FLATIRON INSTITUTE
Center for Computational Mathematics

FWAM Session B: Function Approximation and Differential Equations

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Wed, 10/30/19

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LECTURE 1: interpolation, integration, spectral methods

Motivations

exact func. $f(x)$ described by ∞ number of points
how handle approximately (but accurately) in computer, using least cost (bytes)?

- Interpolation:
  given exact data $f(x_i)$ at some x_i, model $f(x)$ at other points x?
  cheap but accurate look-up table for expensive $f(x)$

  Contrast: fit noisy data = learning (pdf for) params in model, via likelihood/prior
- (Numerical) integration:
  eg computing expectation values given a pdf, or their quantum version

  Contrast: Monte Carlo (random, high-dim.) integration, Thurs am
- Differentiation:

  get gradient ∇f: for optimization, or get matrix which approx. an ODE/PDE
- Spectral (often Fourier) methods:
  If $f(x)$ is smooth, handle very accurately without much extra cost

Deterministic (non-random) methods.
Integr/diff crucial for numerical ODEs and PDEs topic of LECTURE II

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Goals for LECTURE I

TODO

teach range of practical methods focusing on 1D

pointers to dimensions $d > 1$

Concepts:

convergence order — how does accuracy improve w/ number of discretization points?

global — (one expansion formula for the whole domain)

vs local — (different expansions for x in different regions)

spectral method — global, often use FFT, converge very fast

adaptivity — automatically placing degrees of freedom only where they need to be

rounding error & catastrophic cancellation — how not shoot self in the foot

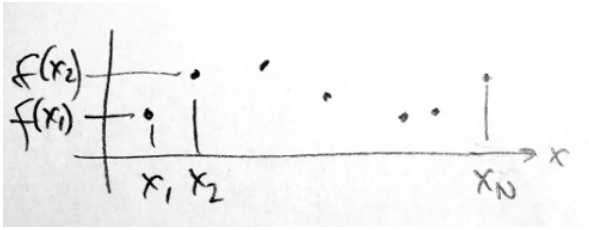
interpolation = func. representation, is key to all else

Interpolation in 1D ($d = 1$)

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

exact data, not noisy

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



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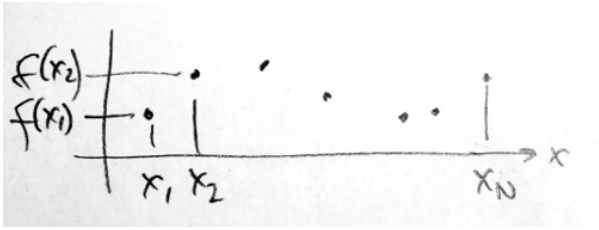
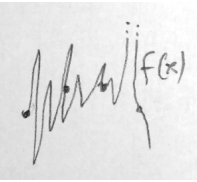


hopeless w/o assumptions on f, eg smoothness, otherwise...

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



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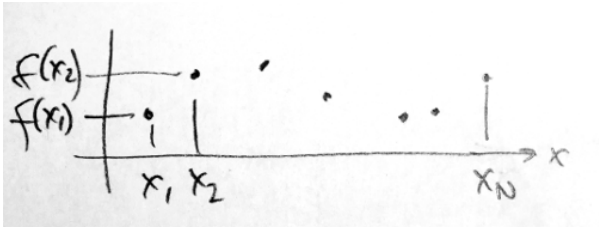

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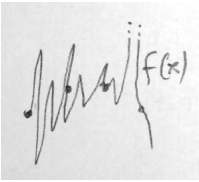
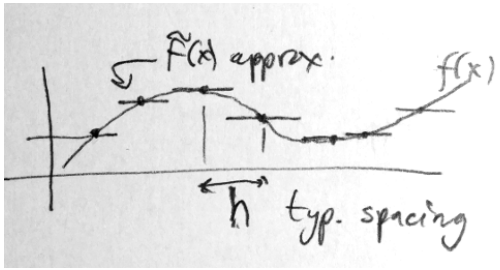


Simplest: use value at x_j nearest to x

"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



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

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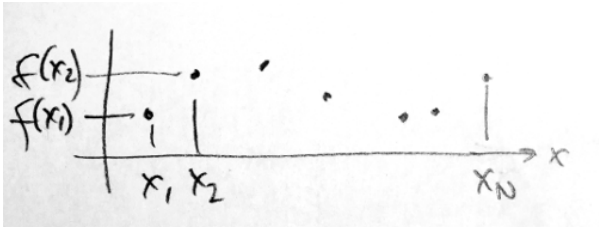

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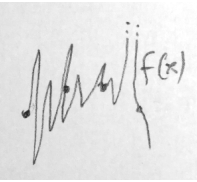

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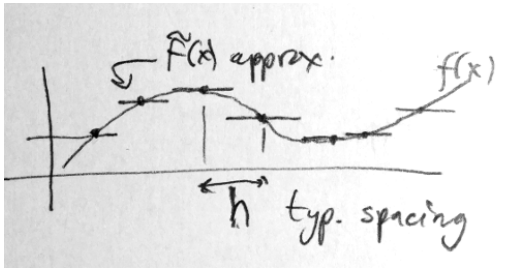
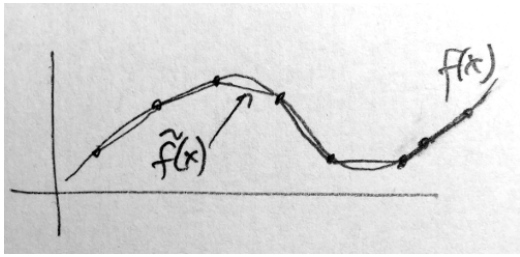


Recall notation "$\mathcal{O}(h)$": exists $C, h_0 > 0$ s.t. error $\leq Ch$ for all $h < h_0$

