Eigenvalue Analysis of Spectral-Galerkin Discretisation of IVPs and Space-Time Spectral Methods

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Outline

Motivation I: Parallel-in-Time (PinT)[1]

- Consider a system of ODEs resulting from spatial discretisation

$$u'(t) + Au(t) = f(t), \quad t > 0; \quad u(0) = u_0; \quad A \in \mathbb{R}^{M\times M} \tag{1}$$

[1] Maday-Ronquist, Parallelization in time via tensor-product space-time solvers'08.

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- Central difference + last step implicit Euler **(Liu-Wang-Wu-Zhou'22)**

$$\begin{cases} \dfrac{u_{j+1} - u_{j-1}}{2\tau} + Au_j = f_j, & j = 1, 2, \ldots, n-1, \\ \dfrac{u_n - u_{n-1}}{\tau} + Au_n = f_n, & \text{given } u_0 \end{cases}$$

- Matrix of all-at-once system

$$B = \begin{bmatrix} 0 & \frac{1}{2} & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} \\ & & & -1 & 1 \end{bmatrix}$$

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- Diagonalising $B = VDV^{-1}$ with $D = \mathrm{diag}(\lambda_1, \cdots, \lambda_N)$:

$$\left(\tau^{-1} B \otimes I_x + I_t \otimes A\right) \boldsymbol{u} = \boldsymbol{b} \quad \Rightarrow \quad (\lambda_j I_x + \tau A) \boldsymbol{w}_j = h_j$$

Note: For a normal matrix $C = U \Lambda U^*$ with $U^{-1} = U^*$, but this diagonalisation for non-normal B involves V^{-1}.

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- Liu et al.'22 showed eigenvalues: $\lambda_j = \mathrm{i} x_j$ and zeros $\{x_j\}$ are

$$U_{n-1}(x) - \mathrm{i} T_n(x) = 0,$$

  eigenvectors $\boldsymbol{v}_j = (U_0(x_j), \cdots, \mathrm{i}^{n-1} U_{n-1}(x_j))^\top$ & $\mathrm{cond}(V) \sim N^2$.

  Stable but first-order!

- **Question: What about spectral methods in time?** Expect to have high accuracy and match spectral method in space!

PinT: Chen-Liu[2]

- Legendre spectral approximation to the ODE system (1):

$$u_N' + A\pi_{N-1}^L u_N = \pi_{N-1}^L f, \quad u_N(-1) = u_0,$$

where

$$u_N(t) = \sum_{k=0}^{N} \hat{u}_k P_k(t), \quad \pi_{N-1}^L f(t) = \sum_{k=0}^{N-1} \hat{f}_k P_k(t).$$

- Testing by $(1-t^2)P_j'(t)$ for $0 \le j \le N-1$ gives

$$\phi_N(A)\hat{\boldsymbol{u}} := \begin{pmatrix} A & -I & -\frac{1}{5}A & & & \\ & \frac{1}{3}A & -I & -\frac{1}{7}A & & \\ & & \ddots & \ddots & \ddots & \\ & & \frac{1}{2N-5}A & -I & \frac{1}{2N-1}A & \\ & & & \frac{1}{2N-3}A & -I & 0 \\ & & & & \frac{1}{2N-1}A & -I \\ I & -I & I & -I & \cdots & (-1)^N I \end{pmatrix} \hat{\boldsymbol{u}} = \boldsymbol{b}.$$

[2] Chen-Liu, Efficient and parallel solution of high-order continuous time Galerkin for dissipative and wave propagation problems, SISC, 2024

Implementation

- Given $\mathbb{X} = (X_{ij})_{i,j=1}^{d}$, the property about the adjugate matrix

$$(\det \mathbb{X})\boldsymbol{I} = \mathbb{X}\,\mathrm{adj}(\mathbb{X}) \quad \Rightarrow \quad (\det \mathbb{X})\delta_{i,j} = \sum_{k=1}^{d}(-1)^{i+k}(\det \mathbb{X}_{k,i})X_{k,j},$$

  where $\mathbb{X}_{i,j}$ is obtained by removing the ith row and jth column.

