FWAM Session B: Function Approximation and Differential Equations

Alex Barnett[1] and **Keaton Burns**[2]

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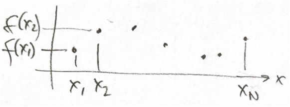
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

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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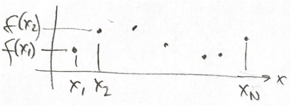
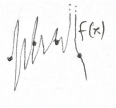


hopeless w/o assumptions on f, eg smoothness, otherwise...

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



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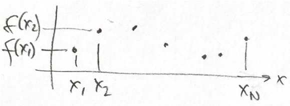

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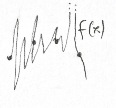
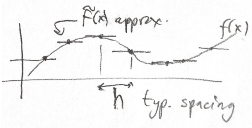


Simplest: use value at x_j nearest to x

"snap to grid"



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

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 $0 < h < h_0$

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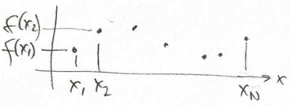

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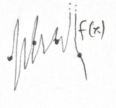

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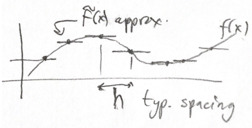

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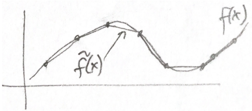
Piecewise linear: "connect the dots"

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

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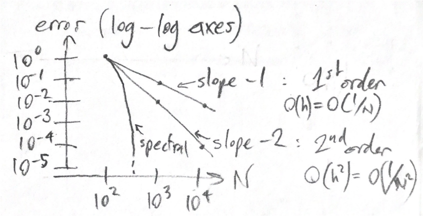

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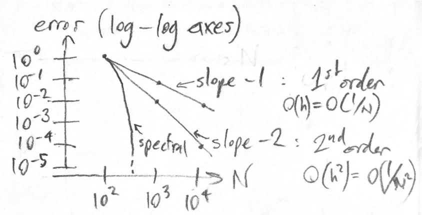

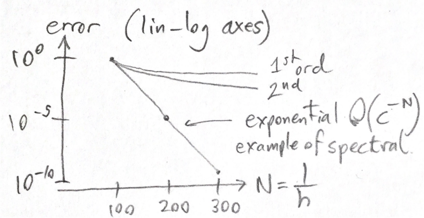

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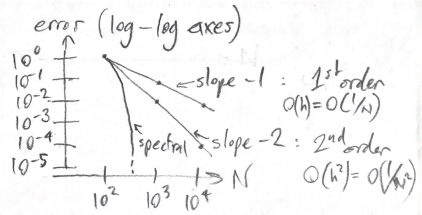

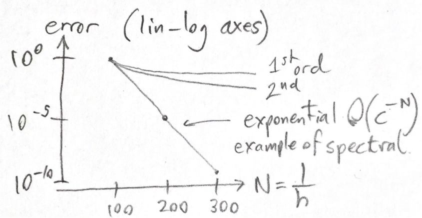

Note how spectral gets many digits for small N crucial for eg 3D prob.

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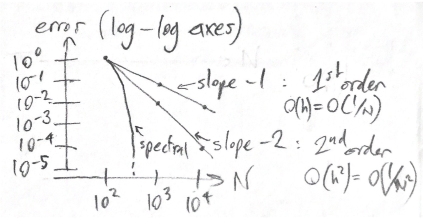

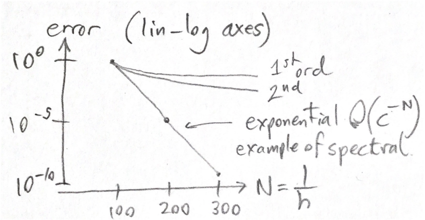

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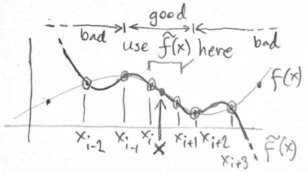
<rant> test your code w/ *known exact soln* to check error conv. <\rant>

How big is prefactor C in error $\leq Ch^p$? Has 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

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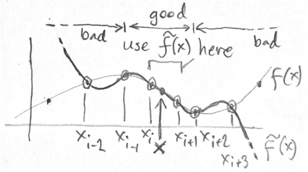

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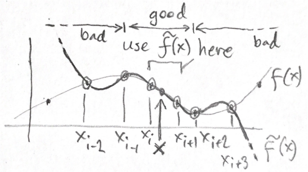

