Spectral Differentiation: Integration and Inversion

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Introduction

- High order differentiation matrices have round-off error
- Can we remove sources of round-off error?

Option 1: Preconditioning by integration

Multiply by integration matrix

Option 2: Inversion

Find inverse of linear operator matrix

Chebyshev differentiation matrices [sec.1]

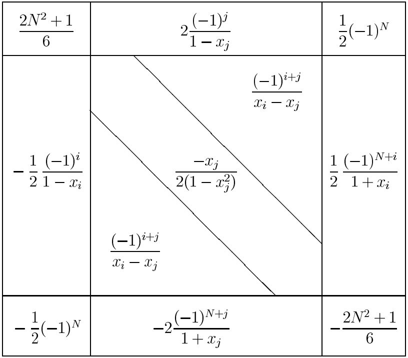

Fig: From pg. 53 of *Spectral Methods in MATLAB* by L.N. Trefethen

$$D^{(2)} = D \cdot D$$

$$D^{(k)} = D \cdot D^{(k-1)} = D^k$$

$$x_k = \cos\left(\frac{k\pi}{N}\right) \in [-1, 1]$$

The general m-th order problem [sec.1]

$$
\begin{aligned}
\mathcal{L}u(x) =& u^{(m)}(x) + \sum_{n=1}^{m} q_n(x) u^{(m-n)}(x) = f(x) \\
\mathcal{B}_k u(1) =& \sum_{n=1}^{m} a_n^k u^{(m-n)}(1) = a_0^k, & k =& 1, \ldots, k_0 \\
\mathcal{B}_k u(-1) =& \sum_{n=1}^{m} a_n^k u^{(m-n)}(-1) = a_0^k, & k =& k_0 + 1, \ldots, m
\end{aligned}
$$

The collocation matrices [sec.1]

$$\bar{A} = D^{(m)} + \sum_{n=1}^{m} Q_n D^{(m-n)}, \qquad Q_n = \begin{bmatrix} q_n(x_0) & & \\ & \ddots & \\ & & q_n(x_N) \end{bmatrix}$$

$$\hat{A}_k = \sum_{n=1}^{m} a_n^k D_0^{(m-n)}, \qquad k = 1, ..., k_0$$

$$\hat{A}_k = \sum_{n=1}^{m} a_n^k D_N^{(m-n)}, \qquad k = k_0 + 1, ..., m$$

$D_0^{(m-n)}$ is the first row of $D^{(m-n)}$, $D_N^{(m-n)}$ the last row and $D^{(0)}$ the identity matrix

Combining $\bar{A}$ and $\hat{A}$ [sec.1]

$\bar{A}$ and $\hat{A}$ can be concatenated to form the full system:

$$\begin{bmatrix} \bar{A} \\ \hat{A} \end{bmatrix} \vec{U} = \begin{bmatrix} \vec{f} \\ a_0^1 \\ \vdots \\ a_0^m \end{bmatrix}$$

However, this system may be overdetermined.
Instead, remove rows of $\bar{A}$ and replace them with the rows of $\hat{A}$.

Combining $\bar{A}$ and $\hat{A}$ [sec.1]

Each row (and column) of $\bar{A}$ is associated with a Chebyshev node.
Choose m of these nodes, $V = \{v_1, ..., v_m\}$.
Then the rows associated with these points will be replaced by boundary conditions.
Define a new matrix A by its rows:

$$A_j = \begin{cases} \bar{A}_j & x_j \notin V \\ \hat{A}_k & x_j = v_k \in V \end{cases}$$

Combining $\bar{A}$ and $\hat{A}$ [sec.1]

Alternatively, define the matrices $\tilde{D}^{(k)}$:

$$\tilde{D}_j^{(m)} = \begin{cases} D_j^{(m)} & x_j \notin V \\ \hat{A}_k & x_j = v_k \in V \end{cases}$$

$$\tilde{D}_j^{(k)} = \begin{cases} D_j^{(k)} & x_j \notin V \\ 0 & x_j \in V \end{cases}$$

Then the matrix A is constructed just like $\bar{A}$:

$$A = \tilde{D}^{(m)} + \sum_{n=1}^{m} Q_n \tilde{D}^{(m-n)}$$

Preconditioning [sec.2]

$\tilde{D}^{(m)}$ is a large source of round-off error.
We would like to remove it by multiplying A by some matrix B:

$$BA = I + \sum_{n=1}^{m} BQ_n \tilde{D}^{(m-n)}$$

Usually, $B\tilde{D}^{(m)} \approx I$ is enough.
In our case, we hope to find $\tilde{D}^{(m)}B = I$.