- An analytic formula of solutions

$$\hat{\boldsymbol{u}}_{i-1} = \frac{1}{\det \phi_N(A)} \sum_{k=1}^{N+1}(-1)^{i+k}(\det \phi_N(A)_{k,i})\boldsymbol{b}_{k-1}, \quad i = 1, \cdots, N+1.$$

- **Chen and Liu'24** proved that

$$\begin{cases} \phi_1(\lambda) = 1 - a_1, \quad \phi_2(\lambda) = 1 - a_1 + a_1 a_2, \\ \phi_k(\lambda) = \phi_{k-1}(\lambda) + a_k a_{k-1}\phi_{k-2}(\lambda), \quad k \geq 3, \end{cases}$$

[Related to Bessel Poly.]

  where $a_k = \frac{\lambda}{2k-1}$, and the recurrence relation of $\det \phi_N(\lambda)_{i,j}$.

Motivation II: Explicit FD + Spectral

- Consider the model problem

$$u_t = \mathcal{L}_x u \quad \Rightarrow \quad u(x,t) = e^{t\mathcal{L}_x} u_0(x), \qquad t \geq 0.$$

- Explicit FD in time by forward Euler + spectral collocation:

$$u^{n+1} = (1 + \tau \boldsymbol{D}) u^n = \cdots = (1 + \tau \boldsymbol{D})^{n+1} u^0.$$

  Stability essentially relies on the spectrum of $\boldsymbol{D}$!

[3] Trefethen-Trummer, An instability phenomenon in spectral methods, SINUM, 1987.

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- Parabolic: $\mathcal{L}_x = \partial_x^2$ with $|\lambda_{\min}| = O(1)$ and $|\lambda_{\max}| = O(N^4)$.
- Under-explored and problematic for IVP or hyperbolic: $\mathcal{L}_x = \partial_x$ (Dubiner'87, Tal-Ezer'86, Trefethen-Trummer'87[3]): CFL: Chebyshev: $O(N^{-2})$, special Legendre: $O(N^{-1})$, in practice (?)

[3] Trefethen-Trummer, An instability phenomenon in spectral methods, SINUM, 1987.

Precision-dependent instability

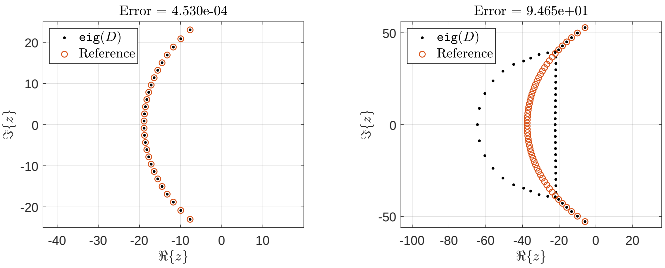


Figure 1: Eigenvalues distributions of the first-order differentiation matrix on Legendre points with $N = 28$ (left) and $N = 56$ (right). The red circles denote the reference values (multi-precision computation), and the black dots denote the eigenvalues computed in double precision. **Why?**

Topics to be addressed ......

- Legendre dual-Petrov-Galerkin (LDPG) spectral method in time for general mth-order IVPs.

- Eigenvalue distributions and eigenvectors of the related spectral matrices. [Bessel & generalised Bessel polynomials]

- Answer some open questions on spectrum of collocation matrix at Legendre points for 1st-order IVP in **Trefethen-Trummer'87**.

- LDPG spectral methods in time: Matrix Diagonalisation or QZ Decomposition. [Waves in oscillatory regions]

Outline

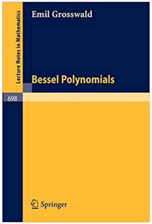
1. Motivations
2. **Bessel & Generalized Bessel Polynomials**
3. Eigenvalue Analysis for First-order IVP
4. Spectral Methods in Time

Generalized Bessel polynomials (GBPs)

Definition: For $\alpha, \beta \in \mathbb{C}, -\alpha \notin \mathbb{N}_0, \beta \neq 0$, the GBP: $B_n^{(\alpha,\beta)}(z), z \in \mathbb{C}$, is a polynomial of degree n that satisfies the 2nd-order ODE:

$$z^2 y''(z) + (\alpha z + \beta) y'(z) = n(n + \alpha - 1) y(z), \quad n \geq 0.$$

If $\alpha = \beta = 2$, $B_n(z) = B_n^{(2,2)}(z)$ is the Bessel polynomial of degree n.