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1) crafty: solve square lin sys for coeffs $\sum_{k<p} x_j^k c_k = y_j$ $\quad j = 1, \ldots, p$

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

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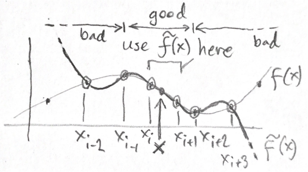

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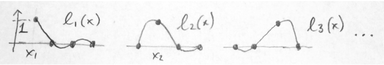
2) traditional: barycentric formula $$\tilde{f}(x) = \frac{\sum_{j=1}^{p} \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^{p} \frac{1}{x-x_j} w_j}$$ $w_j = \frac{1}{\prod_{i \neq j}(x_j - x_i)}$

[?, 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:



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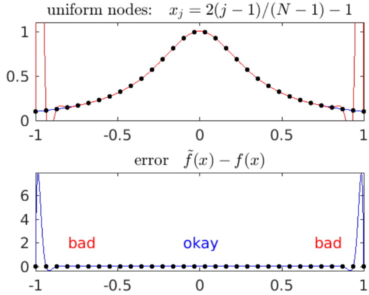

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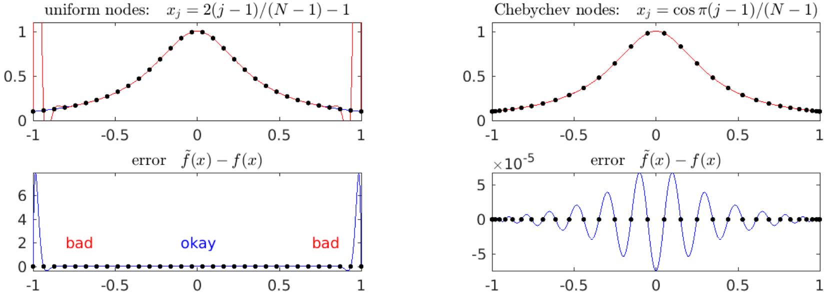

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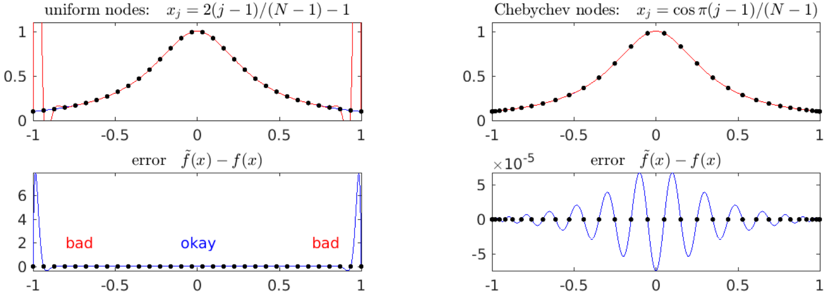

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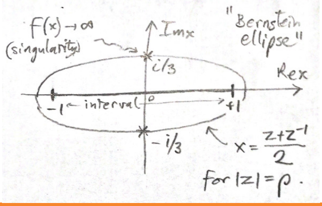
But exists good choice of nodes...

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

- our first spectral method

  max 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)

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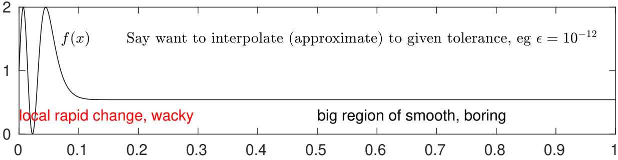

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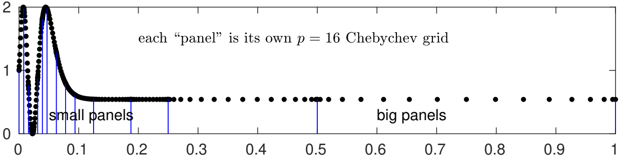

automatically split (recursively) panels until max err $\le \epsilon$

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"

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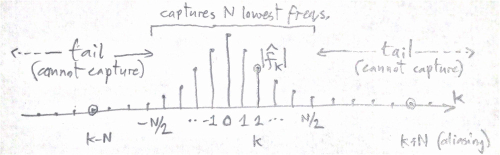

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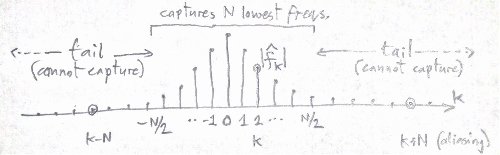

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Just did f on intervals $[a,b]$. global interp. (& integr., etc.) of smooth *periodic* f differs!

