Sparse Spectral Methods

Chebyshev collocation methods achieve spectral accuracy on nonperiodic domains, but the differentiation matrix is

a) dense => expensive direct solve if high-degree poly. is required.

b) ill-conditioned => numerical errors amplify if high-degree poly. is required.

This means that collocation is limited to very smooth problems that can be resolved using relatively low-degree polynomials.

Q: Can we derive spectrally accurate discretizations that are

a) sparse, and b) well-conditioned?

Chebyshev U basis

When we differentiate $T_n(x)$ (for $n=0,1,2,\dots$), we get a new family of orthogonal poly.

$$\partial_x T_n(x) = \frac{\partial\theta}{\partial x}\partial_\theta \cos(n\theta) = n\,\frac{\sin(n\theta)}{\sin\theta}$$

$\underline{n=0}$ $\quad \partial_x T_0(x) = 0$

$\underline{n=1}$ $\quad \partial_x T_1(x) = 1$

$\underline{n=2}$ $\quad \partial_x T_2(x) = 2x$

$\underline{n\geq 2}$ $\quad \partial_x T_{n+1}(x) = 2x\,\overbrace{\frac{\sin(n\theta)}{\sin(\theta)}}^{\partial_x T_n} - \overbrace{\frac{\sin((n-1)\theta)}{\sin(\theta)}}^{\partial_x T_{n-1}}$

$$\Rightarrow \quad U_n(x) = \frac{\sin((n+1)\theta)}{\sin(\theta)} \in \Pi^n \quad \left(\begin{matrix}\text{degree } n\\ \text{polynomial}\end{matrix}\right)$$

These "Chebyshev-U" poly.'s are orthogonal:

$$\langle U_n, U_m\rangle_w = \int_{-1}^{+1} U_n(x)U_m(x)\underbrace{\sqrt{1-x^2}}_{w(x)=\sin(\theta)}\,dx$$

and differentiation maps $T_n \to nU_{n-1}$

$$\partial_x T_n(x) = nU_{n-1}(x) \qquad n=1,2,\dots$$

Sparse Differentiation Matrix

Choose test basis $\{T_n\}$ and trial basis $\{U_n\}$.

Example: $\partial_x u = f$ $\qquad u(1)=0$

Trial basis: $u(x) = \sum_{n=0}^{N-1} \hat{u}_n T_n(x)$, $\quad f(x) = \sum_{n=0}^{N-1} \hat{f}_n T_n(x)$

Test basis: $$\sum_{n=0}^{N-1} \hat{u}_n \underbrace{\langle U_m, \partial_x T_n(x)\rangle_w}_{D_{mn} = \text{diff. mat.}} = \sum_{n=0}^{N-1} \hat{f}_n \underbrace{\langle U_m, T_n\rangle_w}_{S_{mn} = \text{"Conversion matrix"}}$$

$$\underbrace{\begin{bmatrix} 0 & 1 & & & \\ & 0 & 2 & & \\ & & 0 & 3 & \\ & & & \ddots & \ddots \\ & & & & N-1 \\ & & & & 0 \end{bmatrix}}_{D} \begin{bmatrix} \hat{u}_0 \\ \vdots \\ \hat{u}_{N-1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & -1/2 & & \\ & 1/2 & 0 & -1/2 & \\ & & 1/2 & \ddots & \ddots \\ & & & \ddots & -1/2 \\ & & & 1/2 & 0 \end{bmatrix}}_{S} \begin{bmatrix} \hat{f}_0 \\ \vdots \\ \hat{f}_{N-1} \end{bmatrix}$$

~~$S_{mn} = \langle U_m, T_n\rangle$~~

$$T_n(x) = \frac{1}{2}\left(U_n(x) - U_{n-2}(x)\right) \qquad \left(\begin{matrix}\text{trig. identity} \\ \text{for sin/cos}\end{matrix}\right)$$

$$\Rightarrow \underbrace{\langle U_m, T_n\rangle_w}_{S_{mn}} = \frac{1}{2}\delta_{n,m} - \frac{1}{2}\delta_{n-2,m}$$

Boundary Bordering

To enforce B.C. $u(1)=0$, use bordering

$$u(1) = \sum_{n=0}^{N-1} \hat{u}_n \underbrace{T(1)}_{=1} = \sum_{n=0}^{N-1} \hat{u}_n$$

evaluate u at $x=1$ $\Rightarrow$

$$\begin{bmatrix} 1 & 1 & \cdots & & 1 \\ 0 & 1 & & & \\ & 0 & 2 & & \\ & & \ddots & \ddots & \\ & & & 0 & N-2 \end{bmatrix} \begin{bmatrix} \hat{u}_0 \\ \hat{u}_1 \\ \vdots \\ \hat{u}_{N-1} \end{bmatrix} = \begin{bmatrix} 0 & \cdots & & & 0 \\ 1 & 0 & -\tfrac{1}{2} & & \\ & \tfrac{1}{2} & 0 & -\tfrac{1}{2} & \\ & & \tfrac{1}{2} & \ddots & \ddots \\ & & & \ddots & \end{bmatrix} \begin{bmatrix} \hat{f}_0 \\ \hat{f}_1 \\ \vdots \\ \hat{f}_{N-1} \end{bmatrix}$$

$\Leftarrow$ set $u(1)$ to 0

The system is "almost-banded," meaning it is a low-rank (rank 1 here) + banded matrix.

