2 Introduction to spectral methods.

"Big three"

1950s finite difference method

1960s finite element method

1970s Spectral method

Spectral methods: best for

Smooth data, simple domains

collocation methods on { periodic grids
Chebyshev grids

☆ Differentiation Matrices

For a uniform grid $\{x_1, \cdots, x_N\}$ $x_{j+1} - x_j = h$

and data values $\{u_1, \cdots u_N\}$

Q: how to approximate $u'(x_j)$? denoted by w_j.

A1: finite difference

local polynormiall interpolation → differentiation

e.g. find $P_j(x) \in \mathbb{P}_2$ s.t. $P(x_{j+k}) = u_{j+k}$, $k = -1, 0, 1$.

then set $w_j = P_j'(x) = \frac{1}{2h}(u_{j+1} - u_{j-1})$

Note: higher order finite differences. $O(h^p)$

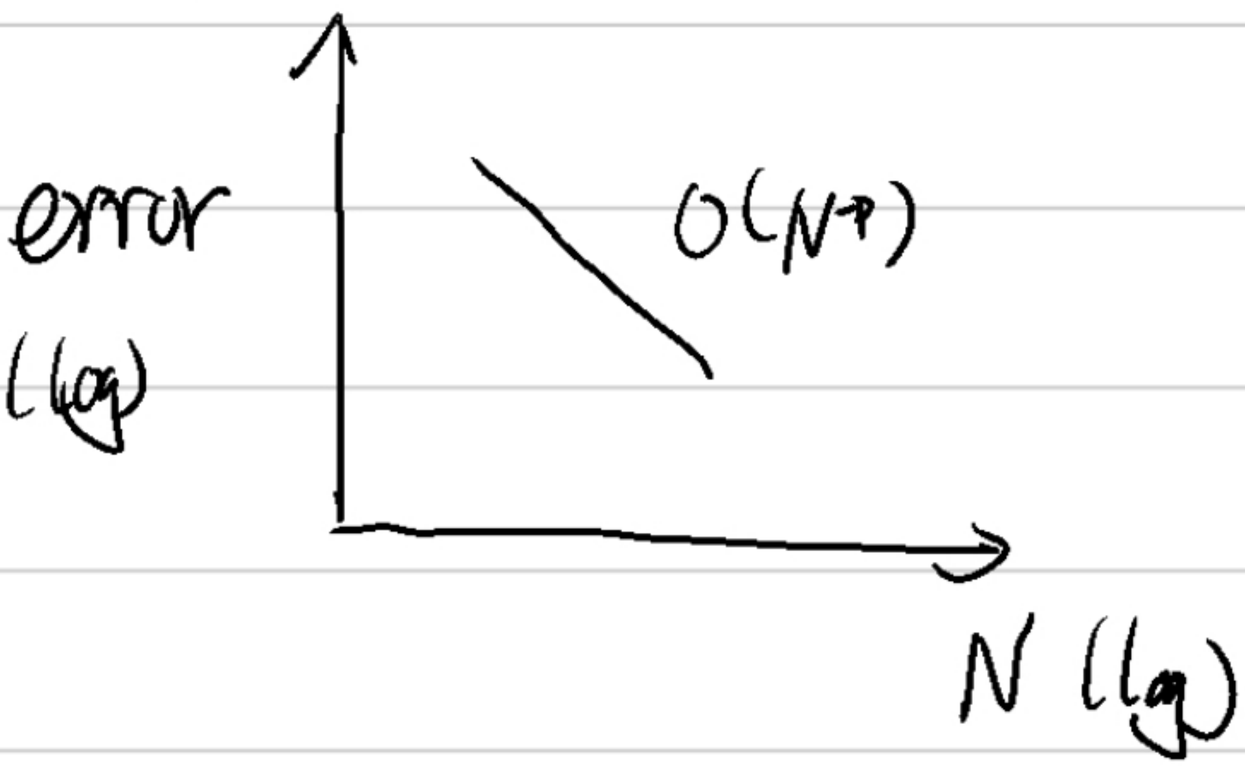
A2: Spectral collocation method.

