FWAM Session B: Function Approximation and Differential Equations

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

Wednesday afternoon, 10/30/19

[1]Center for Computational Mathematics, Flatiron Institute

[2]Center for Computational Astrophysics, Flatiron Institute, and Department of Mathematics, MIT

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)

Goals and plan

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

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

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

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

- Numerical integration:

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

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

- Numerical differentiation:

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

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

Goals and plan

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

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

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

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

- Numerical integration:

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

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

- Numerical differentiation:

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

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

Key concepts:

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

Goals and plan

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

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

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

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

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

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

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

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

Key concepts:

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

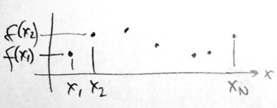
Plus: good 1D tools, pointers to codes, higher dim methods, opinions!

Interpolation in 1D ($d = 1$)

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

note: exact data, not noisy

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

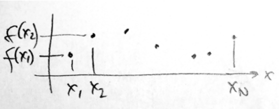


Interpolation in 1D ($d = 1$)

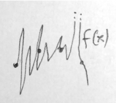
Say $y_j = f(x_j)$ known at nodes $\{x_j\}$ N-pt "grid"

note: exact data, not noisy

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



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



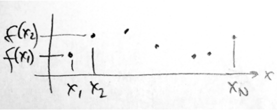
- extra info helps, eg f periodic, or $f(x) = \text{smooth} \cdot |x|^{-1/2}$

Interpolation in 1D ($d = 1$)

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

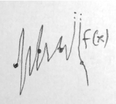
note: exact data, not noisy

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



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

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

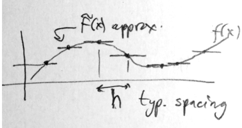


Simplest: use value at x_j nearest to x

"snap to grid"

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

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



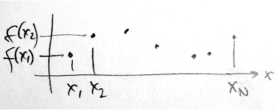
Recap notation "$\mathcal{O}(h)$": exists C, h_0 s.t. error $\leq Ch$ for all $0 < h < h_0$

Interpolation in 1D ($d = 1$)

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

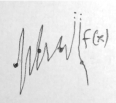
note: exact data, not noisy

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



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

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

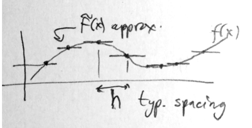


Simplest: use value at x_j nearest to x

"snap to grid"

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

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

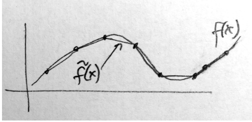


Recap notation "$\mathcal{O}(h)$": exists C, h_0 s.t. error $\leq Ch$ for all $0 < h < h_0$

Piecewise linear: "connect the dots"

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

needs f'' bounded, ie smoother than before



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

Interlude: convergence rates

Should know or measure convergence rate of any method you use

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

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

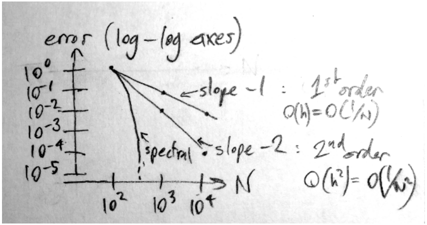
Interlude: convergence rates

Should know or measure convergence rate of any method you use

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

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

There's only one graph in numerical analysis: $\boxed{\text{“relative error vs effort”}}$



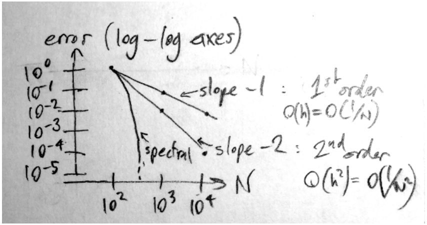
Interlude: convergence rates

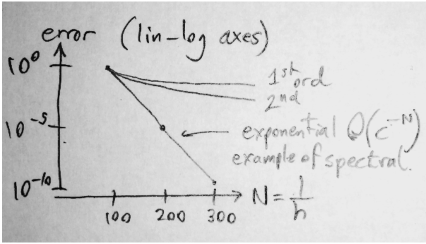
Should know or measure convergence rate of any method you use

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

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

There's only one graph in numerical analysis: $\boxed{\text{"relative error vs effort"}}$