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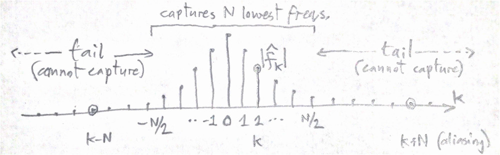

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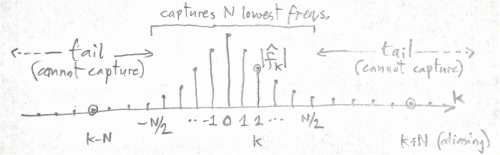

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Summary: given N samples $f(x_j)$, interp. error $=$ truncation $+$ aliasing

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

ie error controlled by sum of tail

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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 $|k| \geq N/2$

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So for a periodic $f \in C^p$, recall first p derivs of f bounded

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

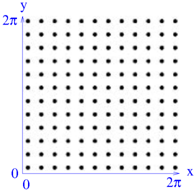
Messages:

- 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 $\hat{f}_k$

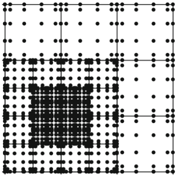
Flavor of interpolation in higher dims $d > 1$

If you *can* choose the nodes:

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



periodic, global



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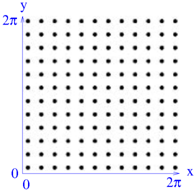

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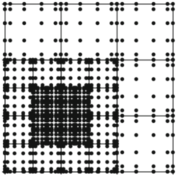

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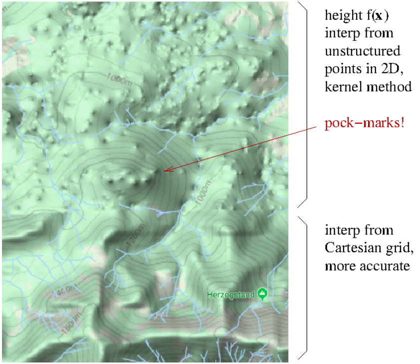
eg google terrain: $f(\mathbf{x})$ rough $\rightarrow$ garbage:



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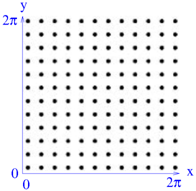

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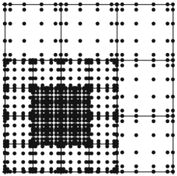

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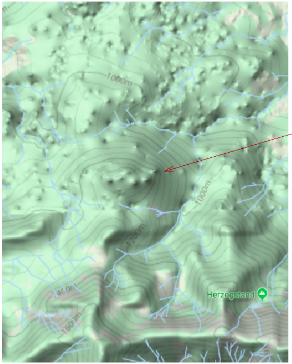

height f(**x**) interp from unstructured points in 2D, kernel method

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 $f(x_j) \rightarrow$ *integrate that exactly*

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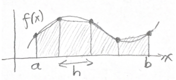

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  $w_j = h$ except $h/2$ at ends. low-order, err $\mathcal{O}(N^{-2})$, avoid!

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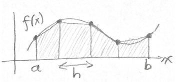

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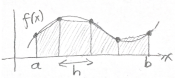

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demo:
```
N=14; sum(exp(cos(2*pi*(1:N)/N)))/N - besseli(0,1)
      ans = 1.3e-15
```

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)
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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.

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...

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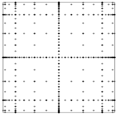

tensor prod: exp. # f evals. $N = n^d$ kills you :("curse of dim."

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

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"centered difference" formula

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

Let's see how that goes...

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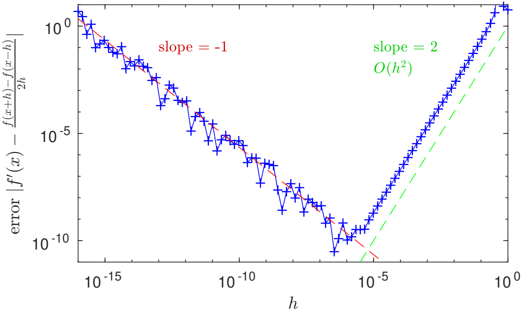