Piecewise linear: "connect the dots"

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

needs f'' bounded, ie smoother than before



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

Interlude: convergence rates

Should know or measure convergence rate of any method you use

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

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

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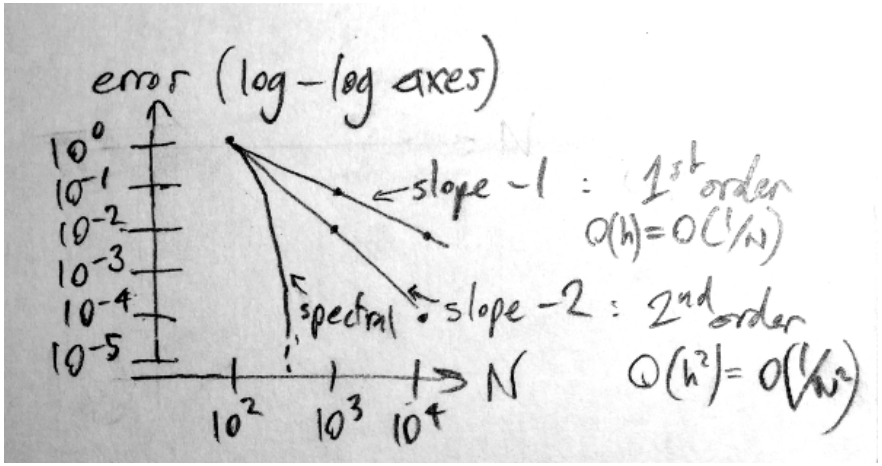

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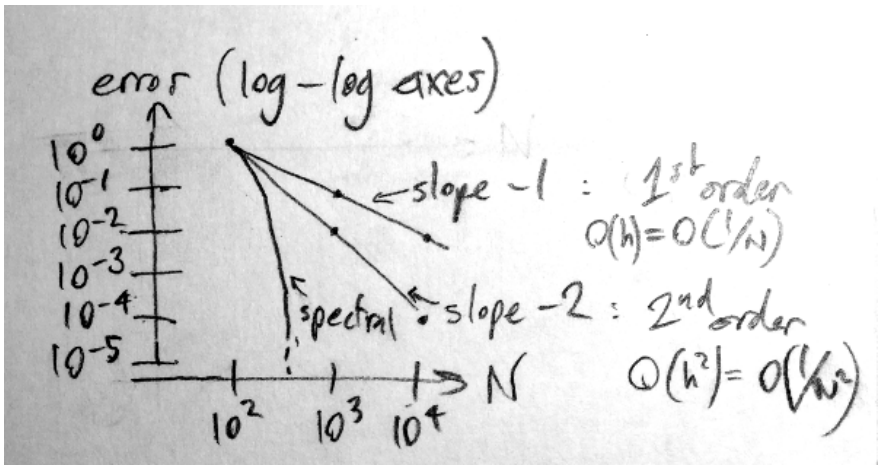

