Spectral Differentiation: Integration and Inversion

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October 16th, 2018

Spectral methods

We want to approximate an infinite dimensional problem with a finite dimensional one:

$$\mathcal{L}u(x) = f(x) \to AU = F$$

We take an orthonormal basis of some finite dimensional space (usually polynomials) and decompose the problem:

$$u(x) \approx \sum_{k=0}^{N} \alpha_k \Phi_k(x), \quad f(x) \approx \sum_{k=0}^{N} \beta_k \Psi_k(x)$$

Three types of spectral methods

- Galerkin: focus on $\Phi_k(x)$ and $\Psi_k(x)$
- Tau: focus on α_k and β_k
- Collocation: focus on $u(x_k)$ and $f(x_k)$

$\{x_k\}_{k=0}^N$ (called collocation points) are specific to the chosen basis and arise from quadrature rules

Spectral collocation

Build a matrix D such that if Φ_j is a vector with entries $\Phi_j(x_k)$ then $D\Phi_j = \Phi_j'$ where the entries of Φ_j' are $\Phi_j'(x_k)$.
Multiply and add D together with coefficient functions to form linear operator matrices. You can now solve $AU = F$.

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

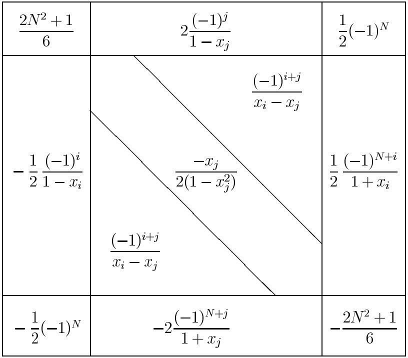


Fig: From pg. 53 of *Spectral Methods in MATLAB* by L.N. Trefethen

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

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

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

The general m-th order problem

$$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{n=1}^{m} q_n(x) u^{(m-n)}(x) = f(x)$$

$$\mathcal{B}_k u(1) = \sum_{n=1}^{m} a_n^k u^{(m-n)}(1) = a_0^k, \qquad k = 1, \ldots, k_0$$

$$\mathcal{B}_k u(-1) = \sum_{n=1}^{m} a_n^k u^{(m-n)}(-1) = a_0^k, \qquad k = k_0 + 1, \ldots, m$$

The collocation matrices

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

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

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

$D_0^{(m-n)}$ 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 $\hat{A}$

$\bar{A}$ 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 $\hat{A}$

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 $\hat{A}$

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

$\tilde{D}^{(m)}$ 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

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

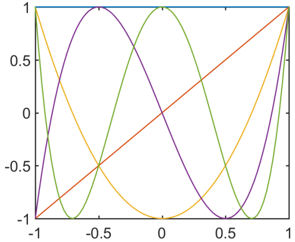


Figure: $T_k(x) = \cos(k \arccos(x))$

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

The Chebyshev polynomials

$T_k(x)$ 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 $B_j(x)$ (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

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

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

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 $\beta_{k,j}$

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

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

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

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

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

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

Fundamental solutions

To solve this problem we need to know the fundamental solutions of $\mathcal{L}$:

$$\mathcal{L}P_k(x) = 0 \quad k = 1, ..., m$$

We then assume the columns of R have the form:

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

Variation of parameters

We proceed by variation of parameters:

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

$$\implies \mathcal{L}R_j(x) = \sum_{k=1}^{m} G'_{k,j}(x) P_k^{(m-1)}(x)$$

Variation of parameters

This leads to the following conditions:

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

$$P_k^{(l)}(v_k) = \begin{cases} 0 & l < m \\ 1 & l = m \end{cases}$$

Therefore, $G_{k,j}(x)$ is a multiple of a Birkhoff interpolant from earlier, and $P_k(x)$ is a particular fundamental solution

Solving for $\beta_{k,j}$ (again)

The system to solve the $\beta_{k,j}$ is:

$$\begin{bmatrix} P_1(x_j) & \dots & P_m(x_j) \\ \vdots & \ddots & \vdots \\ P_1^{(m-1)}(x_j) & \dots & P_m^{(m-1)}(x_j) \end{bmatrix} \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 1 \end{bmatrix}$$

This system is related to the Wronskian of the set $\{P_l(x)\}_{l=1}^m$

The Wronskian

The Wronskian of the set $\{P_l(x)\}_{l=1}^m$ is defined as:

$$W(\{P_l\}_{l=1}^m; x) = \det \left(\begin{bmatrix} P_1(x_j) & \dots & P_m(x_j) \\ \vdots & \ddots & \vdots \\ P_1^{(m-1)}(x_j) & \dots & P_m^{(m-1)}(x_j) \end{bmatrix} \right)$$

By Cramer's rule $\beta_{k,j}$ can be defined as:

$$\beta_{k,j} = (-1)^{j+m} \frac{W(\{P_l\}_{l \neq k}; x_j)}{W(\{P_l\}_{l=1}^m; x_j)}$$