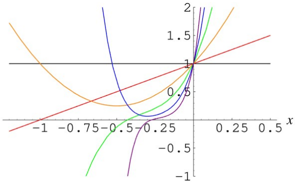


(1978)

Three-term recurrence relation:

$$\begin{cases} B_{n+1}^{(\alpha,\beta)}(z) = \left(a_n \dfrac{z}{\beta} + b_n\right) B_n^{(\alpha,\beta)}(z) + c_n B_{n-1}^{(\alpha,\beta)}(z), \quad n \geq 1, \\ B_0^{(\alpha,\beta)}(z) = 1, \quad B_1^{(\alpha,\beta)}(z) = 1 + \alpha \dfrac{z}{\beta}, \quad \text{where} \end{cases}$$

$$a_n = \frac{(2n+\alpha)(2n+\alpha-1)}{n+\alpha-1}; \; b_n = \frac{(\alpha-2)(2n+\alpha-1)}{(n+\alpha-1)(2n+\alpha-2)}; \; c_n = \frac{n(2n+\alpha)}{(n+\alpha-1)(2n+\alpha-2)}$$



First six Bessel polynomials

Series representation:

$$B_n^{(\alpha,\beta)}(z) = \sum_{k=0}^{n} \binom{n}{k} \frac{\Gamma(n+k+\alpha-1)}{\Gamma(n+\alpha-1)} \left(\frac{z}{\beta}\right)^k.$$

Note: β = scaling factor and wild behaviour of the coefficients!

- **Orthogonality** of GBPs:

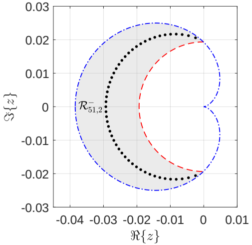
$$\frac{1}{2\pi\mathrm{i}} \int_{|z|=1} B_m^{(\alpha,\beta)}(z) B_n^{(\alpha,\beta)}(z) \rho^{(\alpha,\beta)}(z) \mathrm{d}z = \beta \gamma_n^{(\alpha)} \delta_{mn}, \quad \text{where}$$

$$\rho^{(\alpha,\beta)}(z) := \sum_{k=0}^{\infty} \frac{\Gamma(\alpha)}{\Gamma(k+\alpha-1)} \left(-\frac{\beta}{z}\right)^k = {}_1F_1(1, \alpha-1; -\beta/z).$$

- In particular, for $\alpha = \beta = 2$,

$$\frac{1}{2\pi\mathrm{i}} \int_{|z|=1} B_m(z) B_n(z) \mathrm{e}^{-2/z} \mathrm{d}z = (-1)^{n+1} \frac{2}{2n+1} \delta_{mn}$$

Zeros of GBPs[4]



Zeros of $B_{51}(x)$

Theorem 1 (Important!)

For $\alpha \in \mathbb{R}, n + \alpha - 1 > 0,$ *zeros* $\{z_j^{(\alpha)}\}_{j=1}^n$ *of* $B_n^{(\alpha)}(z) = B_n^{(\alpha,2)}(z)$ *(with* $\beta = 2$*) are*

(i) *Simple, conjugate pairs, and* $\Re\{z_j^{(\alpha)}\} < 0.$

(ii) *Located in the* **crescent-shaped** *region*

$$\mathcal{R}^-_{n,\alpha} := \Big\{ z = \rho e^{i\theta} \in \mathbb{C} : \frac{2}{2n + \alpha - \frac{2}{3}} < \rho \le \frac{1 - \cos\theta}{n + \alpha - 1},$$

$$\theta \in (-\pi, -\Theta_{n,\alpha}) \cup (\Theta_{n,\alpha}, \pi] \Big\}; \quad \Theta_{n,\alpha} := \arccos\left(\frac{-\alpha}{2n + \alpha - 2} \right).$$

- The zeros $|z_j^{(\alpha)}| \sim O(N^{-1})$.
- There is only one real negative zero for odd n.

[4] Bruin et al. On the zeros of generalized Bessel polynomials, I and II, 1981.

Outline

1. Motivations
2. Bessel & Generalized Bessel Polynomials
3. **Eigenvalue Analysis for First-order IVP**
4. Spectral Methods in Time

§1. LDPG scheme for first-order IVPs

- Consider the first-order IVP:

$$u'(t) = \sigma u(t), \quad t \in I := (-1,1); \quad u(-1) = u_0,$$

for given constants $\sigma \neq 0$ and $u_0 \neq 0$.

