat{f}_k = \mathcal{O}(k^{-p}), \text{ tail sum } \mathcal{O}(N^{1-p}) \quad (p-1)\text{th order acc.} \quad (\text{better: [Tre00]})$$

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

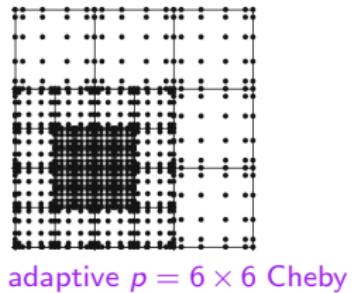
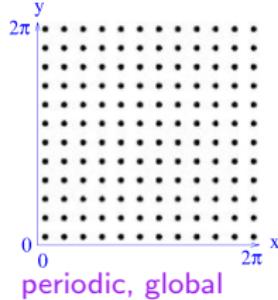
Messages:

- 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:

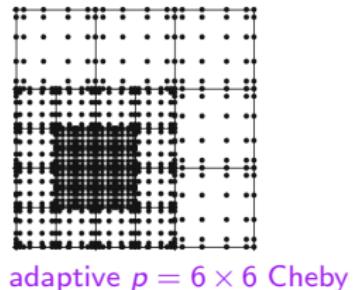
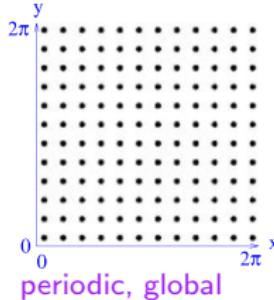
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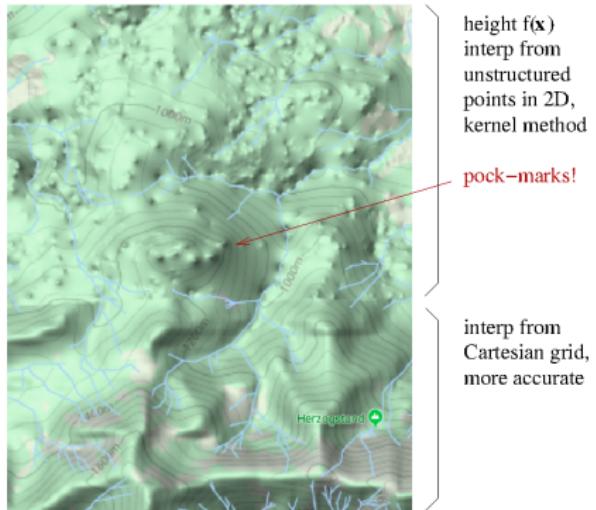
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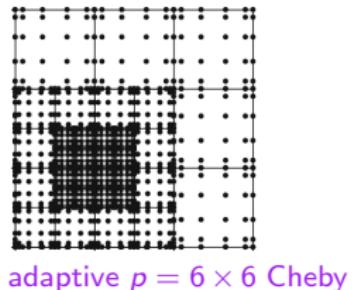
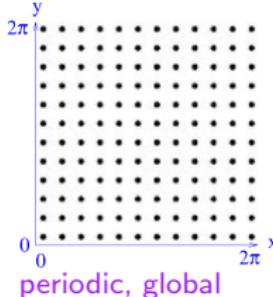
eg google terrain: $f(\mathbf{x})$ rough \rightarrow garbage:



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But if know f smooth:

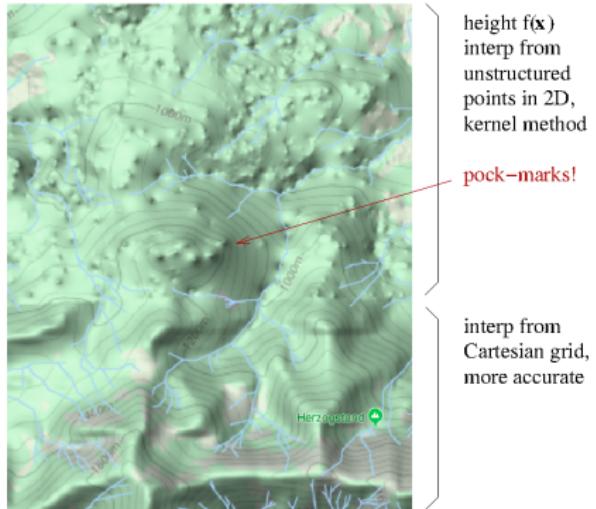
locally fit multivariate polynomials

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 $f(x_j) \rightarrow$ integrate that exactly

“interpolatory quadrature”

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 $w_j = h$ except $h/2$ at ends. low-order, err $\mathcal{O}(N^{-2})$, avoid!
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demo: $N=14$; $\text{sum}(\exp(\cos(2*\pi*(1:N)/N)))/N - \text{besseli}(0,1)$
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)
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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.