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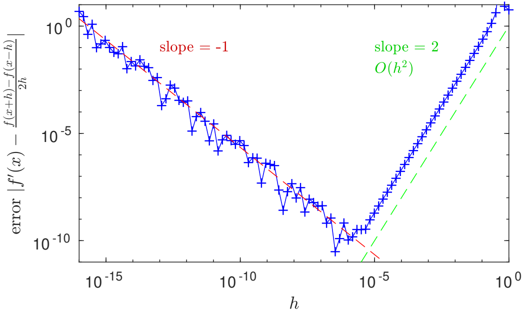

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- CPU arithmetic done only to relative "rounding error" $\epsilon_{\text{mach}} \sim 10^{-16}$
- subtracting v. close $f(x+h)$ and $f(x-h)$: "catastrophic cancellation"
- balance two error types: $h_{\text{best}} \sim \epsilon_{\text{mach}}^{1/3} \sim 10^{-5}$

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

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

As w/ integration: get interpolant $\rightarrow$ differentiate it exactly [**?**, 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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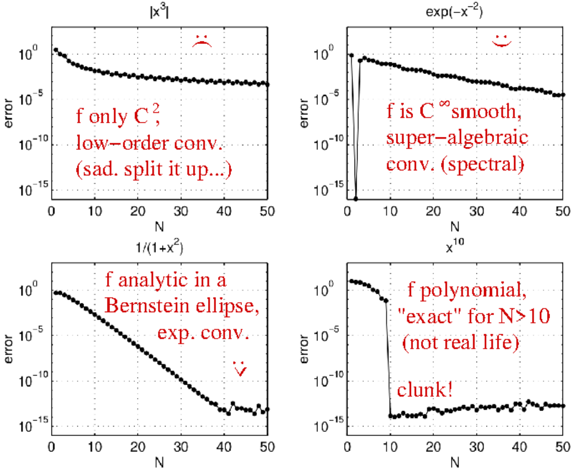
Examples:

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.

LECTURE II: numerical differential equations

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- Boundary Integral Methods Linear problems w/ boundary data

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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. $u(0) = 1,\ u'(0) = 0$

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  Task: solve $u(\boldsymbol{x})$ given forcing, boundary conditions
  Steady state of heat/diffusion, Gauss's law for conservative forces
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  Others: Navier-Stokes, magnetohydrodynamics, ...

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[Mike will overview the three flavors of PDE in next talk]

BCs: simple (eg periodic cube) vs complicated ($u = 0$ on a nasty surface)

Typical solution strategies

Time-independent PDEs:

1. Discretize variables (grid points, cells, basis functions)
2. Discretize operators/equations (derivatives)
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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
- For 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, $x + h$

$$u(x+h) = u(x) + u'(x)h + u''(x)h^2/2 + \mathcal{O}(h^3) \quad (1)$$

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

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$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + \mathcal{O}(h^2) \tag{4}$$

Extra order here due to symmetry

Finite difference methods

Alternate viewpoint:

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

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

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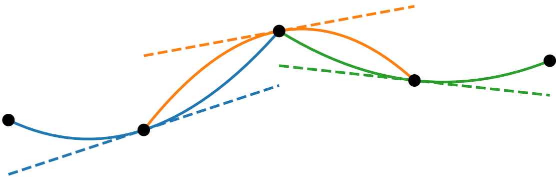

Implicit & Explicit Timestepping

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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Explicit schemes: just need $f(u_n)$. Simple but unstable for large steps

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

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$k\lambda < 2$ for stability

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Implicit schemes: require solving $f(u^{n+1}) = \ldots$ Stable but expensive

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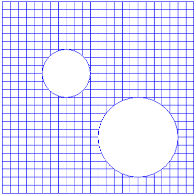
$$u_{n+1} = (1 + k\lambda)^{-1} u_n \tag{10}$$

Finite difference methods

- Extends to multiple dimensions with regular grids
- Simple to adjust order of accuracy
- 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



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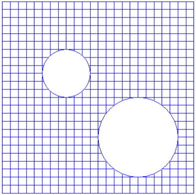
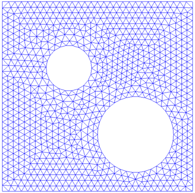


Resources: LeVeque "Finite Difference Methods for ODE/PDE"
Codes: e.g. Pencil code (magnetohydrodynamics)

Finite element methods

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

$$u(\boldsymbol{x}) = \sum_{n=1}^{N} u_n \phi_n(\boldsymbol{x}) \tag{11}$$



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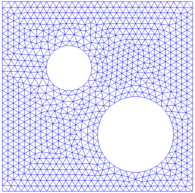