Abel's identity

In many cases using the Wronskians proves neither efficient nor accurate, but one could use Abel's identity to find $W(\{P_l\}_{l=1}^m; x)$:

$$W(\{P_l\}_{l=1}^m; x) = W(\{P_l\}_{l=1}^m; -1) \exp\left(-\int_{-1}^{x} q_1(s) ds\right)$$

BEVP

Consider the boundary eigenvalue problem:

$$u'(x) = \lambda u(x) \quad \forall x \in [-1, 1], \quad u(1) = 0$$

This admits only the eigenpair $u(x) = 0$, $\lambda = 0$

DEVP

Consider the collocation version of this problem with $V = \{1\}$:

$$AU = \tilde{D}U = \lambda U$$

Since $\tilde{D}$ is a $N+1 \times N+1$ nonsingular matrix there are $N+1$ nontrivial eigenpairs

CEVP

The DEVP is not the discrete version of the BEVP; instead, it approximates the following continuous eigenvalue problem:

$$u'(x) = \lambda u(x) \quad \forall x \in [-1, 1), \quad u(1) = \lambda u(1)$$

Either $\lambda = 1$ and $u(x) = e^x$ or $u(1) = u(x) = 0$

Three EVPs

- CEVP admits only one solution not found in BEVP
- DEVP has the nontrivial CEVP eigenpair and N computational eigenpairs (no continuous analogue)
- The computational modes approximate rapidly decaying exponentials

CEVP

Consider the same problem but with $V = \{x_i\}$:

$$u'(x) = \lambda u(x) \quad \forall x \in [-1, 1] \setminus \{x_i\}, \quad u(1) = \lambda u(x_i)$$

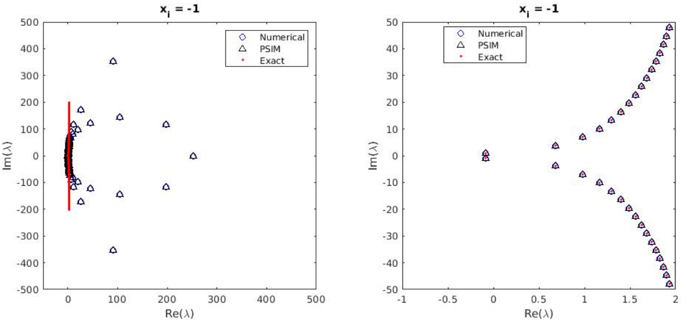
The eigenvalues are then:

$$\lambda = \frac{W(x_i - 1)}{x_i - 1}$$

where $W(x)$ is the Lambert W function, the inverse of xe^x

Eigenvalues

We've gone from one eigenvalue to infinite eigenvalues



The corresponding eigenvectors are spirals in the complex plane

Some notes

- We've reduced the number of computational modes by changing which row we remove
- Eigenvalues of $\tilde{D}$ match those of B
- About 2 thirds of the eigenvalues of $\tilde{D}$ match exact values (Weideman and Trefethen observe a ratio of $2/\pi$ exact to total eigenvalues for a second order example)