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

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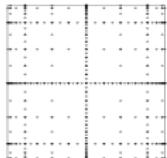
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Much higher $d \gg 1$

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

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Want smallest error:

suggests taking $h \rightarrow 0$?

Let's see how that goes...

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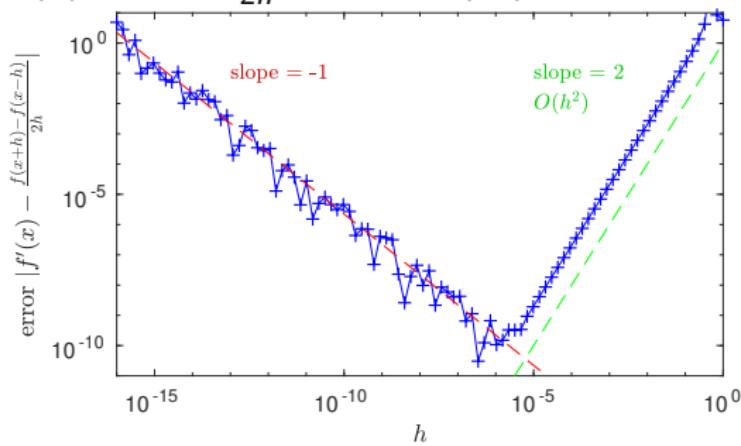
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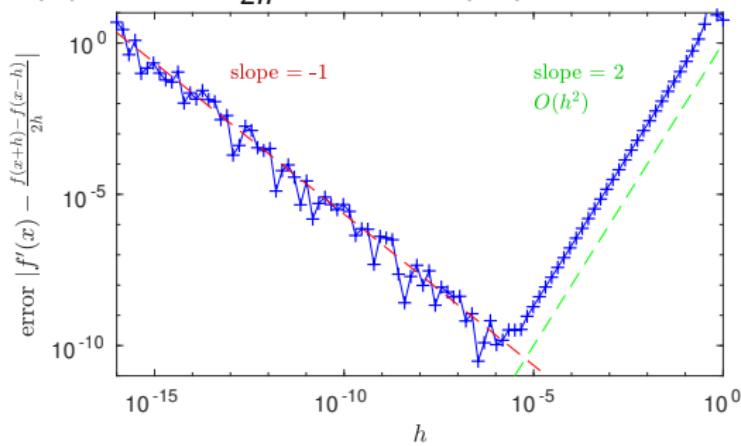
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- shrinking $\mathcal{O}(h^2)$ error gets swamped by a new growing error... what?
- CPU arithmetic done only to relative "rounding error" $\epsilon_{\text{mach}} \sim 10^{-16}$
- subtracting v. close $f(x+h)$ and $f(x-h)$: "catastrophic cancellation"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

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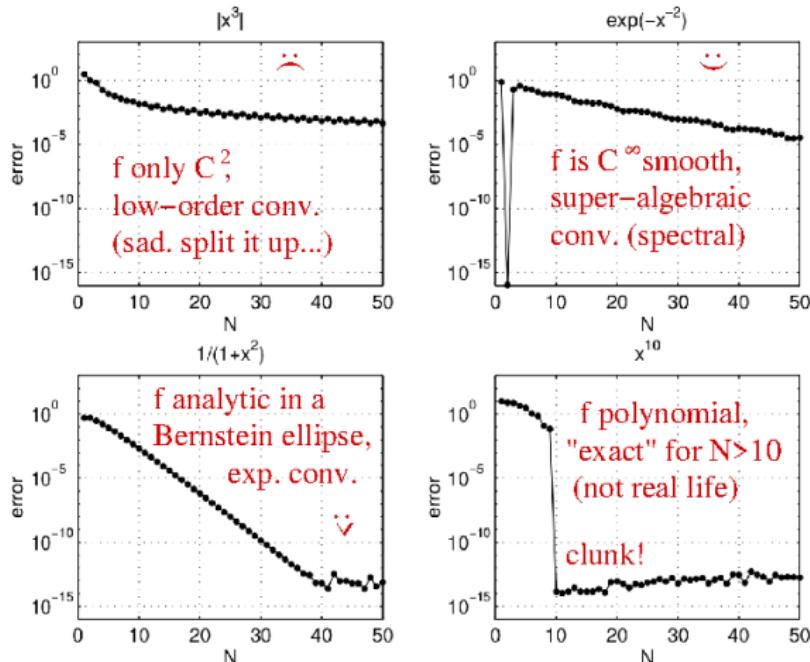
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Examples:

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!

