

On well-conditioned spectral collocation and spectral methods by the integral reformulation

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An m th ODE and its spectral methods

- Consider the m th-order differential equation of the form

$$u^{(m)}(x) + \sum_{k=0}^{m-1} a^k(x)u^{(k)}(x) = f(x),$$

together with m linearly independent constraints

$$\mathcal{B}u = \mathbf{b}.$$

Spectral methods

- Rectangular spectral collocation [1]
- Well-conditioned spectral collocation [5]
- Ultraspherical spectral method [3]
- Chebyshev spectral method by the integral reformulation [2]

Barycentric resampling matrix

- $\{x_j\}_{j=0}^N$: $-1 \leq x_0 < x_1 < \dots < x_{N-1} < x_N \leq 1$.
- The associated barycentric weights

$$w_{j,\mathbf{x}} = \prod_{n=0, n \neq j}^N (x_j - x_n)^{-1}, \quad j = 0, 1, \dots, N.$$

- $\{y_j\}_{j=0}^M$: $-1 \leq y_0 < y_1 < \dots < y_{M-1} < y_M \leq 1$.
- Barycentric resampling matrix $\mathbf{P}^{\mathbf{x} \rightarrow \mathbf{y}} = [p_{ij}^{\mathbf{x} \rightarrow \mathbf{y}}]_{i=0, j=0}^{M, N}$,

$$p_{ij}^{\mathbf{x} \rightarrow \mathbf{y}} = \begin{cases} \frac{w_{j,\mathbf{x}}}{y_i - x_j} \left(\sum_{l=0}^N \frac{w_{l,\mathbf{x}}}{y_i - x_l} \right)^{-1}, & y_i \neq x_j, \\ 1, & y_i = x_j. \end{cases}$$

- If $N \geq M$, then $\mathbf{P}^{\mathbf{x} \rightarrow \mathbf{y}} \mathbf{P}^{\mathbf{y} \rightarrow \mathbf{x}} = \mathbf{I}_{M+1}$.

Pseudospectral differentiation matrix

- Lagrange interpolation basis polynomials of degree N :

$$\ell_{j,\mathbf{x}}(x) = w_{j,\mathbf{x}} \prod_{n=0, n \neq j}^N (x - x_n), \quad j = 0, 1, \dots, N,$$

- Pseudospectral differentiation matrices

$$\mathbf{D}_{\mathbf{x} \mapsto \mathbf{x}}^{(k)} = \left[\ell_{j,\mathbf{x}}^{(k)}(x_i) \right]_{i,j=0}^N, \quad \mathbf{D}_{\mathbf{x} \mapsto \mathbf{y}}^{(k)} = \left[\ell_{j,\mathbf{x}}^{(k)}(y_i) \right]_{i=0, j=0}^{M,N}.$$

- The matrix $\mathbf{D}_{\mathbf{x} \mapsto \mathbf{y}}^{(k)}$ is called a rectangular k th-order differentiation matrix, which maps values of a polynomial defined on $\{x_j\}_{j=0}^N$ to the values of its k th-order derivative on $\{y_j\}_{j=0}^M$.
- There hold

$$\mathbf{D}_{\mathbf{x} \mapsto \mathbf{x}}^{(k)} = \left(\mathbf{D}_{\mathbf{x} \mapsto \mathbf{x}}^{(1)} \right)^k, \quad \mathbf{D}_{\mathbf{x} \mapsto \mathbf{y}}^{(k)} = \mathbf{P}^{\mathbf{x} \mapsto \mathbf{y}} \mathbf{D}_{\mathbf{x} \mapsto \mathbf{x}}^{(k)}, \quad \mathbf{D}_{\mathbf{x} \mapsto \mathbf{y}}^{(0)} = \mathbf{P}^{\mathbf{x} \mapsto \mathbf{y}}.$$

Rectangular spectral collocation

- Consider the m th-order differential equation of the form

$$u^{(m)}(x) + \sum_{k=0}^{m-1} a^k(x)u^{(k)}(x) = f(x), \quad \mathcal{B}u = \mathbf{b}.$$

