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)

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

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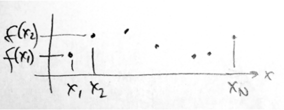
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

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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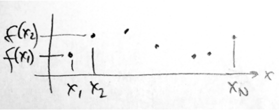
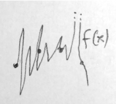


hopeless w/o assumptions on f, eg smoothness, otherwise...

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



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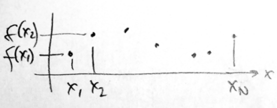

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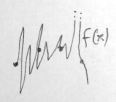
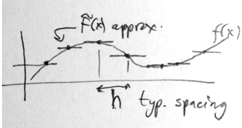


Simplest: use value at x_j nearest to x

"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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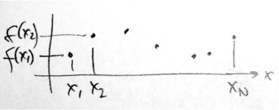

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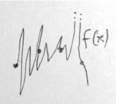

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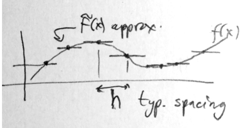

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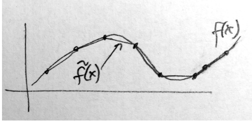
Piecewise linear: "connect the dots"

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

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

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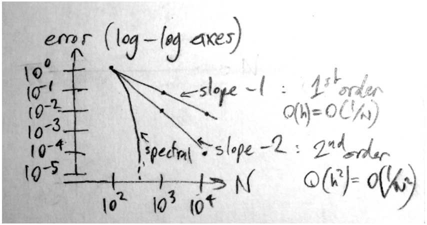

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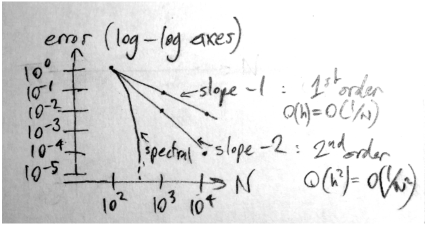

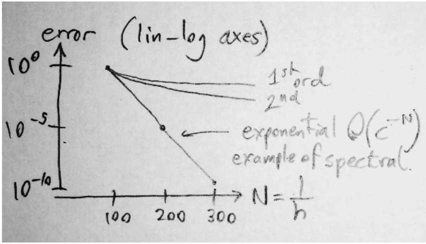

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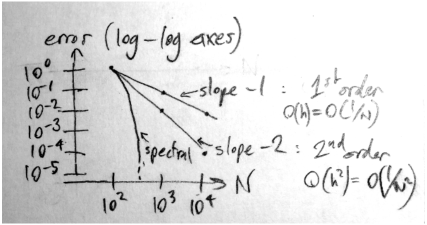
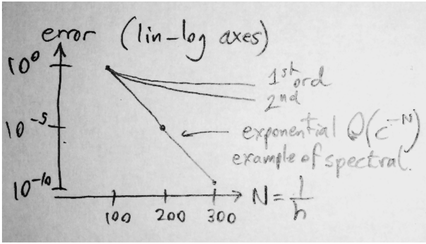




Note how spectral gets many digits for small N crucial for eg 3D prob.

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

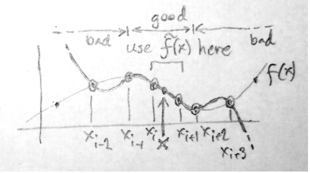
- how many digits to you want? for 1-digit (10% error), low order ok, easier to code

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

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

Higher-order interpolation for smooth f: the local idea

For any target x, use only set of 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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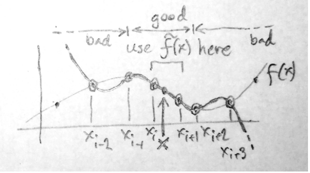

- error $\mathcal{O}(h^p)$, ie high order, but $\tilde{f}$ *not* continuous ($\tilde{f} \notin C$) has small jumps

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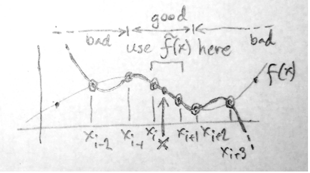

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How to find this degree-$(p-1)$ poly?