- The Legendre-dual Petrov-Galerkin (LDPG) scheme[5] is to

$$\begin{cases} \text{Find } u_N = u_0 + v_N \in \mathbb{P}_N \text{ with } v_N \in {}_0\mathbb{P}_N \text{ such that} \\ (v_N', \psi) - \sigma(v_N, \psi) = \sigma(u_0, \psi), \quad \forall \psi \in {}^0\mathbb{P}_N, \end{cases}$$

where the dual approximation spaces are

$${}_0\mathbb{P}_N := \{\phi \in \mathbb{P}_N : \phi(-1) = 0\}, \quad {}^0\mathbb{P}_N := \{\psi \in \mathbb{P}_N : \psi(1) = 0\}.$$

[5] Shen, SINUM'03; Shen-W., CMAME'07.

Key: Choice of basis polynomials

- Essential to choose the bases so that the derivative matrix is identity, that is, basis functions for $0 \le j, k \le N-1$,

$$\phi_k(t) = \frac{k+1}{\sqrt{2}}\big(P_k(t) + P_{k+1}(t)\big), \quad \psi_j(t) = \frac{1}{\sqrt{2}(j+1)}\big(P_j(t) - P_{j+1}(t)\big).$$

- **Linear system**

$$\big(\boldsymbol{I}_N - \sigma \boldsymbol{M}\big)\boldsymbol{v} = \sqrt{2}\sigma u_0 \boldsymbol{e}_1,$$

where the mass matrix is tri-diagonal with nonzero entries

$$\boldsymbol{M}_{jk} = (\phi_k, \psi_j) = \begin{cases} \dfrac{j}{(j+1)(2j+1)}, & k = j-1, \quad 1 \le j \le N-1, \\ \dfrac{1}{2j+1} - \dfrac{1}{2j+3}, & k = j, \quad 0 \le j \le N-1, \\ -\dfrac{j+2}{(j+1)(2j+3)}, & k = j+1, \quad 0 \le j \le N-2. \end{cases}$$

Key Observation

- Recall the three-term recurrence relation of GBPs $B_j^{(3)}(z)$:

$$\begin{cases} -zB_0^{(3)}(z) = \dfrac{2}{3}B_0^{(3)}(z) - \dfrac{2}{3}B_1^{(3)}(z), \\ -zB_j^{(3)}(z) = \dfrac{j}{(j+1)(2j+1)}B_{j-1}^{(3)}(z) + \dfrac{2}{(2j+1)(2j+3)}B_j^{(3)}(z) \\ \qquad\qquad\qquad - \dfrac{j+2}{(j+1)(2j+3)}B_{j+1}^{(3)}(z), \quad 1 \le j \le N-1. \end{cases}$$

- Matrix form

$$-z\boldsymbol{b}(z) = \boldsymbol{M}\boldsymbol{b}(z) - \frac{N+1}{N(2N+1)}B_N^{(3)}(z)\boldsymbol{e}_N, \quad \text{where}$$

$$\boldsymbol{b}(z) := \left(B_0^{(3)}(z), B_1^{(3)}(z), \cdots, B_{N-1}^{(3)}(z)\right)^{\top}$$

- Zeros of $B_N^{(3)}(z)$ satisfy

$$\boldsymbol{M}\boldsymbol{b}(z_j^{(3)}) = -z_j^{(3)}\boldsymbol{b}(z_j^{(3)}) \;\Rightarrow\; \lambda_j = -z_j^{(3)}, \quad \boldsymbol{v}_j = \boldsymbol{b}(z_j^{(3)}).$$

Theorem 2 (Kong-Shen-W.-Xiang'24)

The eigenvalues of $\boldsymbol{M}$ are $\lambda_j = -z_j^{(3)}$ with $\{z_j^{(3)}\}_{j=1}^N$ being zeros of the GBP: $B_N^{(3)}(z)$. They are simple and within the crescent-shaped region in the right half-plane

$$\lambda_j \in \mathcal{R}_{N,3}^+ := \left\{ z = \rho e^{i\theta} \in \mathbb{C} : \frac{1}{N + 7/6} < \rho \leq \frac{1 + \cos\theta}{N + 2}, \quad |\theta| < \pi - \Theta_{N,3} \right\}.$$

We can also find the eigenvectors: $\left\{ \boldsymbol{v}_j = \boldsymbol{b}(-\lambda_j^{(3)}) \right\}_{j=1}^N$.