$\Rightarrow$ Solve in $\mathcal{O}(N)$ flops with rank-1 update:

"Sherman-Morrison formula"

nonzero row

$$(A + uv^T)^{-1} b = A^{-1}b - \left[\frac{v^T A^{-1} b}{1 + v^T A^{-1} u}\right] A^{-1} u$$

banded

Only need banded solves $A^{-1}b$, $A^{-1}u$ and then vector operations ("dot", "plus").

What about higher-order derivatives?

Ultraspherical Basis

Given ν = integer ≥ 0, the "ultraspherical" polynomials

$\{C_n^{(\nu)}(x)\}_{n=0}^{\infty}$ are orthogonal w.r.t. $w(x) = (1-x^2)^{\nu - 1/2}$.

Differentiation

$$\partial_x^{\lambda} T_n(x) = 2^{(\lambda-1)}(\lambda-1)!\, n\, C_{n-1}^{(\lambda)}(x)$$

banded diff. mat.

$$D^{\lambda} = 2^{(\lambda-1)}(\lambda-1)! \begin{array}{c} \overbrace{\quad\quad}^{\lambda\text{-many}} \\ \left[\begin{matrix} 0 & \cdots & 0 & \lambda & & & \\ & & & & \lambda+1 & & \\ & & & & & \lambda+2 & \\ & & & & & & \ddots \\ 0 & - & - & - & & & 0 \\ \vdots & & & & & & \vdots \\ 0 & - & - & - & & & 0 \end{matrix}\right] \end{array} \left.\vphantom{\begin{matrix}0\\ \vdots\\ 0\end{matrix}}\right\} \lambda\text{-many}$$

$$D_{mn}^{\lambda} = \langle C_m^{(\lambda)}, \partial_x^{\lambda} T_n \rangle$$

Conversion

$$C_n^{(\nu)}(x) = \frac{\nu}{\nu+n}\left(C_n^{(\nu+1)}(x) - C_{n-2}^{(\nu+1)}(x)\right) \quad (\nu > 0)$$

banded convert matrix

$$S^{(\nu)} = \begin{bmatrix} 1 & 0 & -\frac{\nu}{\nu+2} & & & \\ & \frac{\nu}{\nu+1} & 0 & -\frac{\nu}{\nu+3} & & \\ & & \frac{\nu}{\nu+2} & \ddots & \ddots & \\ & & & \ddots & & \end{bmatrix}$$

$S^{(1)} S^{(0)} : \{T_n\} \to \{C_n^{(2)}\}$

Compose maps to go from $T_n \to$ ultraspherical

$$S_{mn}^{(\nu)} = \langle C_m^{(\nu+1)}, C_n^{(\nu)} \rangle$$

Multiplication: $u(x) \to a(x)u(x)$

Need to construct matrix with entries

$$(M_a^{(\nu)})_{mn} = \langle C_m^{(\nu)}, a C_n^{(\nu)} \rangle$$

for "multiplication in $\{C^{(\nu)}\}$ basis."

$\Rightarrow$ For poly. $a(x) = \sum_{n=0}^{M-1} \hat{a}_n C_n^{(\nu)}(x)$ with $M \ll N$, $M_a^{(\nu)}$ has bandwidth $2M+1$.

$\Rightarrow$ Discretizations remain banded so long as we can replace $a(x)$ by a low-degree poly. approx (i.e. a is smooth relative to solution of ODE).

General Discretization Scheme

k^{th}-order linear diff. op.

$$Lu = \sum_{j=0}^{k} a_k(x)\, \partial_x^k u(x) = f(x)$$

$$\left[M^{k}_{a_k} D^{k} + S^{k-1} M^{k-1}_{a_{k-1}} D^{k-1} + \cdots + S^{k-1} \cdots S^{1} M^{1}_{a_1} D^{1} + S^{k-1} \cdots S^{0} M^{0}_{a_0}\right] \hat{\underline{u}}$$

$$= S^{k-1} \cdots S^{0} \hat{\underline{f}}$$

$$\text{bandwidth} \approx 2K + 2M_{max}$$

$\uparrow$ poly. deg. for var. coeffs

$\Rightarrow$ Enforce boundary conditions via boundary bordering to get banded + low-rank.

$\Rightarrow$ Solve using fast + stable "almost-banded" QR solver (see Olver ! Townsend reading) or with Woodbury inversion formula

$$(A + UV)^{-1} = A^{-1} - A^{-1} U (I + V A^{-1} U)^{-1} V A^{-1}$$