- The rectangular spectral collocation discretization is given by

$$\mathbf{A}_{M+1}\mathbf{u} = \mathbf{f}, \quad \mathbf{L}_{\mathcal{B}}\mathbf{u} = \mathbf{b},$$

where $\mathbf{L}_{\mathcal{B}}$ denotes the discretization of the linear operator \mathcal{B} ,

$$\begin{aligned} \mathbf{A}_{M+1} &= \mathbf{D}_{\mathbf{x} \rightarrow \mathbf{y}}^{(m)} + \text{diag}\{\mathbf{a}^{m-1}\}\mathbf{D}_{\mathbf{x} \rightarrow \mathbf{y}}^{(m-1)} + \cdots \\ &\quad + \text{diag}\{\mathbf{a}^1\}\mathbf{D}_{\mathbf{x} \rightarrow \mathbf{y}}^{(1)} + \text{diag}\{\mathbf{a}^0\}\mathbf{D}_{\mathbf{x} \rightarrow \mathbf{y}}^{(0)}, \\ \mathbf{a}^k &= \begin{bmatrix} a^k(y_0) & a^k(y_1) & \cdots & a^k(y_M) \end{bmatrix}^T, \\ \mathbf{f} &= \begin{bmatrix} f(y_0) & f(y_1) & \cdots & f(y_M) \end{bmatrix}^T \end{aligned}$$

- $\mathbf{u} \approx \begin{bmatrix} u(x_0) & u(x_1) & \cdots & u(x_N) \end{bmatrix}^T$.

Birkhoff-type interpolation problem

- Given $\{y_j\}_{j=0}^M$ and \mathbf{b} : Find $p(x) \in \mathbb{P}_{M+m}$ such that

$$\begin{cases} p^{(m)}(y_j) = u^{(m)}(y_j), & j = 0, \dots, M, \\ \mathcal{B}p = \mathbf{b}. \end{cases}$$

- Define the integral operators:

$$\partial_x^{-1}\phi(x) = \int_{-1}^x \phi(t)dt; \quad \partial_x^{-k}\phi(x) = \partial_x^{-1}\left(\partial_x^{-(k-1)}\phi(x)\right), \quad k \geq 2.$$

- The Birkhoff-type interpolation polynomial takes the form

$$p(x) = \sum_{j=0}^M u^{(m)}(y_j) \partial_x^{-m} \ell_{j,\mathbf{y}}(x) + \sum_{i=0}^{m-1} \alpha_i x^i,$$

- After obtaining α_i , we can rewrite the last equation as

$$p(x) = \sum_{j=0}^M u^{(m)}(y_j) B_{j,\mathbf{y}}(x) + \sum_{j=1}^m b_j B_{M+j,\mathbf{y}}(x).$$

First-order Birkhoff-type interpolation problem

- Find $p(x) \in \mathbb{P}_{M+1}$ with $\begin{cases} p'(y_j) = u'(y_j), & j = 0, 1, \dots, M, \\ \mathcal{B}p = b_1. \end{cases}$
- Given $\mathcal{B}p := ap(-1) + bp(1)$ with $a + b \neq 0$, we have

$$B_{j,\mathbf{y}}(x) = \partial_x^{-1} \ell_{j,\mathbf{y}}(x) - \frac{b}{a+b} \int_{-1}^1 \ell_{j,\mathbf{y}}(x) dx,$$

$$B_{M+1,\mathbf{y}}(x) = \frac{1}{a+b}.$$

- Given $\mathcal{B}p := \int_{-1}^1 p(x) dx$, we have

$$B_{j,\mathbf{y}}(x) = \partial_x^{-1} \ell_{j,\mathbf{y}}(x) - \frac{1}{2} \int_{-1}^1 \partial_x^{-1} \ell_{j,\mathbf{y}}(x) dx,$$

$$B_{M+1,\mathbf{y}}(x) = \frac{1}{2}.$$

Second-order Birkhoff-type interpolation problem

- Find $p(x) \in \mathbb{P}_{M+2}$ with $\begin{cases} p''(y_j) = u''(y_j), & j = 0, 1, \dots, M, \\ \mathcal{B}p = \mathbf{b}. \end{cases}$
- Given

$$\mathcal{B}p = \begin{bmatrix} ap(-1) + bp(1) \\ \int_{-1}^1 p(x) dx \end{bmatrix}, \quad a \neq b,$$