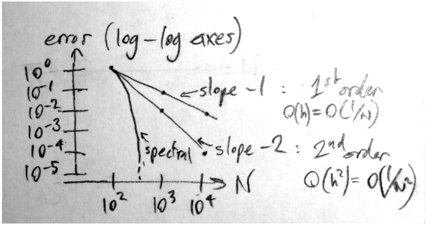
Interlude: convergence rates

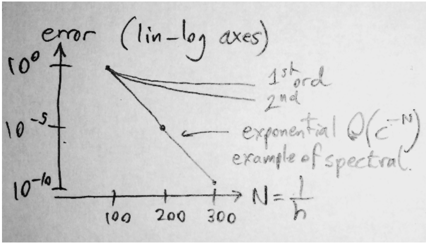
Should know or measure convergence rate of any method you use

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

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

There's only one graph in numerical analysis: $\boxed{\text{"relative error vs effort"}}$





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

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

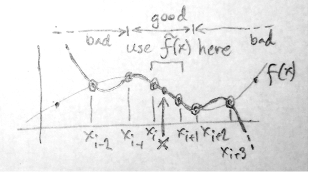
- how many digits to you want? for 1-digit (10% error), low order ok, easier to code

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

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

Higher-order interpolation for smooth f: the local idea

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!

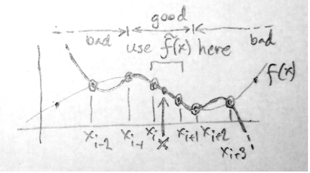
Higher-order interpolation for smooth f: the local idea

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!



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

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

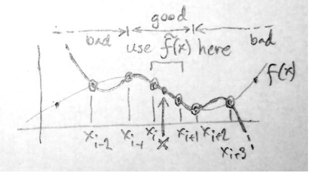
Higher-order interpolation for smooth f: the local idea

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!



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

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

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

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

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

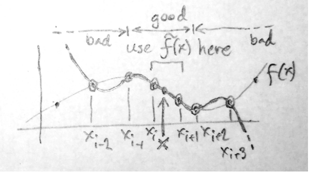
Higher-order interpolation for smooth f: the local idea

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!



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

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

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

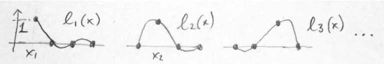
1) crafty: solve square lin sys for coeffs $\sum_{k<p} x_j^k c_k = y_j$ $\quad j = 1, \ldots, p$

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

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

[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:

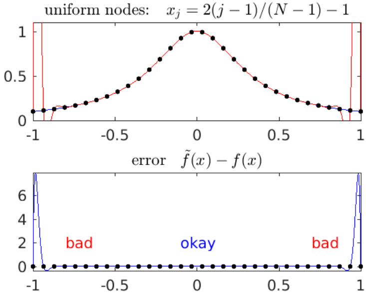


FLATIRON INSTITUTE Center for Computational Mathematics

Global polynomial (Lagrange) interpolation?

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

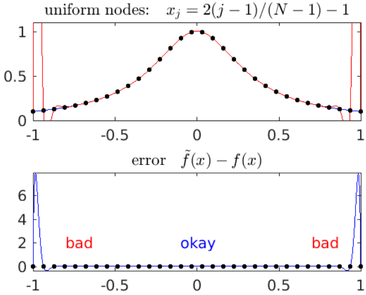
$p = N = 32$, smooth (analytic) $f(x) = \frac{1}{1+9x^2}$ on $[-1, 1]$: (Runge 1901)



Global polynomial (Lagrange) interpolation?

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

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

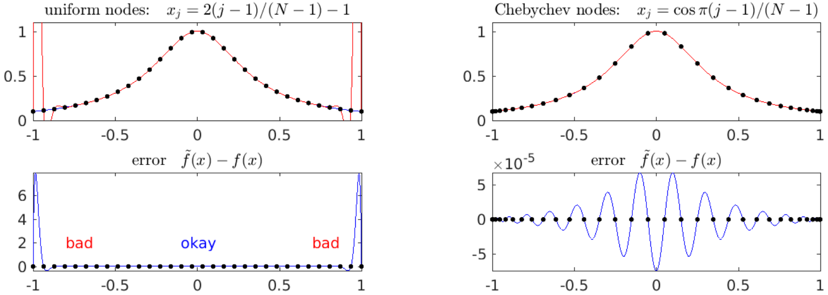


- warning: unif. grid, global interp. fails $\to$ only use locally in central region

Global polynomial (Lagrange) interpolation?