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

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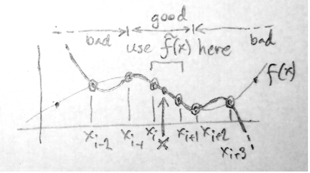

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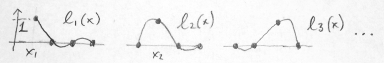
2) traditional: barycentric formula $\tilde{f}(x) = \dfrac{\sum_{j=1}^{p} \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^{p} \frac{1}{x-x_j} w_j}$ $\quad w_j = \frac{1}{\prod_{i \neq j}(x_j - x_i)}$

[Tre13, Ch. 5]

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



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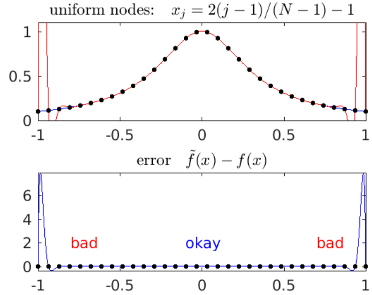
Global polynomial (Lagrange) interpolation?

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)



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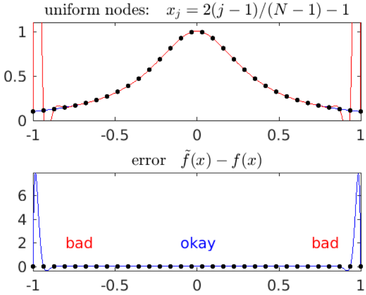

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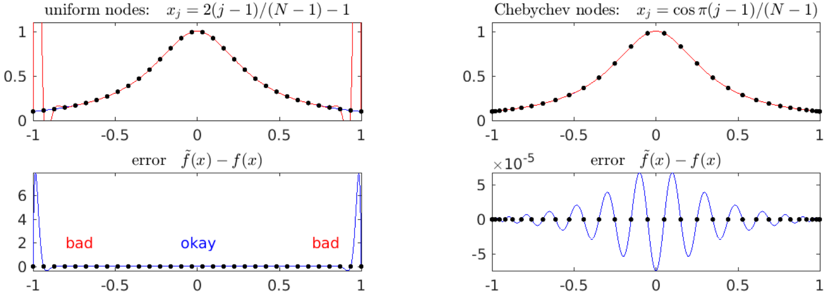

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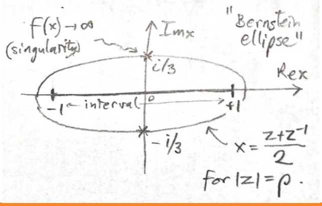
But exists good choice of nodes...

"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 $[a, b]$ has 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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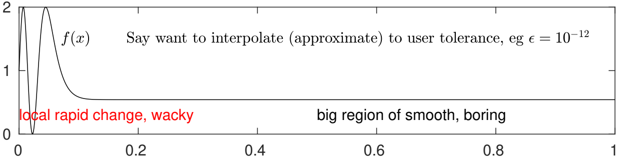

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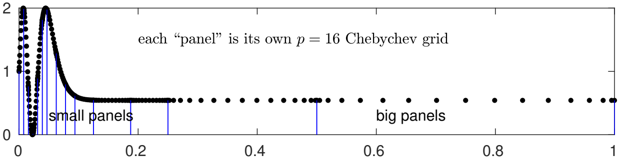

automatically split (recursively) panels until max err $\leq \epsilon$

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

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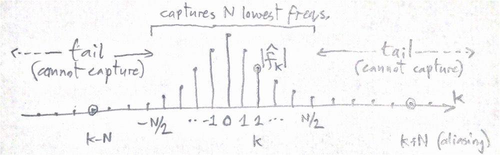

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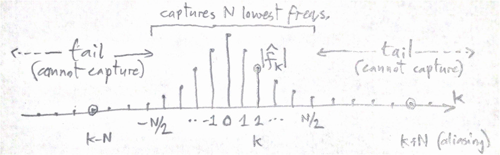

How read off c_k from *samples* of f on a grid?

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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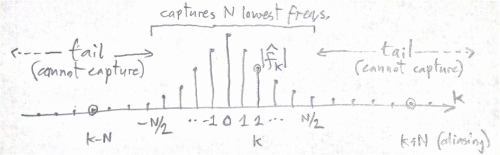

How read off c_k from *samples* of f on a grid?

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 $c_k = \frac{1}{N}\sum_{j=1}^{N} e^{ikx_j} f(x_j)$ $\quad$ 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

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

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

What's best you can do?