we have

$$B_{j,\mathbf{y}}(x) = \partial_x^{-2} \ell_{j,\mathbf{y}}(x) - \frac{bx}{b-a} \int_{-1}^1 \partial_x^{-1} \ell_{j,\mathbf{y}}(x) dx \\ + \left(\frac{(a+b)x}{2(b-a)} - \frac{1}{2} \right) \int_{-1}^1 \partial_x^{-2} \ell_{j,\mathbf{y}}(x) dx,$$

$$B_{M+1,\mathbf{y}}(x) = \frac{x}{b-a},$$

$$B_{M+2,\mathbf{y}}(x) = \frac{1}{2} - \frac{(a+b)x}{2(b-a)}.$$

Pseudospectral integration matrix

- Define the m th-order *pseudospectral integration matrix* (PSIM) as:

$$\mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)} = [B_{j,\mathbf{y}}(x_i)]_{i,j=0}^N, \quad N = M + m.$$

- Define the matrices

$$\mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(k-m)} = [B_{j,\mathbf{y}}^{(k)}(x_i)]_{i,j=0}^N, \quad k \geq 1.$$

- There hold

$$\mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(k-m)} = \mathbf{D}_{\mathbf{x} \mapsto \mathbf{x}}^{(k)} \mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)}, \quad k \geq 1,$$

and, if for any $p(x) \in \mathbb{P}_N$,

$$\mathcal{B}p = \mathbf{L}_{\mathcal{B}} \begin{bmatrix} p(x_0) & \cdots & p(x_N) \end{bmatrix}^T,$$

then

$$\begin{bmatrix} \mathbf{D}_{\mathbf{x} \mapsto \mathbf{y}}^{(m)} \\ \mathbf{L}_{\mathcal{B}} \end{bmatrix} \mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)} = \mathbf{I}_{N+1}.$$

Preconditioning rectangular spectral collocation

- The global collocation system $\mathbf{A}\mathbf{u} = \mathbf{g}$ where

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{M+1} \\ \mathbf{L}_{\mathcal{B}} \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} \mathbf{f} \\ \mathbf{b} \end{bmatrix}.$$

- Consider the matrix $\mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)}$ as a right preconditioner,

$$\mathbf{A}\mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)}\mathbf{v} = \mathbf{g}, \quad \Rightarrow \quad \mathbf{v} = \begin{bmatrix} \mathbf{v}_{M+1} \\ \mathbf{b} \end{bmatrix}, \quad \tilde{\mathbf{A}}_{M+1}\mathbf{v}_{M+1} = \tilde{\mathbf{f}},$$

where \mathbf{v}_{M+1} is an approximation of the vector

$$\left[u^{(m)}(y_0) \quad u^{(m)}(y_1) \quad \cdots \quad u^{(m)}(y_M) \right]^T,$$

$$\tilde{\mathbf{A}}_{M+1} = \mathbf{I}_{M+1} + \text{diag}\{\mathbf{a}^{m-1}\}\tilde{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(m-1-m)} + \cdots + \text{diag}\{\mathbf{a}^0\}\tilde{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(0-m)},$$

Preconditioning rectangular spectral collocation

$$\tilde{\mathbf{f}} = \mathbf{f} - \left(\text{diag}\{\mathbf{a}^{m-1}\} \widehat{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(m-1-m)} + \cdots + \text{diag}\{\mathbf{a}^0\} \widehat{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(0-m)} \right) \mathbf{b},$$

and, for $k = 0, 1, \dots, m-1$,

$$\tilde{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(k-m)} = \left[B_{j,\mathbf{y}}^{(k)}(y_i) \right]_{i,j=0}^M,$$

$$\widehat{\mathbf{B}}_{\mathbf{y} \mapsto \mathbf{y}}^{(k-m)} = \left[B_{j,\mathbf{y}}^{(k)}(y_i) \right]_{i=0, j=M+1}^{M, M+m}.$$

- We obtain \mathbf{u} by

$$\mathbf{u} = \mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)} \mathbf{v} = \mathbf{B}_{\mathbf{y} \mapsto \mathbf{x}}^{(-m)} \begin{bmatrix} \mathbf{v}^{M+1} \\ \mathbf{b} \end{bmatrix}.$$

Numerical examples

- Consider the equation

$$\varepsilon u''(x) - xu'(x) - u(x) = f(x)$$

with the linear constraints

$$u(-1) - u(1) = \sigma_1, \quad \int_{-1}^1 u(x) dx = \sigma_2.$$

The function $f(x)$, σ_1 and σ_2 are chosen such that the exact solution is

$$u(x) = \exp\left(\frac{x^2 - 1}{2\varepsilon}\right).$$

Numerical results

Table: Condition numbers, maximum errors and iterations for $\varepsilon = 1$.