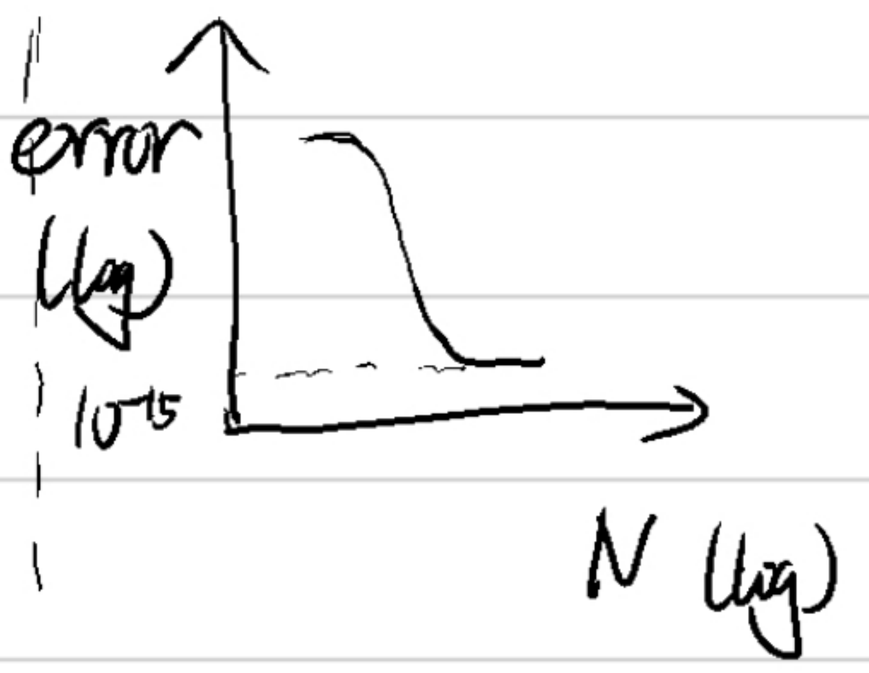
For a finite grid $\{x_j\}$ $\{u_j\}$ (may not be uniform)

find a global function P, s.t. $P(x_j) = u_j$ $\forall j$

then set $w_j = P'(x_j)$.

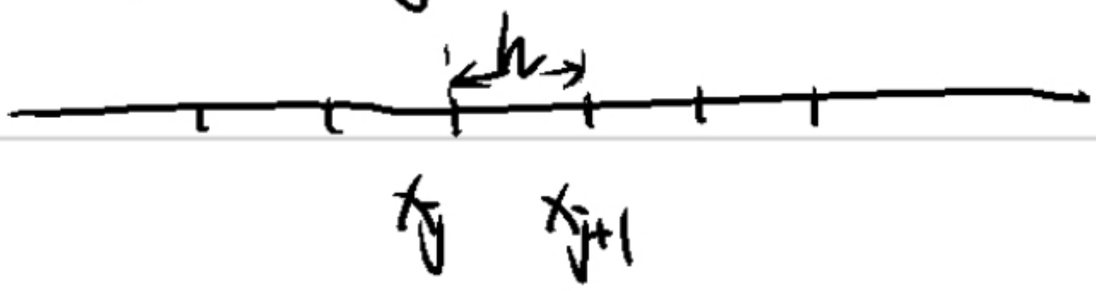
$h = \frac{b-a}{N}$ $e = Ch^p$ $\log e = c_2 - c_3 p \log N$ "spectral accuracy"





✡ Unbounded Domain, semidiscrete Fourier Transform

Consider infinite grid: $h\mathbb{Z}$, $x_j = jh$, $j \in \mathbb{Z}$



Recall, for $u(x)$, $x \in \mathbb{R}$.