Integration matrix [sec.2]

If the columns of B are representations of polynomials $B_j(x)$, then:

$$\tilde{D}_i^{(m)} \vec{B}_j = \begin{cases} B_j^{(m)}(x_i) & x_i \notin V \\ \mathcal{B}_k B_j(\pm 1) & x_i = v_k \in V \end{cases}$$

$$\implies B_j^{(m)}(x_i) = \begin{cases} \delta_{ij} & x_j \notin V \\ 0 & x_j \in V \end{cases}$$

$$\mathcal{B}_k B_j(\pm 1) = \begin{cases} 1 & x_j = v_k \in V \\ 0 & x_j \neq v_k \end{cases}$$

The Chebyshev polynomials [sec.1]

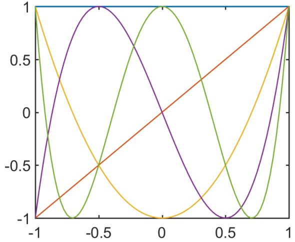

Figure:
$T_k(x) = \cos\left(k \arccos(x)\right)$

$$\partial_x^{-1} T_0(x) = T_1(x)$$
$$\partial_x^{-1} T_1(x) = T_2(x)/4$$
$$\partial_x^{-1} T_k(x) = \frac{1}{2}\left(\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1}\right).$$

The Chebyshev polynomials [sec.1]

$T_k(x)$ satisfy a discrete orthogonality relation on the nodes:

$$\langle T_k, T_j \rangle_c = \sum_{i=0}^{N} \frac{1}{c_i} T_k(x_i) T_j(x_i) = \frac{c_j}{2} N \delta_{jk}$$

$$c_j = \begin{cases} 2 & k = 0, N \\ 1 & 1 \leq k < N \end{cases}$$

Decomposing $B_j(x)$ [sec.2] (adapted from Wang et al.)

$B_j(x)$ is a polynomial of at most degree N, then its m-th derivative can be represented as

$$B_j^{(m)}(x) = \sum_{k=0}^{N} b_{k,j} T_k(x), \quad b_{k,j} = 0 \quad \forall \quad k = N - m + 1, \ldots, N$$

$$\langle B_j^{(m)}, T_k \rangle_c = b_{k,j} c_k N/2$$

Let $\beta_{k,j} = B_j^{(m)}(v_k)/c_n$ where $v_k = x_n \in V$; these values are unknown

$$b_{k,j} = \frac{2}{c_k N} \langle B_j^{(m)}, T_k \rangle_c = \frac{2}{c_k N} \left(\frac{1}{c_j} T_k(x_j) + \sum_{n=1}^{m} \beta_{n,j} T_k(v_n) \right).$$

Solving for $\beta_{k,j}$ [sec.2]

Since $b_{k,j} = 0$ for $k = N - m + 1, ..., N$, we can make a system to solve for $\beta_{k,j}$:

$$\begin{bmatrix} T_N(v_1) & \dots & T_N(v_m) \\ \vdots & \ddots & \vdots \\ T_{N-m+1}(v_1) & \dots & T_{N-m+1}(v_m) \end{bmatrix} \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = -\frac{1}{c_j} \begin{bmatrix} T_N(x_j) \\ \vdots \\ T_{N-m+1}(x_j) \end{bmatrix}$$

Boundary conditions [sec.2]

For $x_j \notin V$

$$B_j(x) = \sum_{k=0}^{N-m} b_{k,j} \left(\partial_x^{-m} T_k(x) - p_k(x) \right)$$

$$\mathcal{B}_n p_k(\pm 1) = \mathcal{B}_n \partial_x^{-m} T_k(\pm 1)$$

For $x_j \in V$, $B_j(x)$ is a polynomial of degree at most $m-1$ satisfying

$$\mathcal{B}_k B_j(\pm 1) = \begin{cases} 1 & x_j = v_k \\ 0 & x_j \neq v_k \end{cases}$$