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.

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- Boundary Integral Methods Linear problems w/ boundary data

Reminder of types and applications of diff. eq.

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Task: solve $u(x)$ given forcing, boundary conditions
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 $u(x)$ is chemical concentration, gravitational/electric potential
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Others: Stokes eqn for velocity field \mathbf{u} in viscous fluid
Others: t-indep. Schrödinger eqn for quantum systems: $\Delta\psi = (V - E)\psi$

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 $g(\mathbf{x})$ = 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, ...

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

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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

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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 $\mathcal{O}(h^{N-d})$)

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

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

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Extra order here due to symmetry

Finite difference methods

Alternate viewpoint:

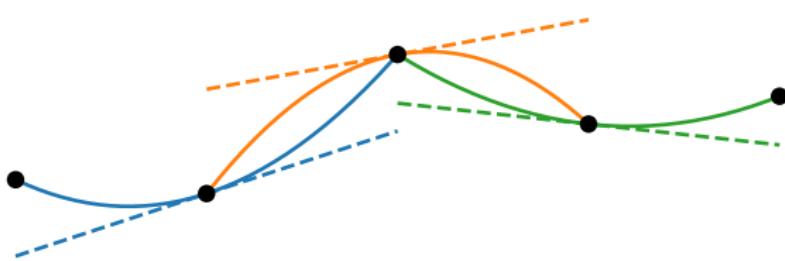
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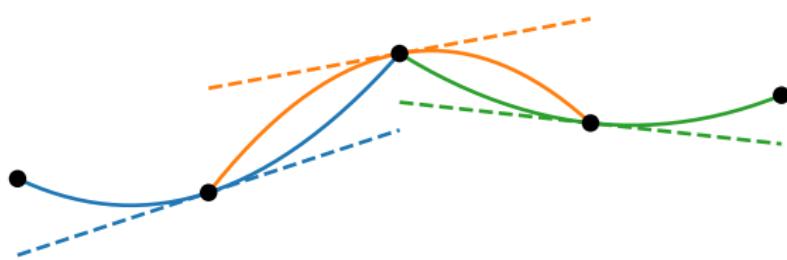


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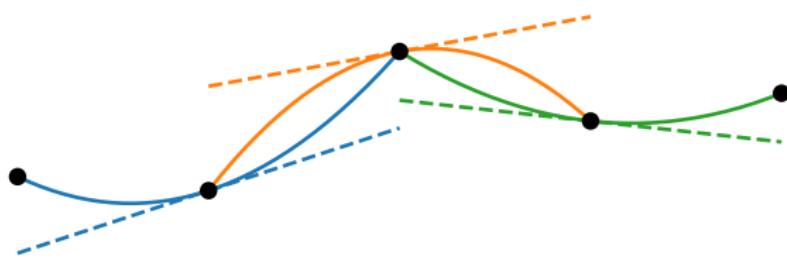
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$$\partial_t u(x) = \Delta u(x) + f(x) \rightarrow \partial_t \mathbf{u} = D_2 \cdot \mathbf{u} + \mathbf{f}$$

Implicit & Explicit Timestepping

Consider temporal ODE $u'(t) = f(u(t))$.

Timesteppers solve using finite differences to advance $u_n \rightarrow u_{n+1}$

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E.g. forward Euler: use 1st-order forward difference

$$u'(t) = -\lambda u(t) \quad \lambda > 0$$

$$u_{n+1} - u_n = -k\lambda u_n$$

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

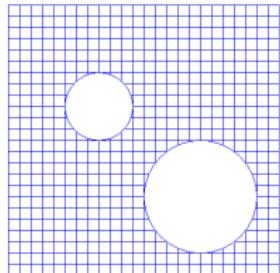
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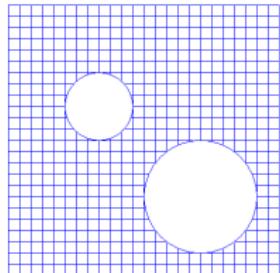
Finite difference methods