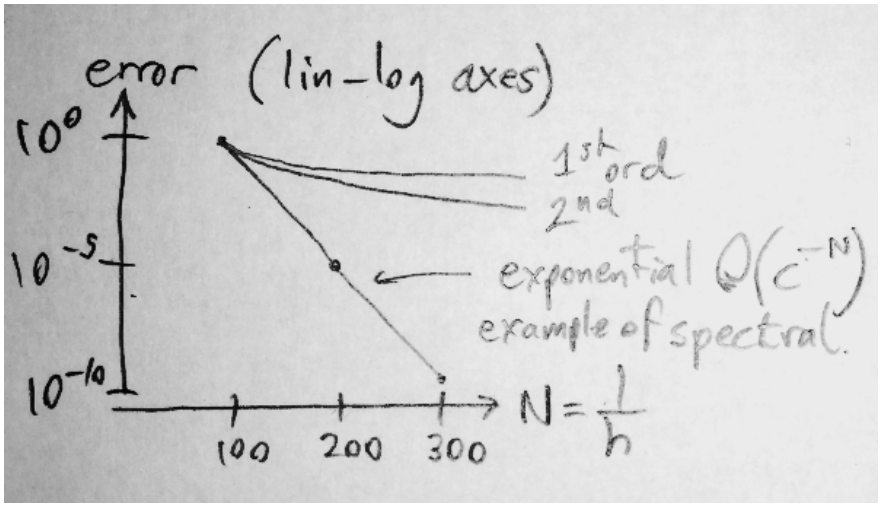

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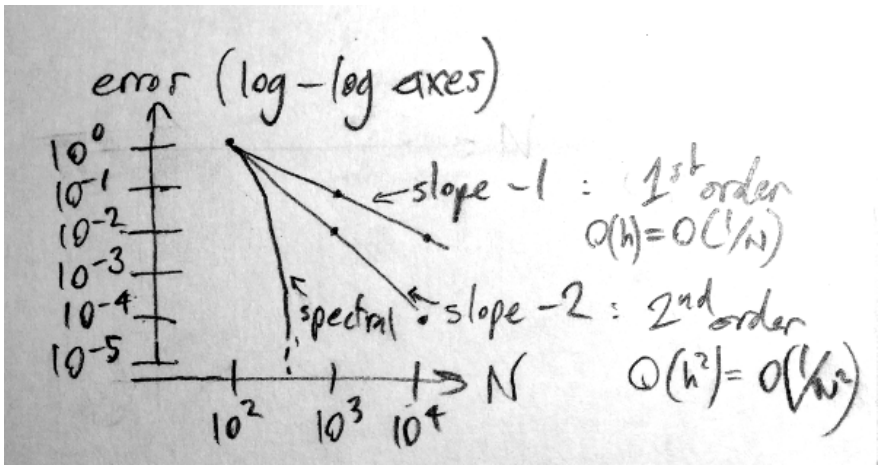
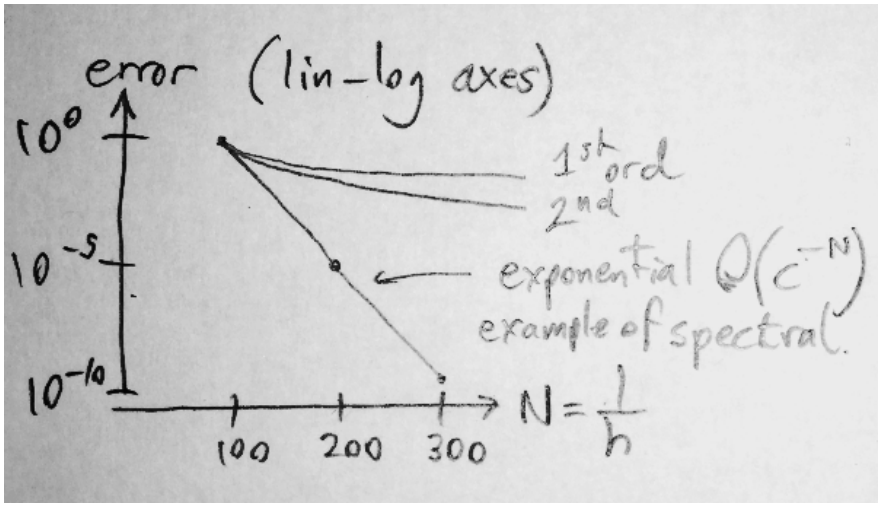




Note how spectral gets many digits for small N crucial for eg 3D prob.

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

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

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

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

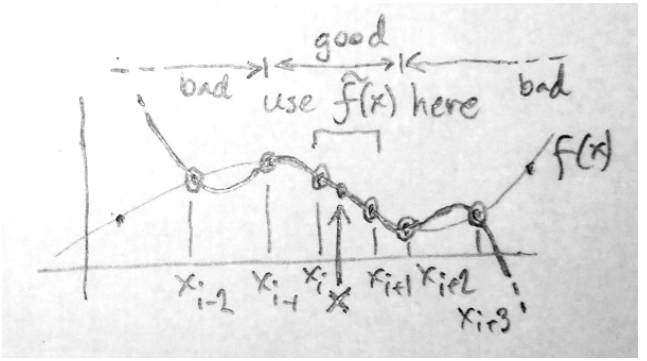
Higher-order interpolation for smooth f: the local idea

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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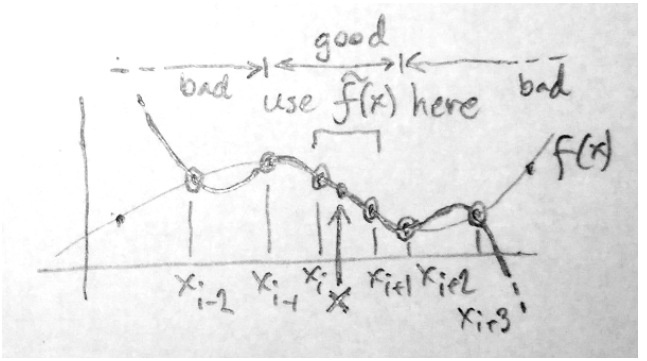

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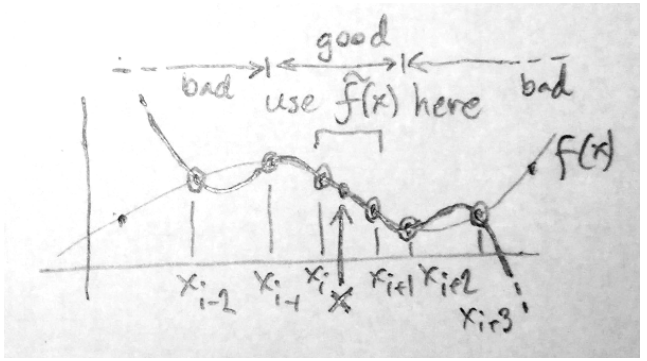

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How to find this degree-$(p-1)$ poly?

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

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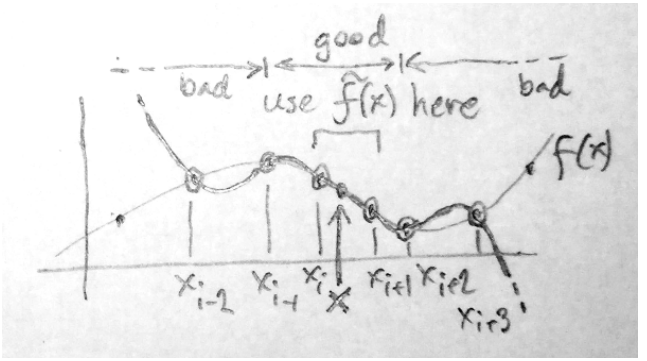

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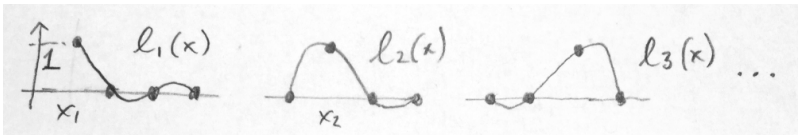
2) traditional: barycentric formula $\tilde{f}(x) = \dfrac{\sum_{j=1}^{p} \frac{y_j}{x-x_j} w_j}{\sum_{j=1}^{p} \frac{1}{x-x_j} w_j}$ $\qquad w_j = \frac{1}{\prod_{i \neq j}(x_j - x_i)}$

   [Tre13, Ch. 5]