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

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



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

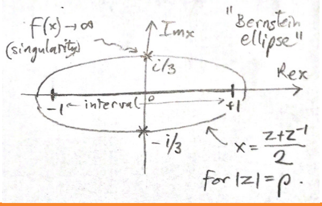
But exists good choice of nodes...

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

- our first spectral method

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

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



Node choice and adaptivity

Recap: poly approx. $f(x)$ on $[a, b]$ 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!

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!

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

Node choice and adaptivity

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

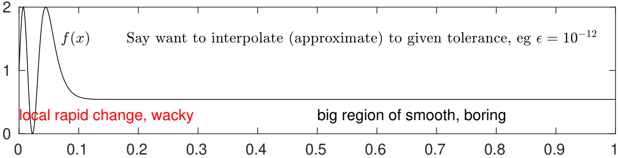
Question: Do *you* get to choose the set of nodes at which f known?

- 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!

Adaptivity idea

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



Node choice and adaptivity

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

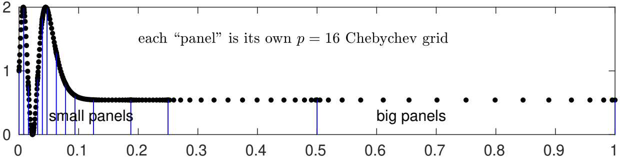
Question: Do *you* get to choose the set of nodes at which f known?

- 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!

Adaptivity idea

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



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

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"

Global interpolation of periodic functions I

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

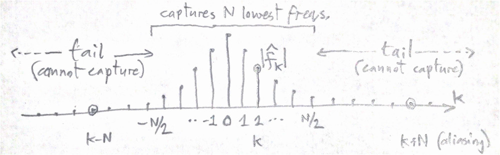
Periodic: $f(x + 2\pi) = f(x)$ for all x, $f(x) = \sum_{n\in\mathbb{Z}} \hat{f}_k e^{ikx}$ Fourier series

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?

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

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



Global interpolation of periodic functions I

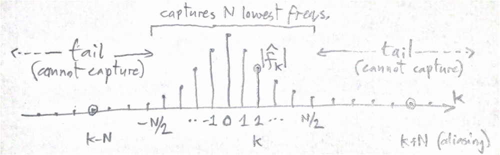
Just did f on intervals $[a, b]$. global interp. (& integr., etc.) of smooth *periodic* f differs!

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?

- get N coeffs right $c_k = \hat{f}_k$
- error $\sim$ size of tail $\{\hat{f}_k\}_{|k|\ge N/2}$



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

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

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

Global interpolation of periodic functions I

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

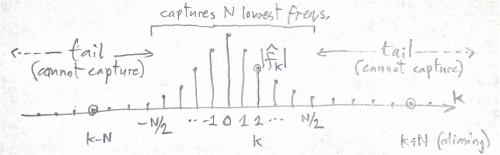
Periodic: $f(x + 2\pi) = f(x)$ for all x, $f(x) = \sum_{n\in\mathbb{Z}} \hat{f}_k e^{ikx}$ Fourier series

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?

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

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



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

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

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

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!

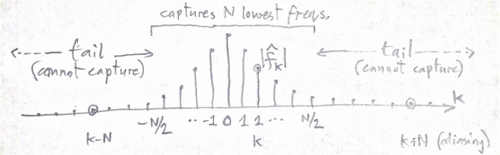
Periodic: $f(x + 2\pi) = f(x)$ for all x, $f(x) = \sum_{n\in\mathbb{Z}} \hat{f}_k e^{ikx}$ Fourier series

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?

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

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



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

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

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

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

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

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

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

ie error controlled by sum of tail

Global interpolation of periodic functions II

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

Now $\quad \hat{f}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-ikx}dx = \frac{1}{2\pi}\int_0^{2\pi} f^{(p)}(x)\frac{e^{-ikx}}{(ik)^p}dx$ 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 $\mathcal{O}(N^{1-p})$ $\quad (p-1)$th order acc. (better: [Tre00])

Global interpolation of periodic functions II

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

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

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

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

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

Global interpolation of periodic functions II

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

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

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

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

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

Even smoother case: f analytic, so $f(x)$ analytic in some complex strip $|\operatorname{Im} x| \leq \alpha$

then $\hat{f}_k = \mathcal{O}(e^{-\alpha|k|})$, exp. conv. $\mathcal{O}(e^{-\alpha N/2})$ (fun proof: shift the contour)

as with Bernstein ellipse, to get exp. conv. *rate* need understand f *off its real axis* (wild!)