- 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”
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Resources: LeVeque “Finite Difference Methods for ODE/PDE” [LeV07]

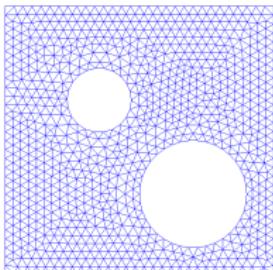
Codes: e.g. Pencil code (magnetohydrodynamics)

Finite element methods

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

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

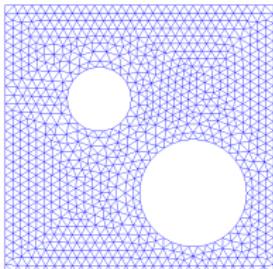
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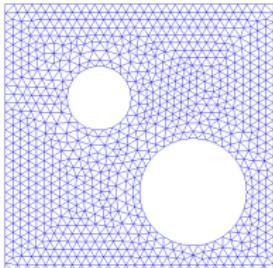
$$\int \psi_m(\mathbf{x}) [\partial_t u(\mathbf{x}) + L u(\mathbf{x}) - f(\mathbf{x})] \, d\mathbf{x} = 0$$

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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

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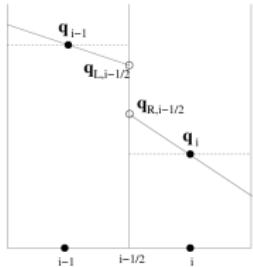
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Many methods for Riemann solvers/flux reconstruction: TVD, ENO, WENO, ...



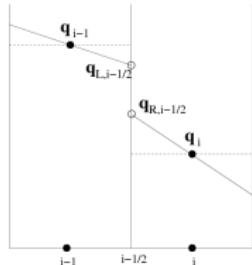
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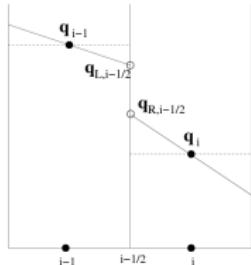
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Codes: Arepo, Athena, OpenFOAM

Many local experts in CCA!

Finite element methods

Traditional FEM

- Use piecewise linear “tent” functions.
Continuous, 2nd order
- “Weak form” from integrating by parts:

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

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Codes: FEniCS, deal.II

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- Solve Galerkin projection of equations. *But don't integrate by parts*
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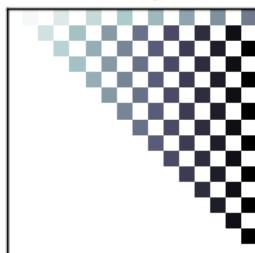
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Non-periodic intervals: Chebyshev polynomials $T_n(x)$. Fast w/ DCT

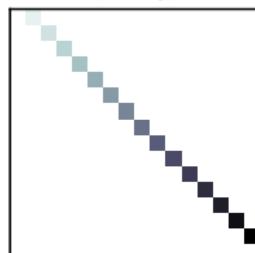
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Modern: M and S banded with right choice of test functions.

$$\langle T_i | \partial_x T_j \rangle$$



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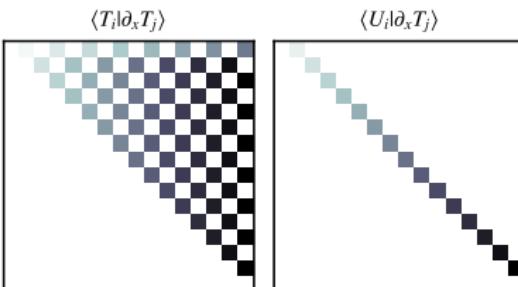
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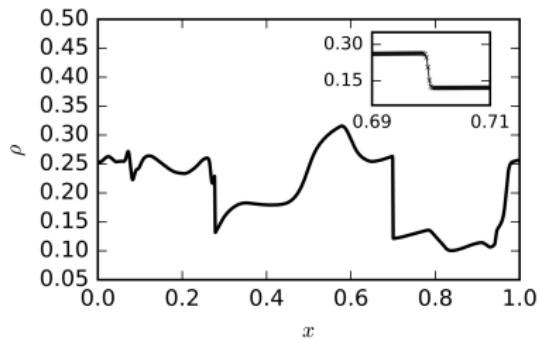
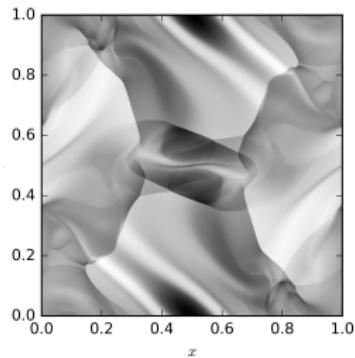
Other geometries: other polynomials, spherical harmonics, ...