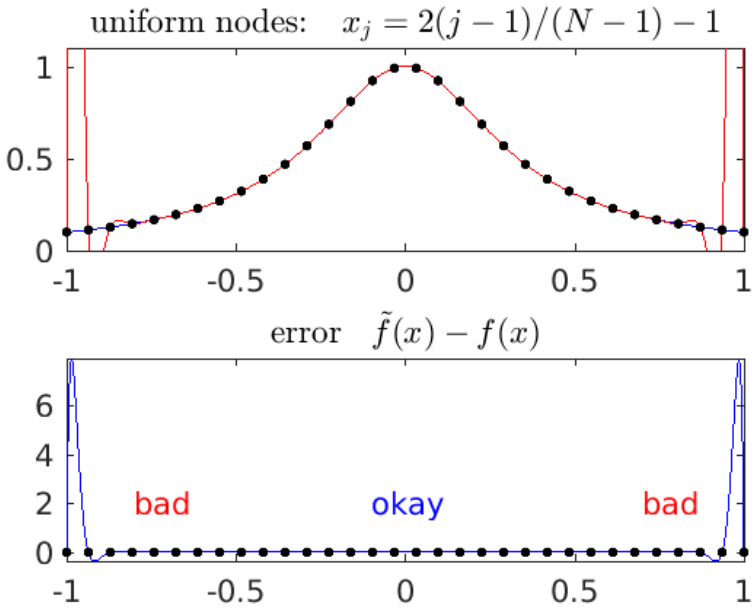
Either way, $\tilde{f}(x) = \sum_{j=1}^{p} y_j \ell_j(x)$ where $\ell_j(x)$ is jth Lagrange basis func:



Global polynomial (Lagrange) interpolation?

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

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



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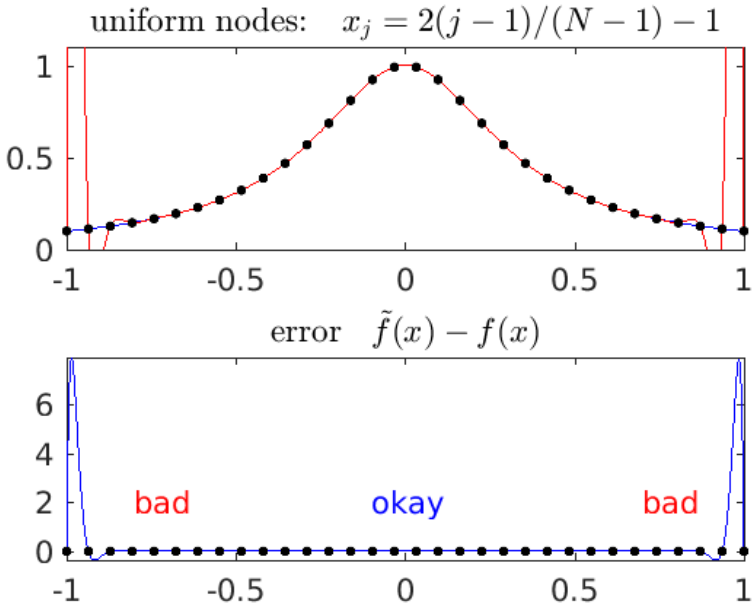

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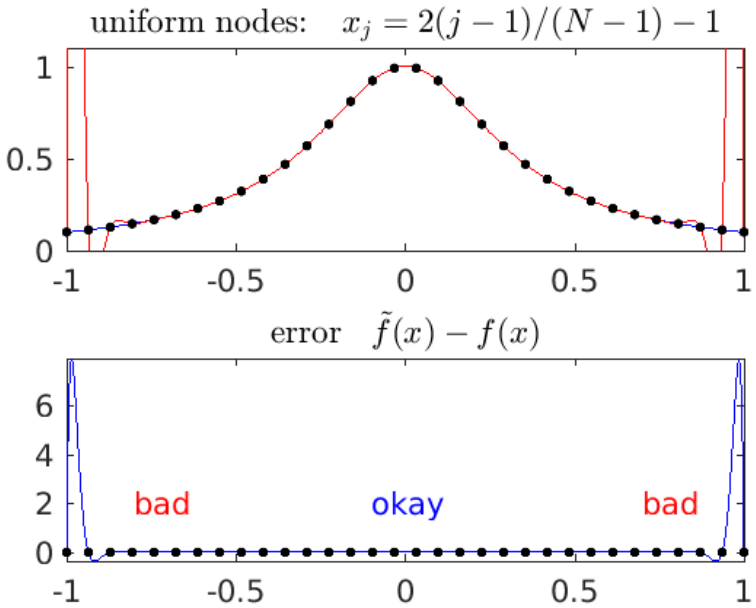