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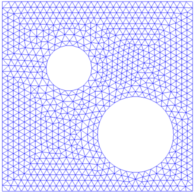

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- Solve resulting algebraic system:

$$M \cdot \partial_t \boldsymbol{u} + S \cdot \boldsymbol{u} = M \cdot \boldsymbol{f} \tag{14}$$

"Mass matrix" M, "stiffness matrix" S

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Finite volume methods

- Piecewise constants inside elements as test/trial functions

  $M = I$, easy explicit formulation

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- Integrate flux terms by parts:

$$\int \psi_m \nabla \cdot \boldsymbol{j} \, d\boldsymbol{x} = \int_{\Omega_i} \nabla \cdot \boldsymbol{j} \, d\boldsymbol{x} = \int_{\delta\Omega_i} \boldsymbol{n} \cdot \boldsymbol{j} \, dS \tag{15}$$

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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:

$$\int \psi_m \nabla^2 u \, d\boldsymbol{x} = - \int \nabla \psi_m \cdot \nabla u \, d\boldsymbol{x} \tag{16}$$

Lowers order of derivatives, allows piecewise linear representation

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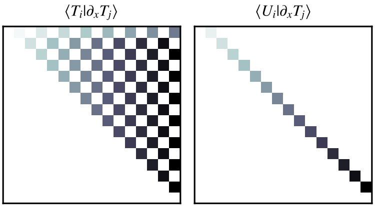
Non-periodic intervals: Chebyshev polynomials $T_n(x)$. Fast w/ DCT

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

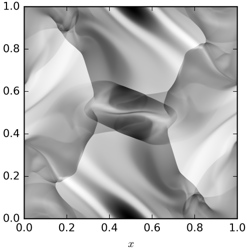
Modern: M and S banded with right choice of test functions.

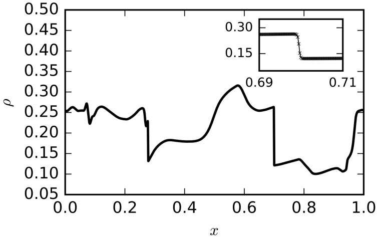


Other geometries: other polynomials, spherical harmonics, ...

Spectral methods

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





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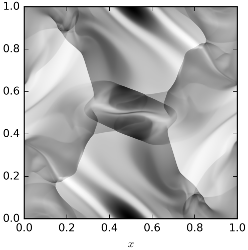

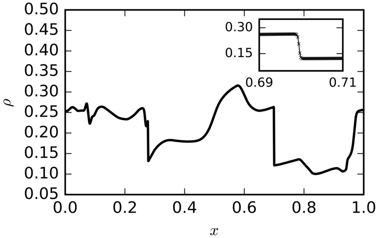

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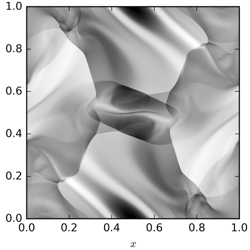

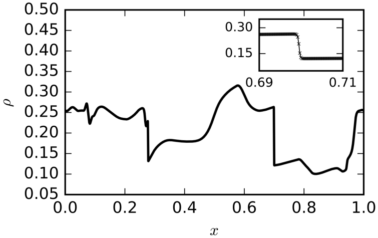

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Modern research: sparse methods for arbitrary equations in more geometries.

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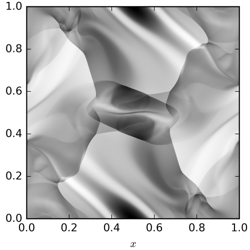

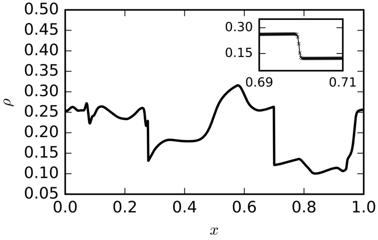

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Resources: Boyd "Chebyshev and Fourier Spectral Methods"
Codes: Chebfun (MATLAB), ApproxFun (julia), Dedalus (Python)

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Boundary integral methods

Use knowledge of PDEs in constructing solutions:

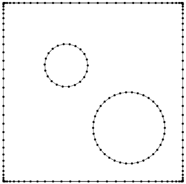
- Linear PDEs dominated by boundary terms
- Solutions involve integrals of fundamental solution (Green's function):

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

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

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

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



Examples: Stokes flow, Helmholtz equation, Maxwell equations

Usually homogeneous media

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

Summary

Recommended accessible reading

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

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