Fourier transform: $\hat{u}(k) = \int_{-\infty}^{+\infty} e^{-ikx} u(x)\,dx$

inverse Fourier transform: $u(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}\hat{u}(x)\,dx$

When $x \in h\mathbb{Z}$, consider $f = \exp(ik_1x)$, $g = \exp(ik_2x)$

Clearly $f = g$ on $h\mathbb{Z}$ when $k_1 - k_2 = j\frac{2\pi}{h}$, $j \in \mathbb{Z}$

"aliases" of k (k period $\frac{2\pi}{h}$)

Def: For a function v on $h\mathbb{Z}$ with value v_j at x_j the semidiscrete Fourier transform (SFT)

$$\hat{v}(k) = h\sum_{j=-\infty}^{+\infty} e^{-ikx_j} v_j, \quad k \in [-\tfrac{\pi}{h}, \tfrac{\pi}{h}].$$

inverse $v_j = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} e^{ikx_j}\hat{v}(k)\,dk$, $j \in \mathbb{Z}$

Def interpolant

$$p(x) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{ikx} \hat{v}(k)\, dk, \quad x \in \mathbb{R}.$$

Clearly, $\hat{p}(k) = \begin{cases} \hat{v}(k) & k \in [-\pi/h, \pi/h] \\ 0 & \text{otherwise} \end{cases}$.

p is the band-limited interpolant of v

Note: such interpolation is unique (sampling thm)

⛤ Spectral differentiation

— given v on hZ, find band-limited interpolant p.

— set $w_j = p'(x_j)$.

Equivalently

— given v on hZ, compute SFT $\hat{v}(k)$

— Define $\hat{w}(k) = ik\,\hat{v}(k)$

— Compute w from $\hat{w}$ by inverse SFT.

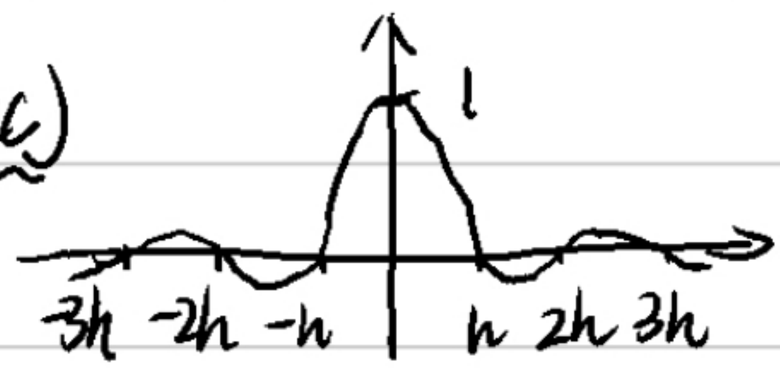
Consider Kronecker delta func. δ_j, $j \in \mathbb{Z}$

$$\delta_0 = 1, \qquad \delta_j = 0, \quad \text{for } j \neq 0.$$

One can compute $\hat{\delta}(k) \equiv h$, $k \in [-\frac{\pi}{h}, \frac{\pi}{h}]$

its interpolant (sinc func)

$$S_h(x) = \frac{\sin(\pi x/h)}{\pi x/h}$$



In general for V on $h\mathbb{Z}$

interpolant $p(x) = \sum_{m=-\infty}^{+\infty} V_m S_h(x - x_m)$

and $w_j = p'(x_j) = \sum_{m=-\infty}^{+\infty} V_m S_h'(x_j - x_m)$

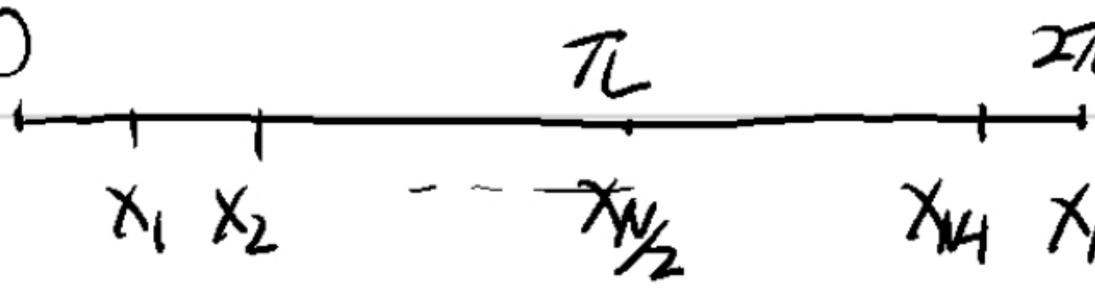
By calculation $S_h'(x_j) = \begin{cases} 0 & j = 0 \\ \frac{(-1)^j}{jh}, & j \neq 0, \end{cases}$

Note: similarly, one can approximate higher order derivatives.