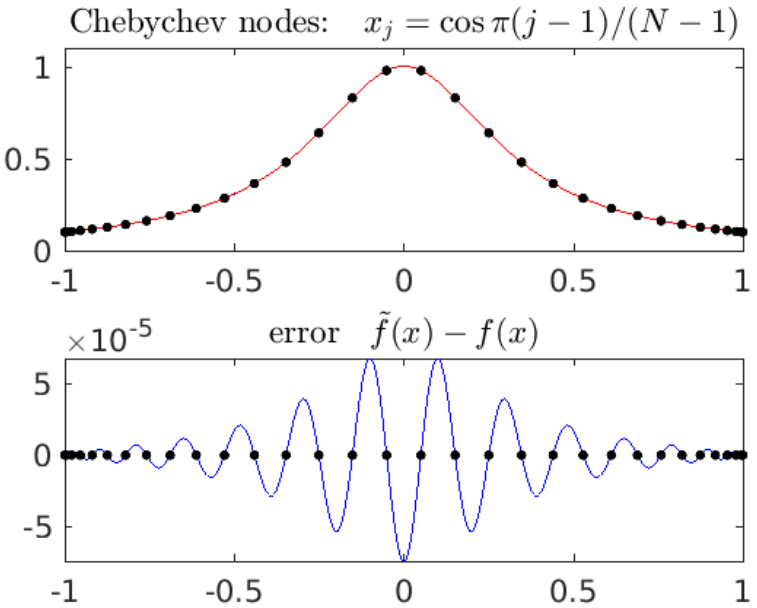

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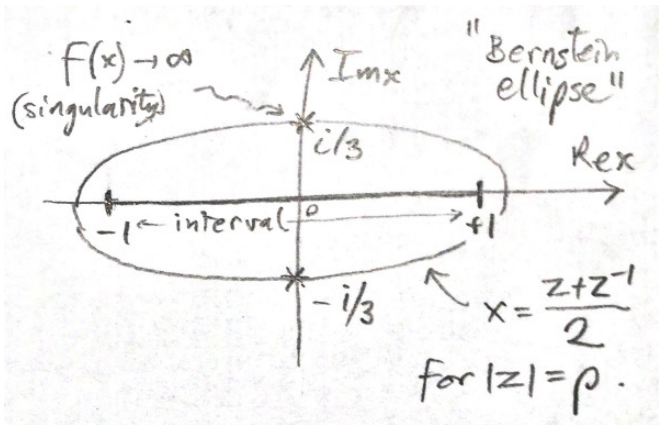
But exists good choice of nodes...

"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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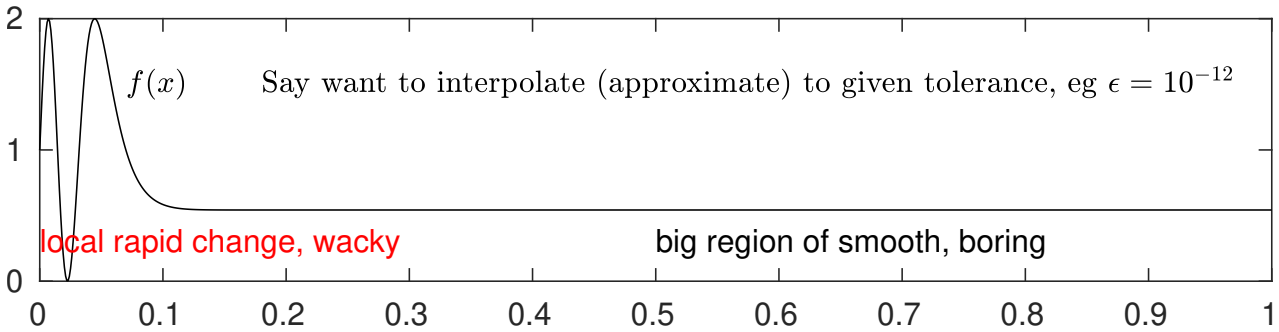

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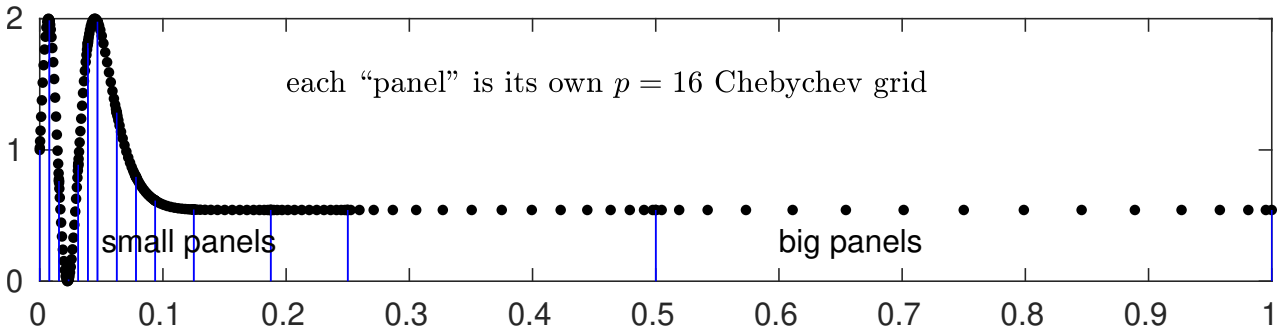

automatically split (recursively) panels until max err $\leq \epsilon$

via tests for local error

1D adaptive interpolator codes to try:

- `github/dbstein/function_generator` py+numba, fast (Stein '19)
- `chebfun` for MATLAB big-p Cheb. grids can exploit 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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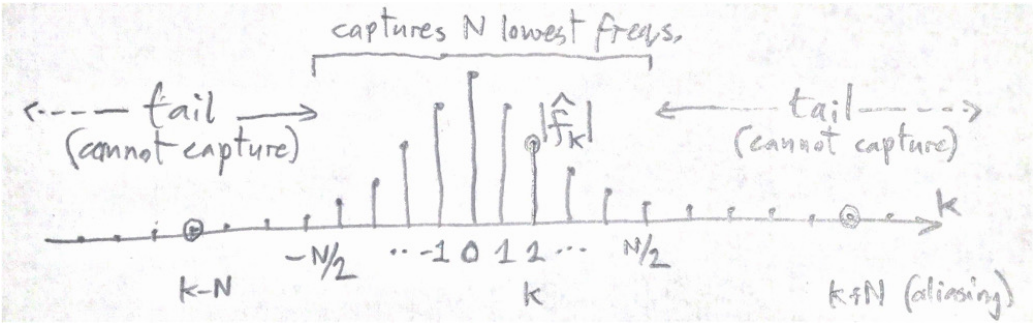
What's best you can do?