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

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

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

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

Even smoother case: f analytic, so $f(x)$ analytic in some complex strip $|\operatorname{Im} x| \leq \alpha$

then $\hat{f}_k = \mathcal{O}(e^{-\alpha|k|})$, exp. conv. $\mathcal{O}(e^{-\alpha N/2})$ (fun proof: shift the contour)

as with Bernstein ellipse, to get exp. conv. *rate* need understand f *off its real axis* (wild!)

Smoothest case: "band-limited" f with $\hat{f}_k = 0$, $|k| > k_{\max}$,

then interpolant *exact* once $N > 2k_{\max}$

Global interpolation of periodic functions II

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

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

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

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

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

Even smoother case: f analytic, so $f(x)$ analytic in some complex strip $|\operatorname{Im} x| \leq \alpha$

then $\hat{f}_k = \mathcal{O}(e^{-\alpha|k|})$, exp. conv. $\mathcal{O}(e^{-\alpha N/2})$ (fun proof: shift the contour)

as with Bernstein ellipse, to get exp. conv. *rate* need understand f *off its real axis* (wild!)

Smoothest case: "band-limited" f with $\hat{f}_k = 0$, $|k| > k_{\max}$,

then interpolant *exact* once $N > 2k_{\max}$

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

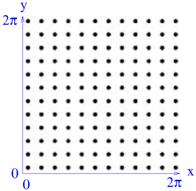
Take-home:

- 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 $\hat{f}_k$

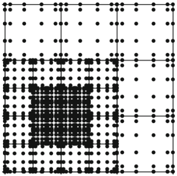
Flavor of interpolation in higher dims $d > 1$

If you *can* choose the nodes:

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



periodic, global

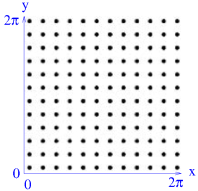


adaptive $p = 6 \times 6$ Cheby

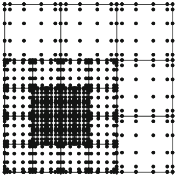
Flavor of interpolation in higher dims $d > 1$

If you *can* choose the nodes:

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



periodic, global



adaptive $p = 6 \times 6$ Cheby

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

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

Or if know f smooth

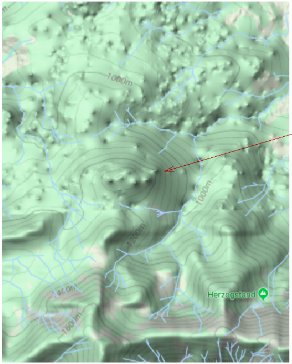
locally fit multivariate polynomials

If also data noisy, many methods:

kriging (Gauss. proc.), NUFFT, RBFs

If also high dim $d \gg 1$:

neural networks, tensor networks



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

pock–marks!

interp from Cartesian grid, more accurate

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"

Numerical integration (back to $d = 1$)

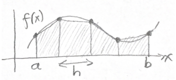
Task: eval. $\int_a^b f(x)dx$ accurately w/ least number of func. evals, N

"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*

"intepolatory quadrature"

Examples:



- local piecewise linear $\rightarrow$ composite trapezoid rule

  $w_j = h$ 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

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

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

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

Numerical integration (back to $d = 1$)

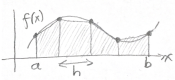
Task: eval. $\int_a^b f(x)dx$ accurately w/ least number of func. evals, N

"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*

"intepolatory quadrature"

Examples:



- local piecewise linear $\rightarrow$ composite trapezoid rule

  $w_j = h$ 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

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

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

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

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

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

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

Numerical integration (back to $d = 1$)

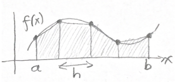
Task: eval. $\int_a^b f(x)dx$ accurately w/ least number of func. evals, N

"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 $f(x_j)$ → *integrate that exactly*

"intepolatory quadrature"

Examples:



- local piecewise linear → composite trapezoid rule

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

- N-node global poly → 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–Cotes)

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

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

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

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

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

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

```
ans = 1.3e-15
```

Advanced integration

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

$\vdots$

Advanced integration

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

⋮

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

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

Numerical differentiation

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

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

"centered difference" formula

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

Let's see how that goes...