N	RSC			P-RSC		
	Condition	Error	Iterations	Condition	Error	Iterations
128	1.95e+08	8.41e-10	>1000	2.73	6.66e-16	8
256	4.39e+09	9.23e-09	>1000	2.73	6.66e-16	8
512	9.94e+10	7.84e-08	>1000	2.73	8.88e-16	8
1024	2.25e+12	2.49e-06	>1000	2.73	1.11e-15	8

Table: Condition numbers, maximum errors and iterations for $\varepsilon = 0.1$.

N	RSC			P-RSC		
	Condition	Error	Iterations	Condition	Error	Iterations
128	6.74e+07	2.65e-10	>1000	5.11e+02	1.14e-14	16
256	1.50e+09	5.95e-10	>1000	5.11e+02	1.62e-14	16
512	3.35e+10	4.12e-09	>1000	5.11e+02	1.58e-14	16
1024	7.55e+11	1.69e-07	>1000	5.11e+02	1.49e-14	16

Chebyshev spectral method by integral reformulation

- Consider the m th-order differential equation of the form

$$u^{(m)}(x) + \sum_{k=0}^{m-1} a^k(x)u^{(k)}(x) = f(x), \quad \mathcal{B}u = \mathbf{b}.$$

- Let $v(x) = \partial_x^m u(x)$, we can write

$$u(x) = \partial_x^{-m} v(x) + \mathcal{X}(\mathcal{B}\mathcal{X})^{-1}(\mathbf{b} - \mathcal{B}\partial_x^{-m} v(x)),$$

where

$$\mathcal{X} = \begin{bmatrix} 1 & x^1 & \dots & x^{m-1} \end{bmatrix}.$$

- Integral reformulation

$$v(x) + \sum_{k=0}^{m-1} a^k(x)\partial_x^{k-m} v(x) - \mathcal{A}(\mathcal{B}\mathcal{X})^{-1}\mathcal{B}\partial_x^{-m} v(x) = f(x) - \mathcal{A}(\mathcal{B}\mathcal{X})^{-1}\mathbf{b},$$

where

$$\mathcal{A} = \begin{bmatrix} a^0(x) & a^0(x)x + a^1(x) & \dots & \sum_{k=0}^{m-1} \frac{(m-1)!}{(m-1-k)!} a^k(x)x^{m-1-k} \end{bmatrix}.$$

Chebyshev spectral (CS) method:

- Representing $v(x)$ and $\partial_x^{-k}v(x)$ by Chebyshev series

$$v(x) = \sum_{j=0}^{\infty} v_j T_j(x), \quad \partial_x^{-k}v(x) = \sum_{j=0}^{\infty} v_j^{(-k)} T_j(x),$$

we have

$$\mathbf{v}^{(-k)} = \mathcal{Q}^k \mathbf{v},$$

where for $i, j = 0, 1, \dots, \infty$,

$$\mathcal{Q} = \begin{bmatrix} 1 & -\frac{1}{4} & -\frac{1}{3} & \frac{1}{8} & -\frac{1}{15} & \frac{1}{24} & \dots & \frac{(-1)^{j+1}}{(j-1)(j+1)} & \dots \\ 1 & 0 & -\frac{1}{2} & 0 & 0 & 0 & \dots & 0 & \dots \\ 0 & \frac{1}{4} & 0 & -\frac{1}{4} & 0 & 0 & \dots & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots & \ddots \\ \vdots & \ddots & \ddots & \frac{1}{2i} & \ddots & -\frac{1}{2i} & \ddots & \vdots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots & \ddots \end{bmatrix},$$

$$\mathbf{v} = [v_0 \quad v_1 \quad \dots]^T, \quad \mathbf{v}^{(-k)} = [v_0^{(-k)} \quad v_1^{(-k)} \quad \dots]^T.$$