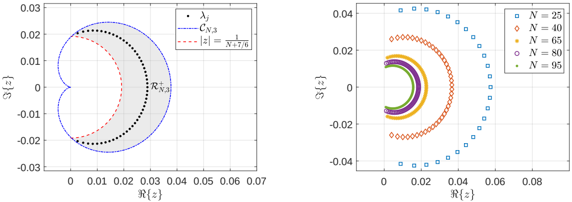


Figure 2: Eigenvalues of $\boldsymbol{M}$. Left: Distribution of $\lambda_j = \lambda_{N,j}$ with $N = 51$ in the crescent-shaped region (left). Right: Distributions of the eigenvalues with various N.

Important remarks

- Continuous "eigenvalue" problem:

$$u'(t) = \rho u(t), \quad t \in (-1, 1); \quad u(-1) = 0,$$

whose continuous spectrum is "empty"!

[6] Z. Zhang, How many numerical eigenvalues can we trust? JSC, 2015

Important remarks

- Continuous "eigenvalue" problem:

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whose continuous spectrum is "empty"!

- LDPG approximation:

$$\rho_N^{-1}\, \boldsymbol{u} = \boldsymbol{M}\, \boldsymbol{u},$$

whose discrete spectrum exist, since

$$\rho_{N,j} = \frac{1}{\lambda_{N,j}} = \frac{\bar{\lambda}_{N,j}}{|\lambda_{N,j}|^2}.$$

- This is different from the 2nd-order: $-u''(x) = \lambda u(x), u(\pm 1) = 0.$[6]

[6] Z. Zhang, How many numerical eigenvalues can we trust? JSC, 2015

§2. Collocation at Special Legendre Points

- Let $t_1 < t_2 < \cdots < t_N$ be Legendre-Gauss points (i.e., zeros of $P_N(t)$). **Collocate** at $\{-1\} \cup \{t_j\}_{j=1}^N$ (neither Radau nor Lobatto):

$$\begin{cases} \text{Find } u_N \in \mathbb{P}_N \text{ such that} \\ u_N'(t_j) = \sigma u_N(t_j), \quad 1 \le j \le N; \quad u_N(-1) = u_0. \end{cases}$$

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- **Linear system**:

$$\big(\boldsymbol{D} - \sigma \boldsymbol{I}_N\big)\,\boldsymbol{u} = -u_0\, \boldsymbol{h}_0',$$

where the spectral differentiation matrix $\boldsymbol{D} \in \mathbb{R}^{N\times N}$.

- **Trefethen-Trummer'87 & Tal-Ezer'86** claimed special Legendre points are better than other points: $|\lambda_j(\boldsymbol{D})| = O(N)$ (vs. $O(N^2)$), but eigen-pairs of $\boldsymbol{D}$ are unknown.

Equivalent Petrov-Galerkin Formulation

- Collocation is equivalent to the Petrov-Galerkin scheme

$$\begin{cases} \text{Find } \ u_N = u_0 + v_N \in \mathbb{P}_N \ \text{ with } \ v_N \in {}_0\mathbb{P}_N \ \text{ s.t.} \\ (v_N', \psi) - \sigma(v_N, \psi) = \sigma(u_0, \psi), \quad \forall \psi \in \mathbb{P}_{N-1}. \end{cases}$$

- Choose the bases so that the derivative matrix is identity:

$$\left(\boldsymbol{I}_N - \sigma \overline{\boldsymbol{M}}\right) \bar{\boldsymbol{v}} = \sqrt{2}\sigma\, u_0\, \boldsymbol{e}_1,$$

where $\overline{\boldsymbol{M}}$ is tri-diagonal with nonzero entries

$$\overline{\boldsymbol{M}}_{jk} = \begin{cases} 1, & k = j = 0, \\ -\dfrac{1}{2j+1}, & k = j+1, \\ \dfrac{1}{2j+1}, & k = j-1. \end{cases}$$

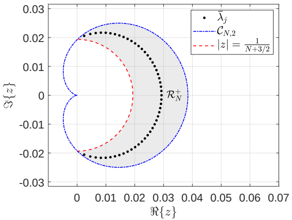
Eigenvalue distributions of $\overline{\boldsymbol{M}}$ and $\boldsymbol{D}$