Numerical differentiation

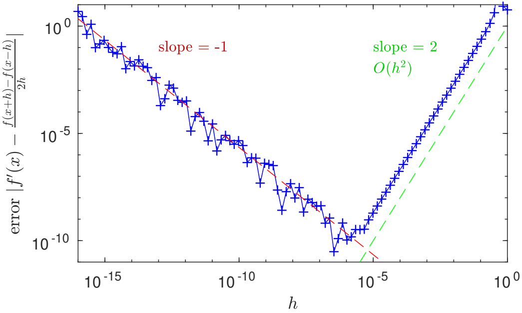
Task: given ability to eval. $f(\boldsymbol{x})$ anywhere, how get $\nabla f(\boldsymbol{x})$? assume smooth

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

"centered difference" formula

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

Let's see how that goes...



- shrinking $\mathcal{O}(h^2)$ error gets swamped by a new growing error... what?

Numerical differentiation

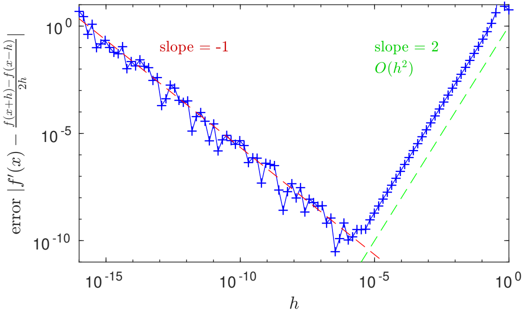
Task: given ability to eval. $f(\boldsymbol{x})$ anywhere, how get $\nabla f(\boldsymbol{x})$? assume smooth

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

"centered difference" formula

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

Let's see how that goes...



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

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

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

As w/ integration: get interpolant $\rightarrow$ 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

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

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

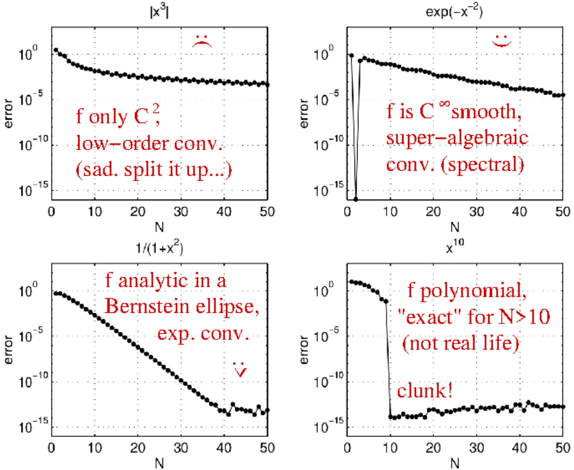
Get $N \times N$ matrix D acting on func. values $\{f(x_j)\}$ to give $\{f'(x_j)\}$. Has simple formula

Examples:

N Chebychev nodes

in $[-1, 1]$

shown: max error in f'



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

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

Summary: we scratched the surface

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

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

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

Concepts:

convergence order/rate — how much effort will you have to spend to get more digits?

smoothness — smooth $\Leftrightarrow$ fast convergence; nonsmooth needs custom methods

global — (one interpolation formula/basis for the whole domain)

vs local — (distinct formulae for x in different regions)

spectral method — global, converge v. fast, even non-per. can exploit FFT

adaptivity — auto split boxes to put nodes only where they need to be

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

tensor products for 2D, 3D — for higher dims: randomized/NN/TN (Th/Fr sessions)

See recommended books at end, and come discuss stuff!

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.

FLATIRON INSTITUTE
Center for Computational Mathematics

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general
  - Finite Volume Methods Fluids

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general
  - Finite Volume Methods Fluids
  - "Traditional" Finite Elements Mechanics

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general
  - Finite Volume Methods Fluids
  - "Traditional" Finite Elements Mechanics
  - "Modern" Finite Elements Higher order

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

- Finite Difference Methods For time & space.
- Finite Element Methods Very general
  - Finite Volume Methods Fluids
  - "Traditional" Finite Elements Mechanics
  - "Modern" Finite Elements Higher order
  - Spectral Methods Best accuracy for smooth solutions

LECTURE II: numerical differential equations

Motivation

Produce numerical approximations to the solutions of ODEs/PDEs.

Goals for today

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

Families of methods:

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

Reminder of types and applications of diff. eq.