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

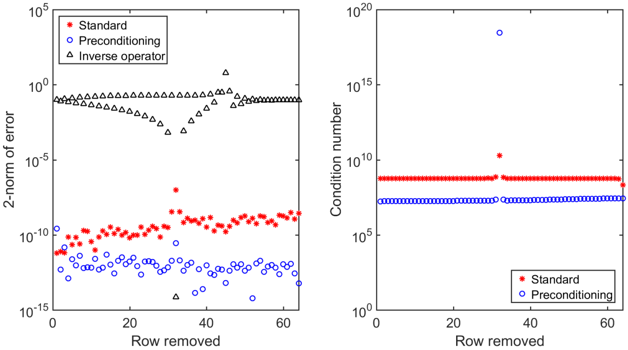


Figure: $xu''(x) - (x+1)u'(x) + u(x) = x^2, \quad u(\pm 1) = 1$

Singular example: function of N

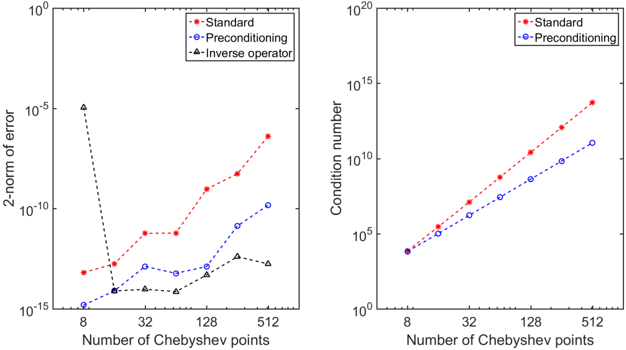


Figure: $xu''(x) - (x+1)u'(x) + u(x) = x^2, \quad u(\pm 1) = 1$

Constant coefficients: function of V

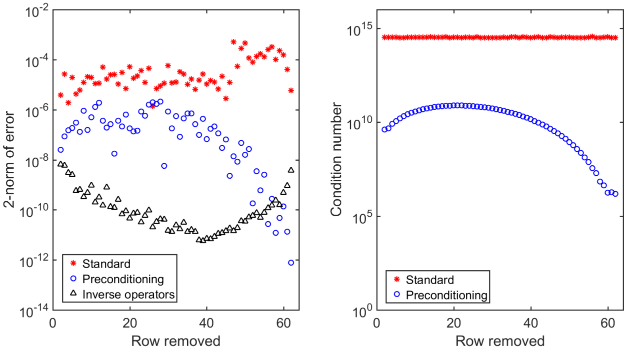


Figure: $u^{(5)}(x) + u^{(4)}(x) - u'(x) - u(x) = f(x)$

Constant coefficients: function of N

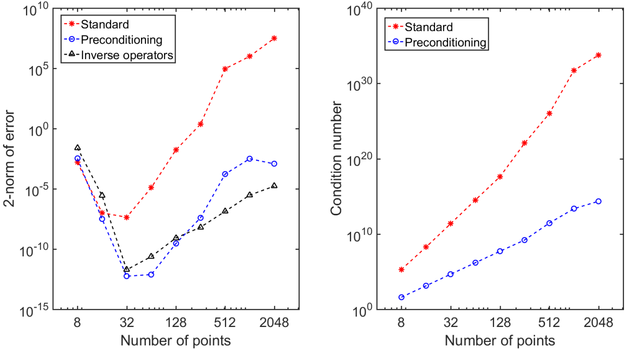


Figure: $u^{(5)}(x) + u^{(4)}(x) - u'(x) - u(x) = f(x)$

Nonconstant coefficients: function of V

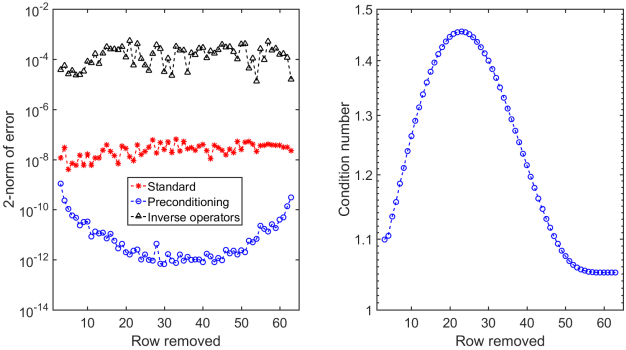


Figure:
$$u^{(5)}(x) + \sin(10x)u'(x) + xu(x) = f(x), \quad u(\pm 1) = u'(\pm 1) = u''(1) = 0$$

Nonconstant coefficients: function of N

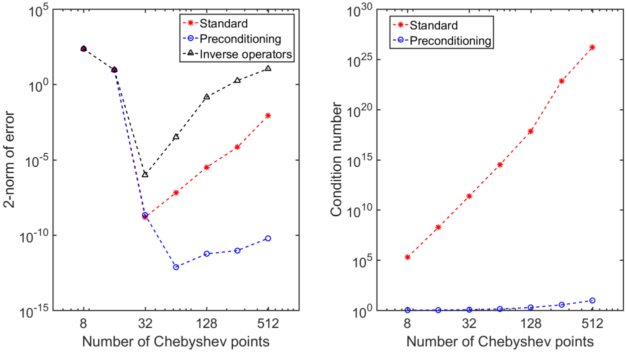


Figure:
$$u^{(5)}(x) + \sin(10x)u'(x) + xu(x) = f(x), \quad u(\pm 1) = u'(\pm 1) = u''(1) = 0$$

Nonlinear

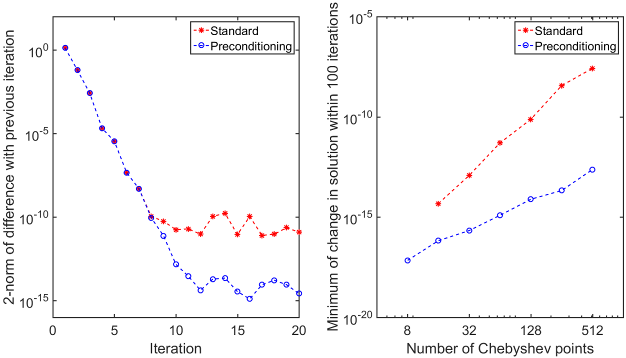


Figure: $u^{(4)}(x) = u'(x)u''(x) - u(x)u^{(3)}(x)$,
$u(\pm 1) = u'(-1) = 0, \quad u'(1) = 1$

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