Bounded, Periodic grids DFT

periodicity: boundary is unrelated/periodic

N is even



periodic grid on $[0, 2\pi L]$

Def. the discrete Fourier transform (DFT)

$$\hat{v}_k = h \sum_{j=1}^{N} e^{-ikx_j} v_j, \quad k = -\frac{N}{2}+1, \cdots, \frac{N}{2}$$

inverse $$v_j = \frac{1}{2\pi L} \sum_{k=-N/2+1}^{N/2} e^{ikx_j} \hat{v}_k, \quad j = 1, \cdots, N.$$

interpolant: $$p(x) = \frac{1}{2\pi L} \sum_{k=-N/2}^{N/2}{}' e^{ikx} \hat{v}_k$$

$$\triangleq \frac{1}{2\pi L} \sum_{k=-N/2+1}^{N/2-1} e^{ikx} \hat{v}_k + \frac{1}{2\pi L}\cdot\frac{1}{2}\left(e^{\frac{iN}{2}x}\hat{v}_{-N/2} + e^{\frac{-iN}{2}x}\hat{v}_{N/2}\right)$$

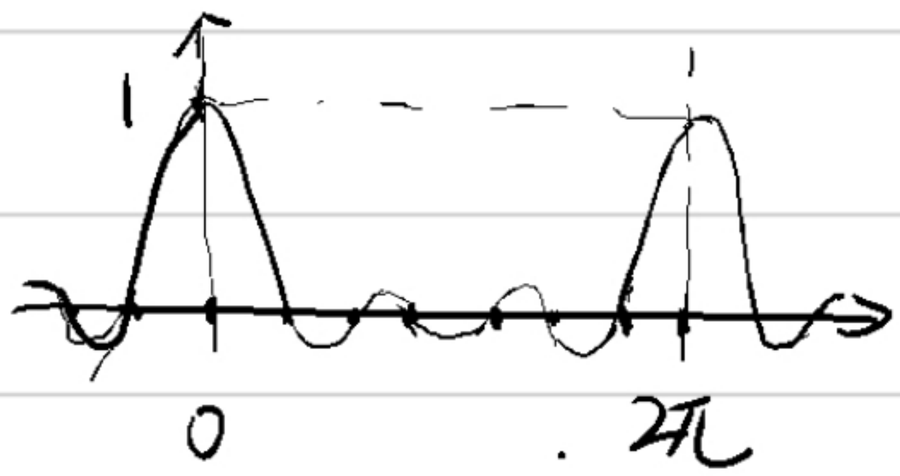
"trigonometric polynomials"

Consider delta fun. $$\delta_j = \begin{cases} 1 & j = 0 \pmod N \\ 0 & j \neq 0 \pmod N \end{cases}$$

its interpolant

periodic sinc

$$S_N(x) = \frac{\sin(\pi x/h)}{(2\pi/h)\tan(\frac{x}{2})}$$



In general, for a period grid func. v

Interpolant $p(x) = \sum_{m=1}^{N} v_m S_N(x - x_m)$

We compute $S_N'(x_j) = \begin{cases} 0 & j \equiv 0 \pmod N \\ \frac{1}{2}(-1)^j \cot\left(\frac{jh}{2}\right) & j \not\equiv 0 \pmod N \end{cases}$

Spectral differentiation matrix $D_N \in \mathbb{R}^{N \times N}$

s.t. $w = D_N v$ $\quad$ $\square$

Equivalently,

- given v, compute $\hat{v}$
- Define $\hat{w}_k = ik\hat{v}_k$, except $\hat{w}_{\frac{N}{2}} = 0$
- Compute w from $\hat{w}$.

Similarly, second-order differentiation matrix $D_N^{(2)} \in \mathbb{R}^{N \times N}$

Note: with the Fast Fourier transform (FFT)

the cost is $O(N \log N)$.

Applications in differential equations.