- ODEs: eg pendulum $u''(t) + \sin(u(t)) = 0$
  Task: solve $u(t)$ given initial conditions e.g. $u(0) = 1$, $u'(0) = 0$

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 ($\boldsymbol{u}(t)$ is vector of multiple components)

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 ($\boldsymbol{u}(t)$ is vector of multiple components)

- Time-independent PDEs: eg Poisson eqn $\Delta u(\boldsymbol{x}) = g(\boldsymbol{x})$

  Task: solve $u(\boldsymbol{x})$ given forcing, boundary conditions

  Steady state of heat/diffusion, Gauss's law for conservative forces

  $u(\boldsymbol{x})$ is chemical concentration, gravitational/electric potential

  Δu means Laplacian $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \cdots =$ curvature of u

  $g(\boldsymbol{x}) =$ volume source of chemical, mass or charge density

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 ($\boldsymbol{u}(t)$ is vector of multiple components)

- Time-independent PDEs: eg Poisson eqn $\Delta u(\boldsymbol{x}) = g(\boldsymbol{x})$

  Task: solve $u(\boldsymbol{x})$ given forcing, boundary conditions

  Steady state of heat/diffusion, Gauss's law for conservative forces

  $u(\boldsymbol{x})$ is chemical concentration, gravitational/electric potential

  Δu means Laplacian $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \cdots =$ curvature of u

  $g(\boldsymbol{x}) =$ volume source of chemical, mass or charge density

  Others: Stokes eqn for velocity field $\boldsymbol{u}$ in viscous fluid

  Others: t-indep. Schrödinger eqn for quantum systems: $\Delta\psi = (V - E)\psi$

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 ($\boldsymbol{u}(t)$ is vector of multiple components)

- Time-independent PDEs: eg Poisson eqn $\Delta u(\boldsymbol{x}) = g(\boldsymbol{x})$

  Task: solve $u(\boldsymbol{x})$ given forcing, boundary conditions

  Steady state of heat/diffusion, Gauss's law for conservative forces

  $u(\boldsymbol{x})$ is chemical concentration, gravitational/electric potential

  Δu means Laplacian $\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 + \cdots =$ curvature of u

  $g(\boldsymbol{x}) =$ volume source of chemical, mass or charge density

  Others: Stokes eqn for velocity field $\boldsymbol{u}$ in viscous fluid

  Others: t-indep. Schrödinger eqn for quantum systems: $\Delta\psi = (V - E)\psi$

- Time-dependent PDEs: eg advection-diffusion $\partial_t c + \nabla \cdot (\boldsymbol{u}c) = \Delta c$

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

[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)
3. Solve resulting algebraic system

Typical solution strategies

Time-independent PDEs:

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

Time-dependent PDEs: "method of lines"

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

Typical solution strategies

Time-independent PDEs:

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

Time-dependent PDEs: "method of lines"

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

ODEs:

- Treat spatial problems as time-indep. PDEs "boundary value problems"

Typical solution strategies

Time-independent PDEs:

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

Time-dependent PDEs: "method of lines"

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

Finite difference methods

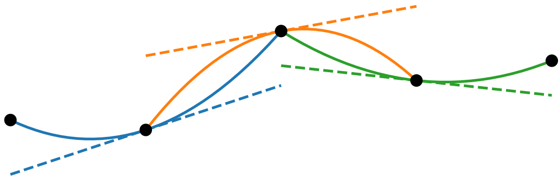
Alternate viewpoint:

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

    Unique, degree N-1.

- Differentiate the local interpolant to approximate derivatives.

E.g. Centered differences using 3 points:



Implicit & Explicit Timestepping

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

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

Implicit & Explicit Timestepping

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

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

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

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

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

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

$k\lambda < 2$ for stability

Implicit & Explicit Timestepping

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

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

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

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

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

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

$k\lambda < 2$ for stability

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

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

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

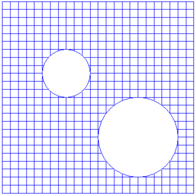
$$u_{n+1} - u_n = -k\lambda u_{n+1} \tag{9}$$

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

FLATIRON INSTITUTE
Center for Computational Mathematics

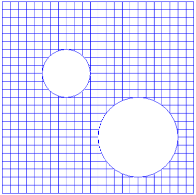
Finite difference methods

- 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"



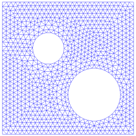
Finite difference methods

- 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"



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

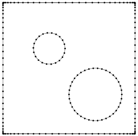
- More flexible in terms of equations
- Still limited to simple geometries: cubes, spheres, cylinders, etc.
- Still a weak method, but don't integrate by parts. Apply Galerkin directly.

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