Inversion matrices [sec.3]

$$A = \tilde{D}^{(m)} + \sum_{n=1}^{m} Q_n \tilde{D}^{(m-n)}$$

We want R such that $AR = I$. If $R_j(x)$ is the polynomial represented by the j-th column of R, then:

$$\mathcal{L}R_j(x_i) = \begin{cases} \delta_{ij} & x_j \notin V \\ 0 & x_j \in V \end{cases}$$

$$\mathcal{B}_k R_j(\pm 1) = \begin{cases} 0 & x_j \neq v_k \in V \\ 1 & x_j = v_k \in V \end{cases}$$

Methods

Standard:

$$AU = F$$

Preconditioning (generalized from Wang et al.):

$$\left(I + \sum_{n=1}^{m} BQ_n \tilde{D}^{(m-n)} \right) U = BF$$

Inverse operator (new):

$$U = RF$$

Singular example: function of V [sec.6.1]

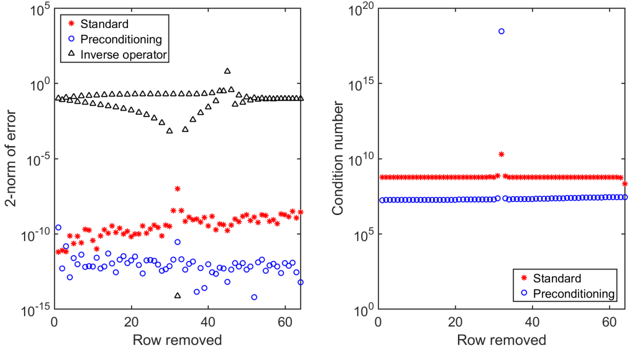

Figure: $xu''(x) - (x+1)u'(x) + u(x) = x^2, \quad u(\pm 1) = 1$

Singular example: function of N [sec.6.1]

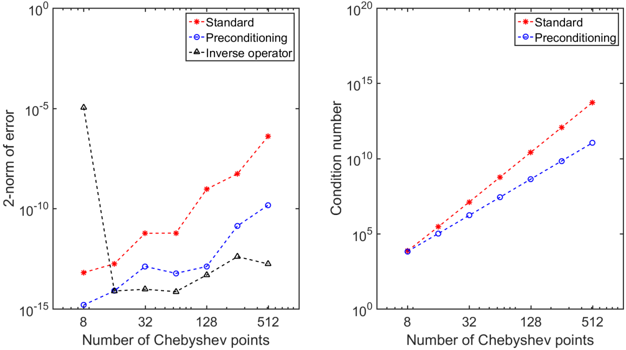

Figure: $xu''(x) - (x+1)u'(x) + u(x) = x^2, \quad u(\pm 1) = 1$

Constant coefficients: function of V [sec.6.2]

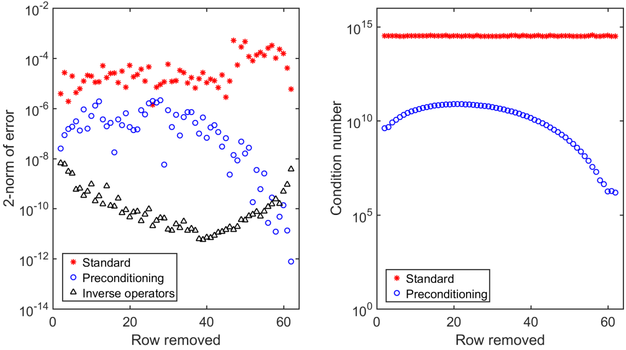

Figure: $u^{(5)}(x) + u^{(4)}(x) - u'(x) - u(x) = f(x)$

Constant coefficients: function of N [sec.6.2]

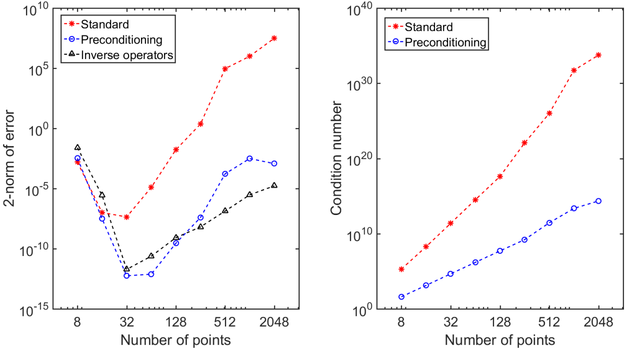

Figure: $u^{(5)}(x) + u^{(4)}(x) - u'(x) - u(x) = f(x)$

Nonconstant coefficients: function of V [sec.6.3]