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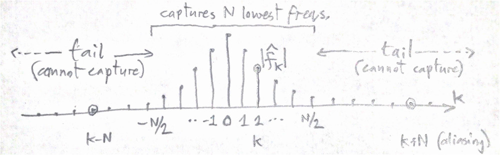

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Summary: given N samples $f(x_j)$, interp. error = truncation + aliasing

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

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 $|k| \geq N/2$

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])

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

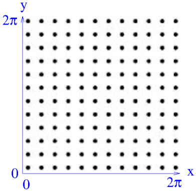
Take-home:

- 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



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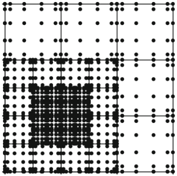

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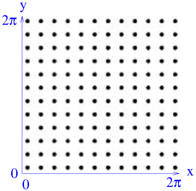

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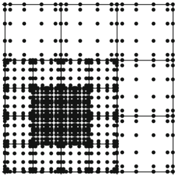

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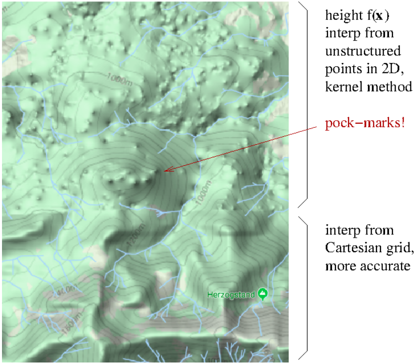

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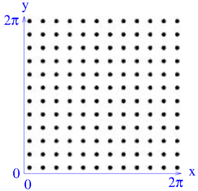

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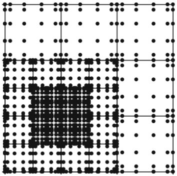

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But if know f smooth:

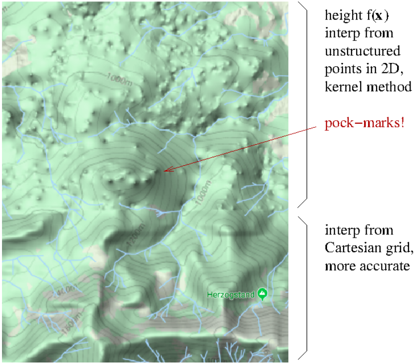
locally fit multivariate polynomials

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

"intepolatory quadrature"

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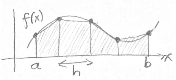

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  $w_j = h$ except $h/2$ at ends. low-order, err $\mathcal{O}(N^{-2})$, avoid!

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

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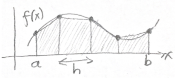

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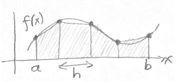

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demo:
```
N=14; sum(exp(cos(2*pi*(1:N)/N)))/N - besseli(0,1)
ans = 1.3e-15
```

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)
- oscillatory functions: deform contour to $\mathbb{C}$ "numerical steepest descent"

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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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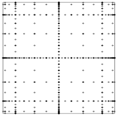

tensor prod: exp. # f evals. $N = n^d$ kills you :("curse of dim."

- "sparse grids" scale better as $N \sim n(\log n)^d$ (Smolyak '63)
- (quasi-)Monte Carlo: $\sum_{j=1}^N f(\mathbf{x}_j)$, 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

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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...

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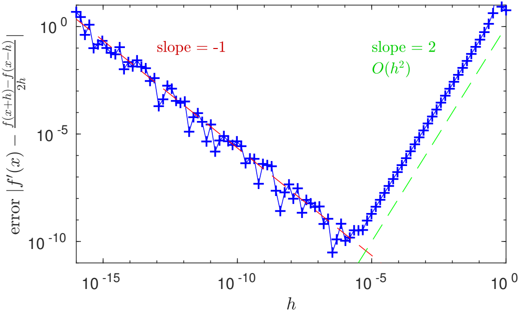

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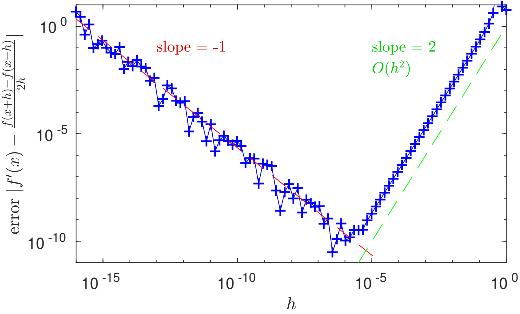

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- CPU arithmetic done only to relative "rounding error" $\epsilon_{\text{mach}} \sim 10^{-16}$
- subtracting v. close $f(x+h)$ and $f(x-h)$: "catastrophic cancellation"
- balance two error types: $h_{\text{best}} \sim \epsilon_{\text{mach}}^{1/3} \sim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