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

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



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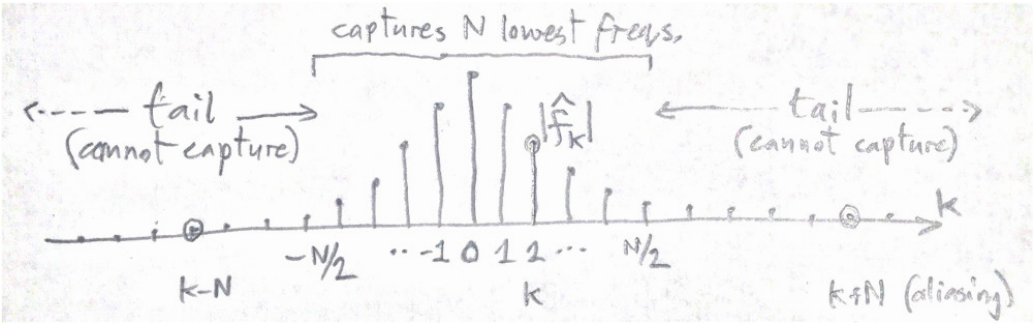

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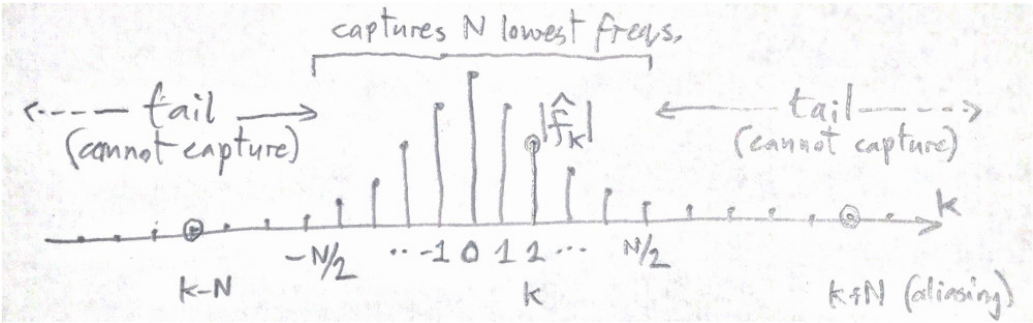

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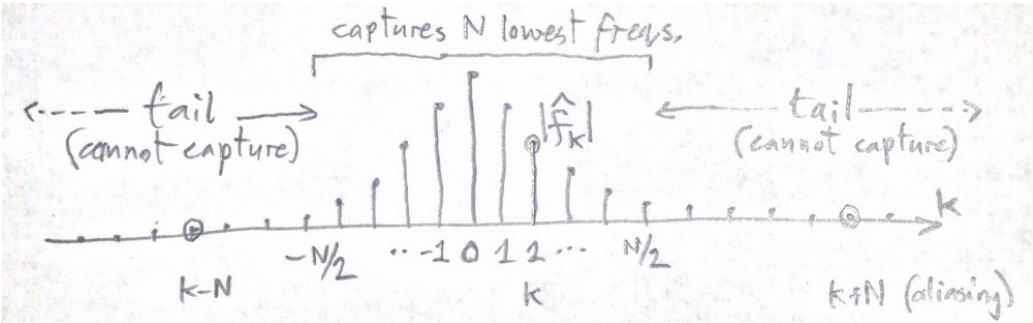

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Summary: given N samples $f(x_j)$, interp. error = truncation + aliasing

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

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!

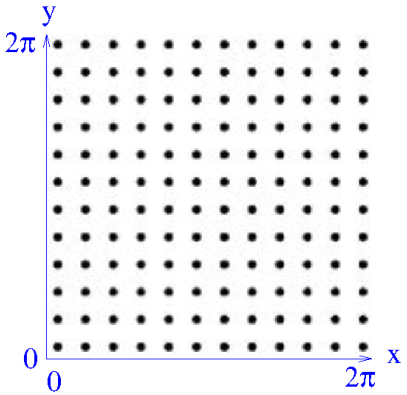
Take-home:

- 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 interp.
- either global
- or adaptively refined boxes



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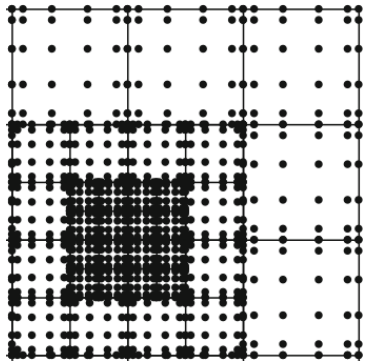
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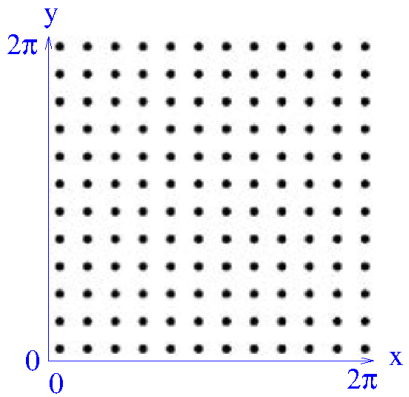