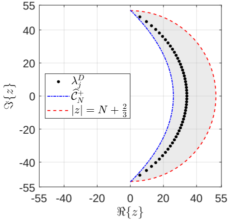
Theorem 3

- $\{-\lambda_j(\overline{\boldsymbol{M}})\}_{j=1}^{N}$ *are zeroes of the BP: $B_N(z)$ so that are simple and lie in a crescent-shaped region:*

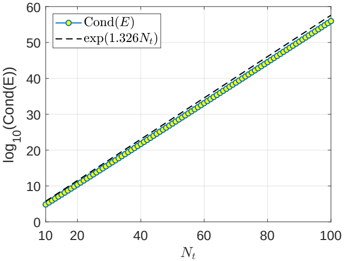
$$\lambda_j(\overline{\boldsymbol{M}}) \in \mathcal{R}_N^+ := \left\{ z = \rho e^{i\theta} \in \mathbb{C} : \frac{1}{N+2/3} < \rho \le \frac{1+\cos\theta}{N+1}, \quad |\theta| < \pi - \Theta_{N,2} \right\}.$$

- *Collocation matrix $\boldsymbol{D}$ is similar to $\overline{\boldsymbol{M}}^{-1}$, so $\lambda_j^{\boldsymbol{D}} = (\lambda_j(\overline{\boldsymbol{M}}))^{-1}$.*
- *Eigenvectors are in term of $\{B_k(-\lambda_j(\overline{\boldsymbol{M}}))\}_{k=0}^{N-1}$.*





- **Why precision instability?** Computing eigenvalues based on the matrix, e.g., `eig()`, is stable for small $N \leq 28$. Eigenvectors are badly behaved.



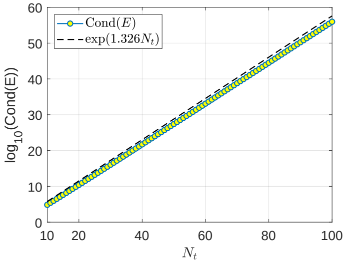
Conditioning of eigenvector matrix

Results for Higher-order IVPs

Order	Method	Eigenvalues
$m = 1$	LDPG	$\{-\lambda_i\}$ are N zeros of $B_N^{(3)}(z)$
	LPG	$\{-\bar{\lambda}_i\}$ are N zeros of $B_N(z)$
	Collocation	$\{-\lambda_i^D = -(\bar{\lambda}_i)^{-1}\}$
$m = 2$	Pseudo-spectral	$\{\mu_i = (z_i^{(4)})^2\}$ with $\{z_i^{(4)}\}$ being N zeros of $B_N^{(4)}(z)$
$m \geq 1$	First-order system	$\{(-\lambda_i)^m\}$
$m \geq 3$	LDPG	Approximate characterisation

Computing eigenvalues for large N

- **Why?** Computing eigenvalues based on the matrix, e.g., `eig()`, is stable for small N and precision-dependent. Eigenvectors are badly behaved.



Conditioning of eigenvector matrix

- Computing GBPs and the zeros are necessary!

Algorithms for computing zeros of GBPs

(1) Pasquini's algorithm (Numer. Math'00) based on iterative methods for nonlinear system obtained from a suitable reformulation of the second-order ODE of GBPs.

(2) Segura's algorithm (Numer. Math'13) based on analytic analysis of the second-order ODE and the connections with Laguerre functions.

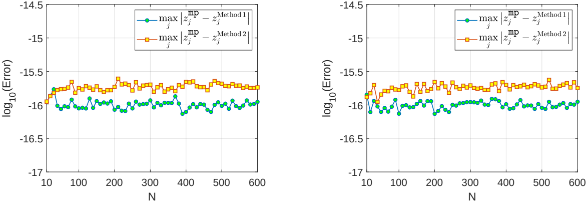


Figure 3: Method 1 and Method 2 (with double precision) and reference values (with multiple precision) for $\alpha = 2$ (left) and $\alpha = 4$ (right).

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4. **Spectral Methods in Time**

Why? Pros & Cons

- Many evolutionary PDEs requires high resolution in time, e.g., oscillatory wave propagations.
- Match with high-order accuracy of spectral methods in space, e.g., for some benchmark simulations.
- However, a spectral method in time is fully and globally implicit. Strategies to alleviate the burden:
  - Matrix-diagonalization in time
  - QZ decomposition in time
  - Suitable iterative solvers for nonlinear problems (inexact Newton's iteration?)