Spectral methods

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

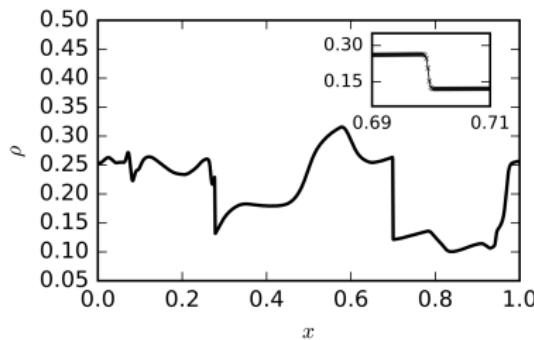
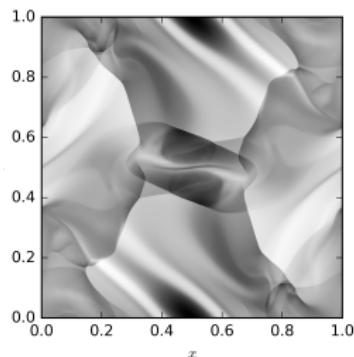
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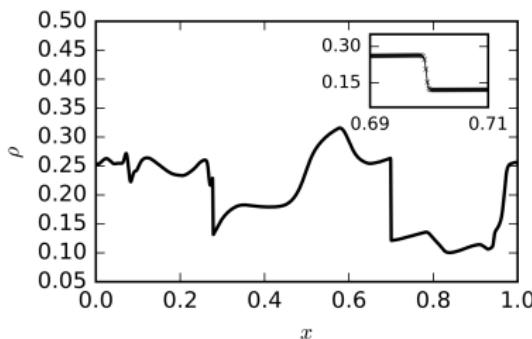
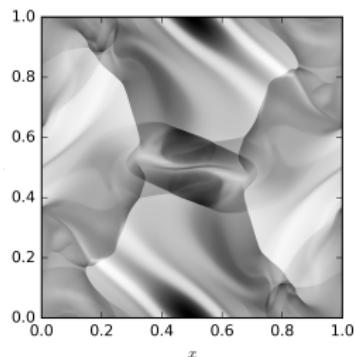
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- Very flexible in terms of equations.
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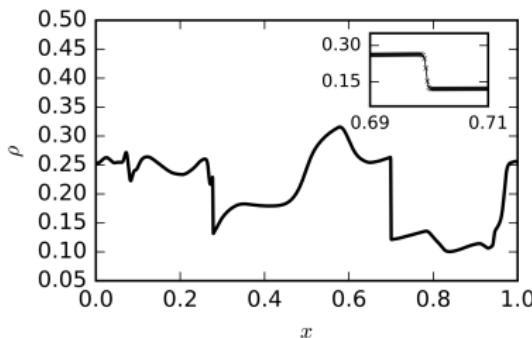
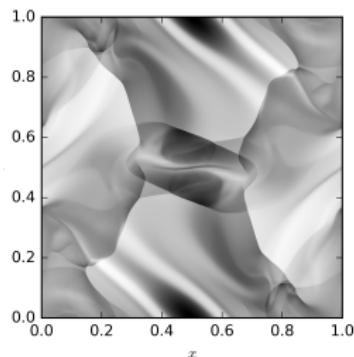


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Resources: Boyd “Chebyshev and Fourier Spectral Methods” [Boy01]

Codes: Chebfun (MATLAB), ApproxFun (julia), Dedalus (Python)

Boundary integral methods

Use knowledge of PDEs in constructing solutions:

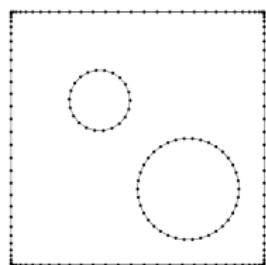
- Linear PDEs dominated by boundary terms
- Solutions involve integrals of fundamental solution (Green's function):

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