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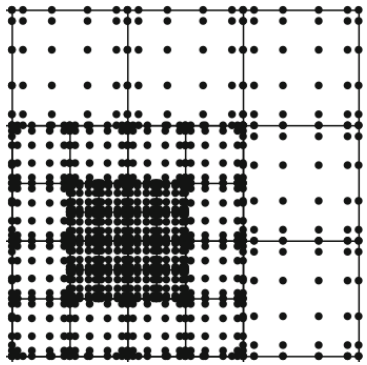
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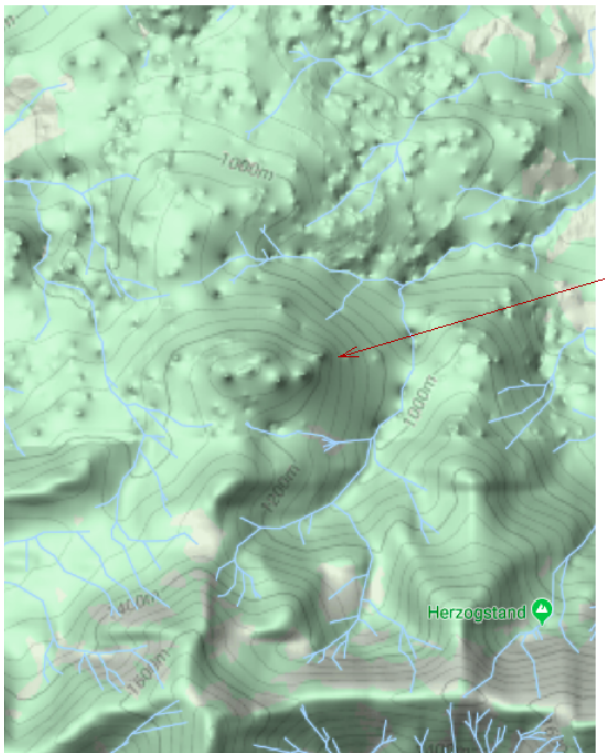
If *cannot* choose the nodes:
interp. $f(\boldsymbol{x})$ from scattered data $\{\boldsymbol{x}_i\}$ is hard

Eg google terrain: $f(\boldsymbol{x})$ rough $\rightarrow$ v. low ord,
see amusing transition in interp. type:



Or if know f smooth
fit local multivariate polynomial

If f noisy and smooth, many methods
kriging, kernels, ***

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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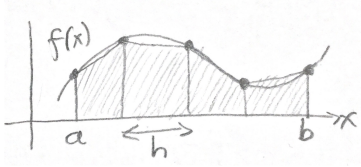

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  $w_j = h$ except $h/2$ at ends. low-order, err $\mathcal{O}(N^{-2})$, avoid!

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

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

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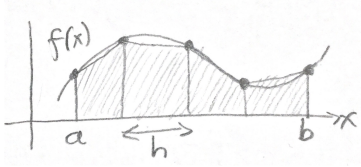

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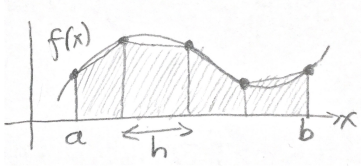

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demo:
```
N=14; sum(exp(cos(2*pi*(1:N)/N)))/N - besseli(0,1)
ans = 1.3e-15
```

Advanced integration

- custom quadr. for singularity eg $f(x) = \text{smooth} \cdot |x|^{-1/2}$
  or for a new set of funcs. "gen. Gaussian quad." (CCM: Manas Rachh)
- high-order end-corrections to trap. rule (Alpert '99)

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Higher dimensions $d > 1$

For d a few, tensor products of 1D n-node grids in each dim

other coord systems, eg sphere, can use tensor product in (θ, ϕ)

adaptivity works: subdivide into boxes same pic as for interp.

Much higher $d \gg 1$

Now exponential cost $N = n^d$ kills you :(

Are "sparse grids" scaling better rely on funcs aligning w/ axes

Monte Carlo methods: sum N values of $f(\boldsymbol{x}_j)$ for $\boldsymbol{x}_j$ random points

error $= \mathcal{O}(N^{-1/2})$ 1/2-order acc, indep of dim d

*** check

Numerical differentiation

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Want smallest error:

suggests taking $h \to 0$?

Let's see how that goes...

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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: $h_{\text{best}} \sim \epsilon_{\text{mach}}^{1/3} \sim 10^{-5}$

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

Better approach to differentiation ($d = 1$)

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

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

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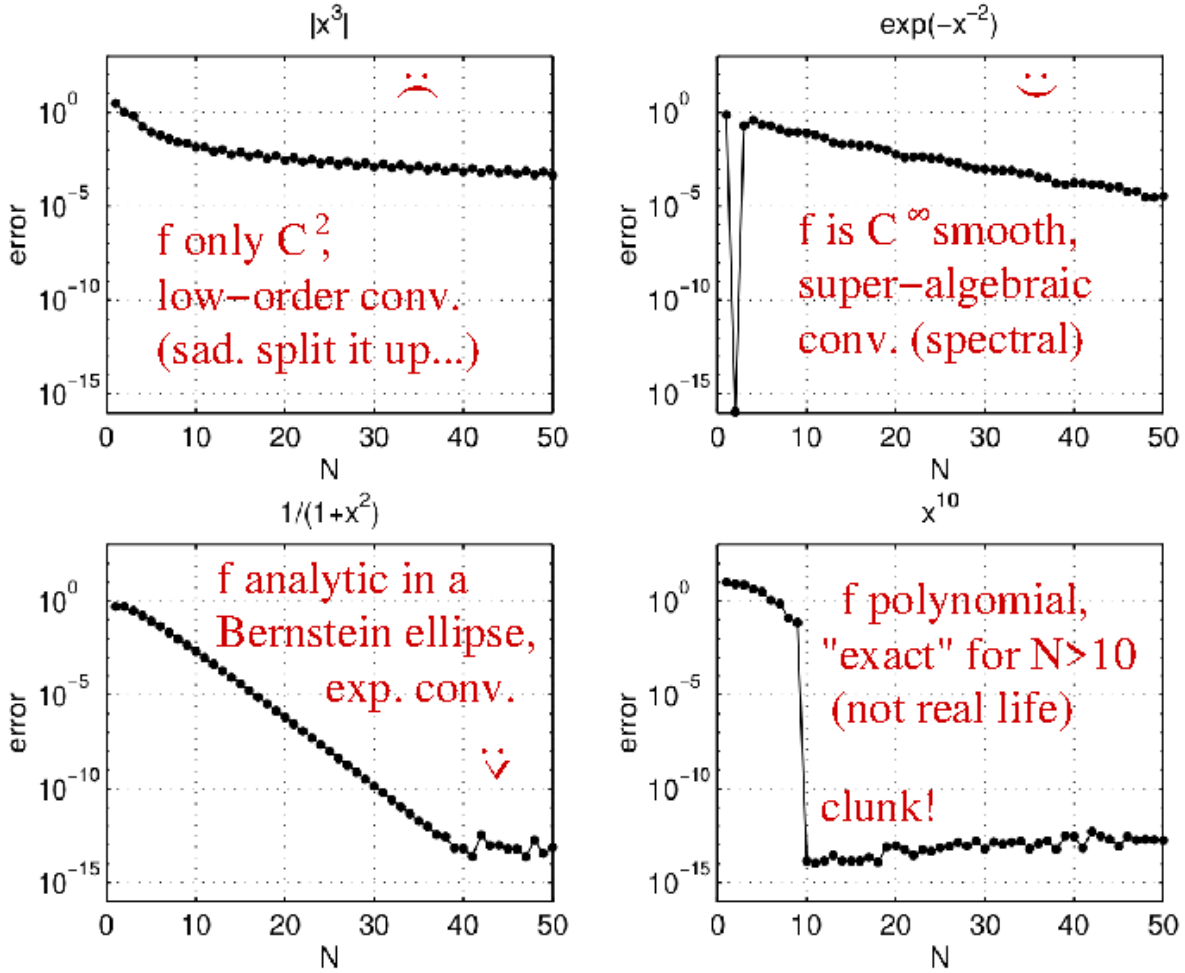
Examples:

N Chebychev nodes

in $[-1, 1]$

shown: max error in f'



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

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

Summary: we scratched the surface

Can integrate & differentiate functions 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
smoothness
spectral method
global vs local interpolant
adaptivity
rounding error & catastrophic cancellation
tensor products for 2D & 3D; higher gets harder

See references at end of slide, and come ask us stuff!

LECTURE II: numerical differential equations

GOALS

***

Reminder of types and applications of diff. eq.

- ODEs: eg pendulum $u''(t) + \sin(u(t)) = 0$ task: solve $u(t)$ efficiently & acc.
  needs initial conditions to kick it off eg $u(0) = 1$, $u'(0) = 0$
  eg kinetics of system of well-mixed chemicals, $\boldsymbol{u}(t)$ is vector

- time-independent PDEs, usually "elliptic" Mike will explain
  eg Poisson eqn $\Delta u = g$, $u(\boldsymbol{x})$ = chemical concentration or electric potential
  $\boldsymbol{x}$ means $(x, y, \dots)$, Δu means Laplacian $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \cdots$ = curvature of u
  $g(\boldsymbol{x})$ = volume source of chemical or charge
  needs boundary conditions (BCs) on u, or decay at infinity
  eg viscous fluid flow: $\boldsymbol{u}$ is velocity field, Stokes eqns
  eg what is ground state of quantum system? solving t-indep. Schrödinger $\Delta u = Eu$

- time-dependent (evolution) PDEs $u(\boldsymbol{x}, t)$ varies in space and time
  eg heat/diffusion equation $\partial u/\partial t + \Delta u = g$ $g(\boldsymbol{x}, t)$ = source
  needs initial and BCs BCs may vary in time...

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

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

IVPs to BVPs

Motivate focus on BVPs by mentioning:

- Most people familiar with method of lines
- Equivalent "propagator" approach: discretize time, then solve BVP
- Most timesteppers are FD methods (some examples)

Finite difference methods

Basic viewpoint:

- Construct Taylor-series approximation to value at neighboring points
- For N points, expand to (N-1) derivatives (error $\mathcal{O}(h^N)$)
- Eliminate system to get approximation to d-th derivative ($d < N$)

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

Alternate viewpoint:

- Differentiate the unique interpolating polynomial of deg N-1

Illustrate with centered forward 1st-order scheme, centered 2nd-order scheme (get extra degree for free).

Timestepping with finite difference methods

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

Explicit methods: simple, just require evaluating $f(u_n)$.

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

Unstable for large timesteps

$$u'(t) = -\lambda u(t) \quad \lambda > 0 \tag{1}$$

$$\frac{u_{n+1} - u_n}{k} = -\lambda u_n \tag{2}$$

$$u_{n+1} = (1 - k\lambda)u_n \tag{3}$$

$$\boxed{k\lambda < 2} \tag{4}$$

Implicit methods: stable, but require solving $f(u^{n+1}) = \ldots$

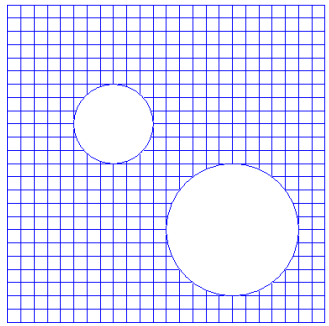
- Backward Euler: use 1st-order backward difference rule

Stability, but potentially at high cost

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

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

Advanced finite difference techniques

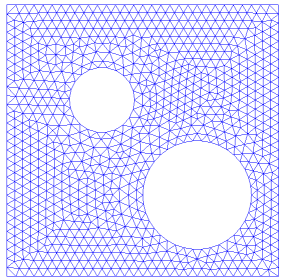


- Selecting stencils term by term (e.g. upwinding)
- Adaptive stencil selection (e.g. WENO)

Resources: ...
Codes: ...

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.

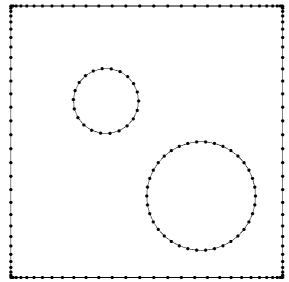
Modern research: sparse methods for arbitrary equations.

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`.