Essential reading: floating point, backward stability [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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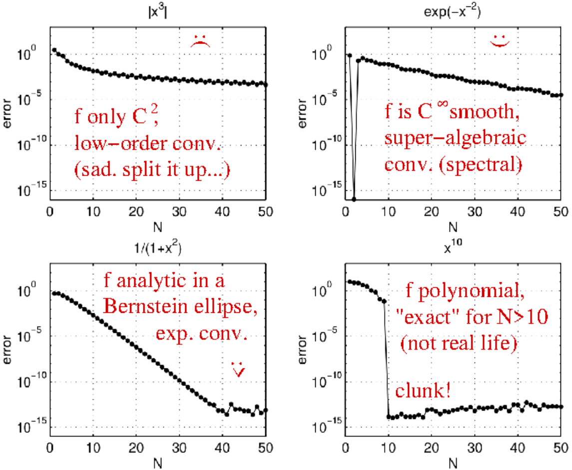
Examples:

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

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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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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

LECTURE II: numerical differential equations

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- Boundary Integral Methods Linear problems w/ boundary data

Reminder of types and applications of diff. eq.

- ODEs: eg pendulum $u''(t) + \sin(u(t)) = 0$

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  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:

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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, $x+h$

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

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

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

Extra order here due to symmetry

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Finite difference methods

Alternate viewpoint:

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  Unique, degree N-1.
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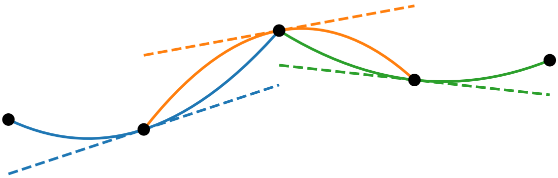

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Implicit & Explicit Timestepping

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

$$u'(t) = -\lambda u(t) \quad \lambda > 0 \tag{5}$$

$$u_{n+1} - u_n = -k\lambda u_n \tag{6}$$

$$u_{n+1} = (1 - k\lambda)u_n \tag{7}$$

$k\lambda < 2$ for stability

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

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

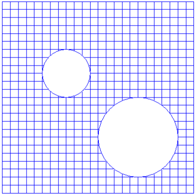
$$u'(t) = -\lambda u(t) \quad \lambda > 0 \tag{8}$$

$$u_{n+1} - u_n = -k\lambda u_{n+1} \tag{9}$$

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

Finite difference methods

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



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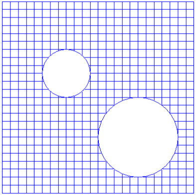
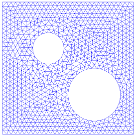


Resources: LeVeque "Finite Difference Methods for ODE/PDE"
Codes: e.g. Pencil code (magnetohydrodynamics)

Finite element methods

Partition domain into elements, represent unknown within each element using basis functions (usually polynomials)



Convert equations to weak form

- Give example
- Weak form advantages: lowers order, works if lower derivs are integrable (good for discontinuities, hyperbolic), can use tent functions

Replace weak form with Galerkin/weighted-residual form to get algebraic system

Traditional FEM methods use tent functions, produce continuous solutions. Fluxes at cell boundaries can be computed from internal representation, but can be discontinuous (non conservative).

Finite volume methods

Case of FEM taking functions to be piecewise constant inside elements
Resulting system is exactly conservative (good for hyperbolic), but requires Riemann solve

- Order increased by using neihgbors to reconstruct higher order internal representations or fluxes (slope/flux reconstruction)
- Reconstruction is nonlinear to control oscillations around discontinuities (TVD, ENO/WENO).

Very common in CFD, CCA

Advanced finite element methods

- Discontinuous Galerkin: allow discontinuities, need Riemann solvers again
- Spectral elements: move towards large p for better internal representations

Resources: ...

Codes: ...

Spectral methods

Limit of very few elements with very large p: exponential accuracy for smooth problems

Traditional techniques: Fourier spectral methods.

- Fast due to FFT: optimal complexity with exponential accuracy
- Limited to simple geometries / equations with symmetries

Polynomial spectral methods

- More flexible in terms of equations
- Still limited to simple geometries: cubes, spheres, cylinders, etc.
- Still a weak method, but don't integrate by parts. Apply Galerkin directly.

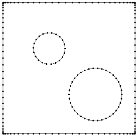
Modern research: sparse methods for arbitrary equations.

Resources: ...

Codes: ...

Boundary integral methods

Use knowledge of PDEs in constructing numerical solutions:
A Green's func G (fundamental soln) needed
eg $\Delta G = \delta$



For linear PDEs dominated by boundary rather than bulk terms, compute solution by forming integral equation of the fundamental solution/Green's function. Reduced dimensionality. Improved conditioning. Low-rank interactions and fast methods. Reconstruct solution in the bulk.
Examples: Stokes flow, Helmholtz, Maxwell, typically with homogeneous media
heavily uses high-order integration methods

- see Jun Wang's talk later today!

Summary

Recommended accessible reading

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

[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