Ex.1. $u_t + c(x) u_x = 0 \quad x \in [0, 2\pi]$

periodic in x, I.C. $u(x,0) = u_0(x)$

Leap-frog: Let $D = D_N \in \mathbb{R}^{N \times N}$

$$\frac{v_j^{n+1} - v_j^{n-1}}{2\Delta t} = -c(x_j)(Dv^{(n)})_j, \quad j = 1, \cdots, N.$$

Ex2. BVP (eigenvalue problem)

Find λ s.t. $-u'' + x^2 u = \lambda u \quad x \in \mathbb{R}$

Since u decays fast at ∞

Choose a sufficiently large L. consider

$-u'' + x^2 u = \lambda u, \quad x \in [-L, L]$ periodic

discretize to: $(-D_N^{(2)} + S) u = \lambda u \quad (\ )' = \cdot'$

where $S = \mathrm{diag}(x_0^2, \cdots, x_N^2)$

approximate eigenvalues: eigenvalues of $-D^{(2)} + S$

Read: Chaper 4 for accuracy analysis.

☆ Polynomial interpolation.

For bounded, nonperiod domain, $[-1,1]$

a smooth func. becomes nonsmooth when periodically extended



Idea: "trigonometric" ⇒ "algebraic" polynomials

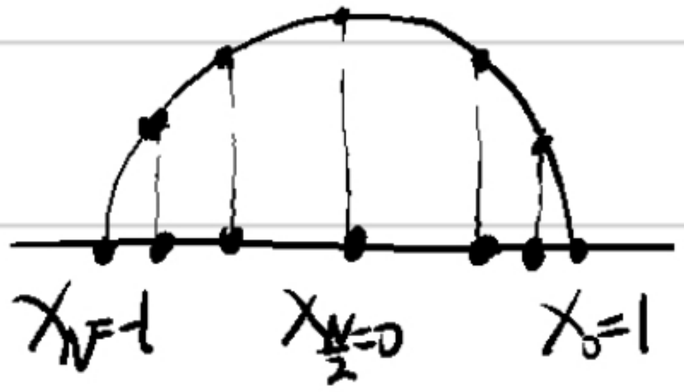
Uniform grid? Bad! Runge-phenomenon.

Instead, we choose Chebyshev points

$$x_j = \cos\left(\frac{j\pi}{N}\right)$$

$j = 0, 1, \cdots, N,$

N: even or odd.



Read: Chapter 5 for accuracy analysis.

✡ Chebyshev Differentiation Matrices

Given v defined on Chebyshev points $\{x_j\}_{j=0}^N$

— Let $p \in P_N$ s.t. $p(x_j) = v_j$, $0 \le j \le N$

— Set $w_j = p'(x_j)$

Differentiation Matrix $D_N \in \mathbb{R}^{(N+1)\times(N+1)}$, $w = D_N v$

where $D_N =$

$$\begin{pmatrix} \frac{2N^2+1}{6} & \cdots & -2\frac{(-1)^j}{1-x_j} & \cdots & \frac{1}{2}(-1)^N \\ \vdots & & \vdots & & \vdots \\ -\frac{1}{2}\frac{(-1)^i}{1-x_i} & \cdots & \frac{(-1)^{i+j}}{x_i - x_j} \text{ or } \frac{-x_j}{2(1-x_j)^2} & \cdots & \frac{1}{2}\frac{(-1)^{N+i}}{1+x_i} \\ \vdots & & \vdots & & \vdots \\ -\frac{1}{2}(-1)^N & \cdots & -2\frac{(-1)^{N+j}}{1+x_j} & \cdots & \frac{2N^2+1}{6} \end{pmatrix}$$

Note: can use FFT to speed up (Chapter 8)

✡ Applications to Boundary Value Problems

Ex1 $u_{xx} = e^{4x}$, $0 < x < 1$, $u(\pm 1) = 0$

Q: with D_N^2, how to impose B.C.?

$x_1, \cdots x_{N+1}$ computational grids

$v = (v_1, \cdots, v_{N+1})^T$ unknown vector

Spectral differentiation

— Let $P(x) \in P_N$ with $P(\pm 1)=0$, $P(x_j)=V_j$, $1 \le j \le N-1$

— Set $W_j = P''(x_j)$, $1 \le j \le N-1$.

Equivalently set $\widetilde{D_N^2} = D_N^2(1:N-1, 1:N-1)$

we obtain $\widetilde{D_N^2} V = f$.