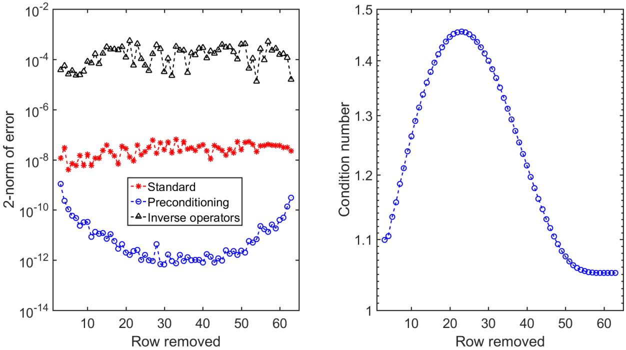

Figure:
$$u^{(5)}(x) + \sin(10x)u'(x) + xu(x) = f(x), \quad u(\pm 1) = u'(\pm 1) = u''(1) = 0$$

Nonconstant coefficients: function of N [sec.6.3]

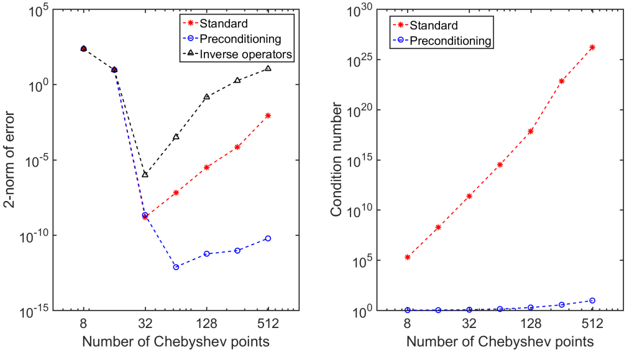

Figure:
$$u^{(5)}(x) + \sin(10x)u'(x) + xu(x) = f(x), \quad u(\pm 1) = u'(\pm 1) = u''(1) = 0$$

Nonlinear [sec.6.4]

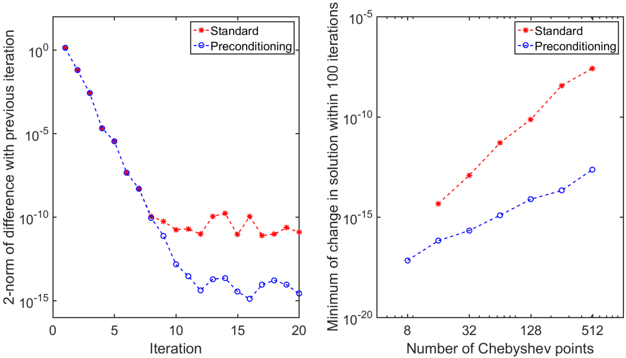

Figure: $u^{(4)}(x) = u'(x)u''(x) - u(x)u^{(3)}(x)$,
$u(\pm 1) = u'(-1) = 0, \quad u'(1) = 1$

Conclusion

- Some sources of round-off error (largest order derivative) are easy to remove
- Remaining derivatives prove challenging
- Inversion operators need homogeneous solutions, which may not be available

Future Works

- A priori row removal
- Alternative methods to calculate integration matrix
- Inversion for constant coefficients
- Preconditioning for perturbed/ boundary layer problems

Variation of parameters [sec.3]

$$R_j(x) = \sum_{k=1}^{m} G_{k,j}(x) P_k(x)$$

$$\sum_{k=1}^{m} G'_{k,j}(x) P_k^{(l)}(x) = 0 \quad l = 0, ..., m-2$$

$$G'_{k,j}(x_i) = \begin{cases} \beta_{k,j} & x_i = x_j \\ 0 & x_i \neq x_j, v_k \end{cases}$$

$$\mathcal{L} P_k(x) = 0, \quad P_k^{(l)}(v_k) = \begin{cases} 0 & l < m \\ 1 & l = m \end{cases}$$