Chebyshev spectral method: Multiplication operator

- Let

$$u(x) = \sum_{j=0}^{\infty} u_j T_j(x), \quad x \in [-1, 1].$$

where $T_j(x)$ is the degree j Chebyshev polynomial. Write the infinite vector

$$\mathbf{u} = \begin{bmatrix} u_0 & u_1 & \cdots \end{bmatrix}^T.$$

- For $a(x)$ with Chebyshev expansion coefficients $\{a_j\}_{j=0}^{\infty}$, the infinite vector $\mathcal{M}_0[a]\mathbf{u}$ is the Chebyshev expansion coefficients of $a(x)u(x)$, where

$$\mathcal{M}_0[a] = \frac{1}{2} \begin{bmatrix} 2a_0 & a_1 & a_2 & a_3 & \cdots \\ a_1 & 2a_0 & a_1 & a_2 & \ddots \\ a_2 & a_1 & 2a_0 & a_1 & \ddots \\ a_3 & a_2 & a_1 & 2a_0 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ a_1 & a_2 & a_3 & a_4 & \cdots \\ a_2 & a_3 & a_4 & a_5 & \ddots \\ a_3 & a_4 & a_5 & a_6 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

Chebyshev spectral (CS) method

- The integral equation can be rewritten as

$$\tilde{\mathcal{L}}\mathbf{v} = \mathbf{f} - \mathcal{A}(\mathcal{B}\mathcal{X})^{-1}\mathbf{b},$$

where

$$\tilde{\mathcal{L}} := \mathcal{I} + \sum_{k=0}^{m-1} \mathcal{M}_0[a^k] \mathcal{Q}^{m-k} - \mathcal{A}(\mathcal{B}\mathcal{X})^{-1} \mathcal{B}\mathcal{Q}^m.$$

- We have

$$\mathbf{u} = \mathcal{Q}^m \mathbf{v} + \mathcal{X}(\mathcal{B}\mathcal{X})^{-1}(\mathbf{b} - \mathcal{B}\mathcal{Q}^m \mathbf{v}).$$

- By truncating the above equations, we obtain

$$\tilde{\mathbf{A}}_n \mathbf{v}_n := \mathcal{P}_n \tilde{\mathcal{L}} \mathcal{P}_n^T \mathcal{P}_n \mathbf{v} = \mathcal{P}_n (\mathbf{f} - \mathcal{A}(\mathcal{B}\mathcal{X})^{-1} \mathbf{b}).$$

and

$$\mathbf{u}_n = \mathcal{P}_n \mathbf{u} \approx \mathcal{P}_n \mathcal{Q}^m \mathcal{P}_n^T \mathbf{v}_n + \mathcal{P}_n \mathcal{X}(\mathcal{B}\mathcal{X})^{-1} (\mathbf{b} - \mathcal{B}\mathcal{Q}^m \mathcal{P}_n^T \mathbf{v}_n).$$

Chebyshev spectral (CS) method

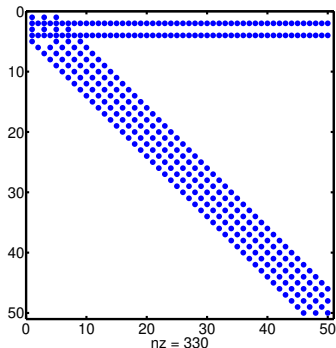
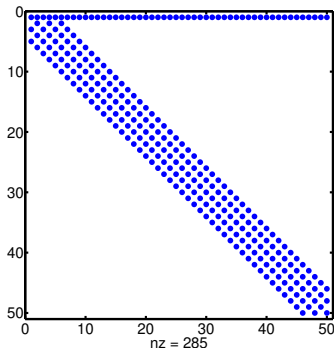
- It converges at the same rate as $\mathcal{P}_n^T \mathcal{P}_n \mathbf{v}$ converges to \mathbf{v} .
- The condition number of the matrix $\tilde{\mathbf{A}}_n$ is independent of n .
- The almost banded structure of $\tilde{\mathbf{A}}_n$ follows from the almost banded structure of \mathcal{Q} and the banded structure of $\mathcal{M}_0[a^k]$.
- The matrix-vector product for the matrix $\tilde{\mathbf{A}}_n$ and an n -vector can be obtained in $\mathcal{O}(n \log n)$ operators.
- The low-rank property still holds for the coefficient matrix $\tilde{\mathbf{A}}_n$, therefore, the fast direct method [4] with the computational complexity $\mathcal{O}(rn \log^2 n) + \mathcal{O}(r^2 n)$ applies, where r is independent of n and small.