Ex2. eigenvalue problem

$$u_{xx} = \lambda u, \quad -1 < x < 1, \quad u(\pm 1)=0$$

$\Rightarrow$ eigens of $\widetilde{D_N^2}$

Ex3 2D Poisson equation

$$\begin{cases} u_{xx} + u_{yy} = f(x,y) & x,y \in \Omega = (-1,1)\times(-1,1) \\ u = 0 & x,y \in \partial\Omega \end{cases}$$

use tensor product $\otimes$

discrete Laplacian $L_N = I \otimes \widetilde{D_N^2} + \widetilde{D_N^2} \otimes I$

☆ Time stepping and stability

Consider explicit methods

ex1 $u_t + u_x = 0$ $[-\pi, \pi]$ Fourier $\Delta t = O(N^{-1})$

ex2. $u_{tt} = u_{xx}$ $[-1, 1]$ Chebyshev $\Delta t = O(N^{-2})$

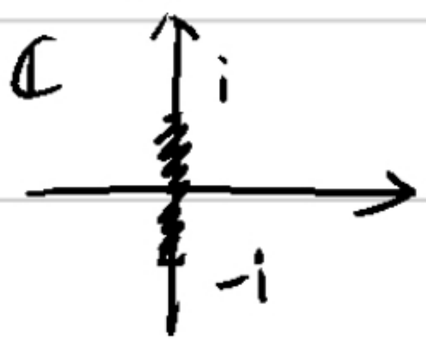
Note: ex1 is similar to FD (CFL condition)

ex2 is worse than FD in stability.

Stability by Method of lines

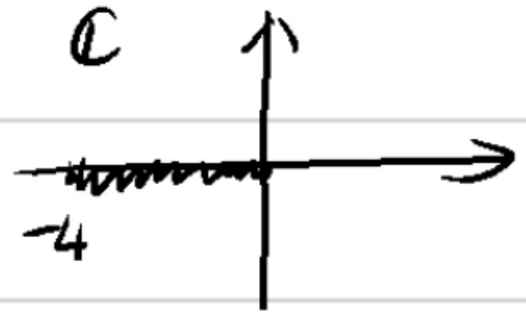
in ex1, eigenvalues of Fourier differentiab matrix D_N are ik, $k = -\frac{N}{2}+1, \cdots, \frac{N}{2}-1$

leapfrog stability region



Thus $\Delta t (\frac{N}{2} - 1) < 1$, $\Delta t = O(N^{-1})$.

In ex2. $u_{tt} = \lambda u$



$$\frac{1}{(\Delta t)^2}\left(U^{n+1} - 2U^n + U^{n-1}\right) = \lambda U^n$$

However, D_N^2 is nonsymmetric

one can show: eigenvalues: real & negative

part of them $\lesssim O(N^2)$ → eigenvalues of $\frac{d^2}{dx^2}$

the rests $O(N^4)$ "outliers"

$$\Rightarrow \quad \Delta t = O(N^{-2})$$

Note: better use implicit / semi-implicit methods.

✡ More on boundary conditions

(I) restrict interpolants on boundary (Dirichlet)

(II) do not restrict interpolants

but add additional equation (Neumann)

ex1 $u_{xx} = f(x)$, $-1<x<1$ $u_x(-1) = u(1) = 0$

Chebyshev points $x_j = \cos\left(\frac{j\pi}{N}\right)$ $j = 0, \cdots, N$

at $x=1$ $(j=0)$ $u=0$, equation not needed

at $x=-1$ $(j=N)$ $u_x = 0$ $(D_N v)_{j=N} = 0$

at x_j, $j = 1 \cdots, N-1$ $(D_N^2 u)_j = f_j$

unknown $u_1, \cdots, u_N$, N equations. ✓

ex2 $u_{tt} = u_{xx} + u_{yy}$, $-3<x<3$, $-1<y<1$

$u_y(x, \pm 1, t) = 0$ + periodic in x

- Fourier in x
- Chebyshev in y
- leap-frog in t

More in this book?

- eigenvalues pseudospectra Ch 9.
- polar coordinates Ch 11
- integral quadrature Ch. 12
- Fourth order problem Ch. 14.