Example 1

$$u'(x) + x^3 u(x) = 100 \sin(20,000x^2), \quad u(-1) = 0.$$

The exact solution is

$$u(x) = \exp\left(-\frac{x^4}{4}\right) \int_{-1}^x 100 \exp\left(\frac{t^4}{4}\right) \sin(20,000t^2) dt.$$

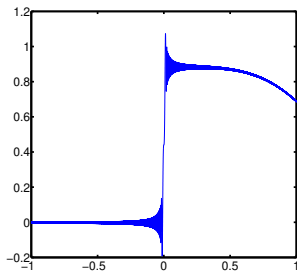


Example 1

Table: Comparison of condition numbers of the matrices for Example 1.

n	US	P-US	CS
128	2.4045e+02	3.9813	2.5955
256	4.8312e+02	3.9864	2.5955
512	9.6846e+03	3.9889	2.5955
1024	1.9391e+04	3.9901	2.5955

The L^2 norm errors $\approx 1.2602 \times 10^{-14}$.

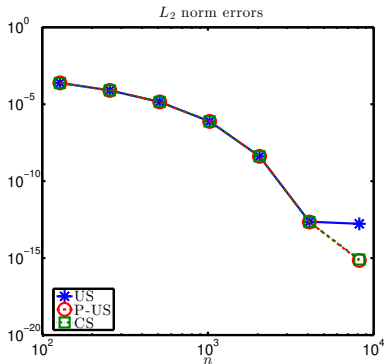
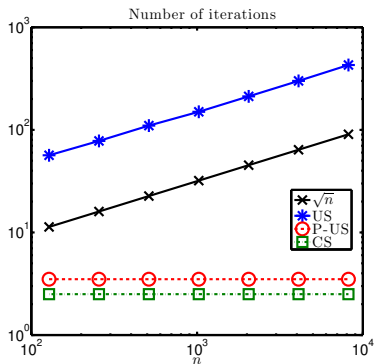


Example 2

$$u'(x) + \frac{1}{ax^2 + 1}u(x) = 0, \quad u(-1) = 1, \quad a = 50000.$$

The exact solution is

$$u(x) = \exp\left(-\frac{\arctan(\sqrt{a}x) + \arctan(\sqrt{a})}{\sqrt{a}}\right).$$



Example 3

$$u^{(10)}(x) + \cosh(x)u^{(8)}(x) + x^2u^{(6)}(x) + x^4u^{(4)} + \cos(x)u^{(2)}(x) + x^2u(x) = 0,$$

with boundary conditions

$$u(\pm 1) = 0, \quad u'(\pm 1) = 1, \quad u^{(k)}(\pm 1) = 0, \quad 2 \leq k \leq 4.$$

The condition number of $\tilde{\mathbf{A}}_n$ remains a constant (about 1.7444) for different values of n . The computed solution is odd to about machine precision,

$$\left(\int_{-1}^1 (\tilde{u}(x) + \tilde{u}(-x))^2 dx \right)^{\frac{1}{2}} = 5.2171 \times 10^{-14}.$$

Extensions

- Nonlinear problems: Newton iteration
- 2D-problem:

$$\mathcal{L}u(x, y) = f(x, y), \quad \mathcal{L} = \sum_{i=0}^2 \sum_{j=0}^2 a_{ij}(x, y) \partial_x^j \partial_y^i.$$






Combining the low-rank singular value expansion of $a_{ij}(x, y)$,

$$a_{ij}(x, y) \approx \sum_{l=1}^{r_{ij}} \sigma_l^{ij} \phi_l^{ij}(x) \psi_l^{ij}(y),$$

and tensor-product techniques.

- Fractional differential equations

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