LDPG method in time: A general setup

- Consider the prototype system of first linear ODEs:

$$\boldsymbol{u}_t + \boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}(t), \quad t \in (-1, 1); \quad \boldsymbol{u}(-1) = \boldsymbol{u}_0,$$

  where $\boldsymbol{A}$ is a matrix resulted from a spatial discretization.

- Employ the LDPG method in time:

$$\left(\boldsymbol{I}_t \otimes \boldsymbol{I}_x + \boldsymbol{M}_t \otimes \boldsymbol{A}\right)\hat{\boldsymbol{u}} = \hat{\boldsymbol{f}},$$

  or

$$\boldsymbol{U} + \boldsymbol{M}_t \boldsymbol{U}\boldsymbol{A} = \boldsymbol{F}.$$

- Equipped with the eigenvalue distributions, we now deal with the time direction.

Important remarks[7]

Theorem 4

The scheme

$$\boldsymbol{u}_N' + \boldsymbol{A}\mathcal{P}_{N-1}\boldsymbol{u}_N = \mathcal{P}_{N-1}\boldsymbol{f}, \quad \boldsymbol{u}_N(-1) = \boldsymbol{u}_0,$$

by testing with $(1-t^2)P_j'(t)$ *is equivalent to the* **LPG** *scheme, and thus to the* **collocation** *scheme at Gauss points.*

- Formulating as LPG scheme, one can simplify the computation of the adjugate matrix and the solution formula.
- Chen-Liu'24 showed that the scheme is unconditionally stable and there exists hp superconvergence.
- **Con:** The adjugate matrix is ill-conditioned.

[7] Chen-Liu, SISC'24

I. Matrix diagonalisation + multiple domain

- Diagonalise $\boldsymbol{M}_t$:

$$\boldsymbol{E} = (\boldsymbol{v}_1, \cdots, \boldsymbol{v}_{N_t}), \quad \boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \cdots, \lambda_{N_t}), \quad \text{so} \quad \boldsymbol{M}_t\boldsymbol{E} = \boldsymbol{E}\boldsymbol{\Lambda},$$

- Substitute $\boldsymbol{U} = \boldsymbol{E}\boldsymbol{V}$:

$$\boldsymbol{V} + \boldsymbol{\Lambda}\boldsymbol{V}\boldsymbol{A} = \boldsymbol{E}^{-1}\boldsymbol{F} =: \boldsymbol{G}.$$

- Decouple and solve the system in space:

$$\left(\boldsymbol{I}_x + \lambda_j\boldsymbol{A}\right)\boldsymbol{v}_j = \boldsymbol{G}_j, \quad 1 \le j \le N_t,$$

  which can be solved in parallel for each j.

- **Con:** The involvement of $\boldsymbol{E}^{-1}$. It is stable for small N_t and should implement sequentially in multiple sub-domains.

2. QZ decomposition

Definition 5 (QZ decomposition)

Given square matrices $\boldsymbol{A}, \boldsymbol{B}$, the QZ decomposition is

$$\boldsymbol{QAZ} = \boldsymbol{S}, \quad \boldsymbol{QBZ} = \boldsymbol{T},$$

where $\boldsymbol{Q}$ and $\boldsymbol{Z}$ are unitary (i.e., $\boldsymbol{Q}^{-1} = \boldsymbol{Q}^{\mathrm{H}}, \boldsymbol{Z}^{-1} = \boldsymbol{Z}^{\mathrm{H}}$, where $\boldsymbol{Q}^{\mathrm{H}}$ is the conjugate transpose of $\boldsymbol{Q}$), and $\boldsymbol{S}$ and $\boldsymbol{T}$ are upper triangular.

- Set $\boldsymbol{A} = \boldsymbol{I}_t$ and $\boldsymbol{B} = \boldsymbol{M}_t$. Substitute $\boldsymbol{U} = \boldsymbol{ZW}$:

$$\boldsymbol{SW} + \boldsymbol{TWA} = \boldsymbol{QF} =: \boldsymbol{G}.$$

- Backward substitution: for $j = N_t - 1, \cdots, 1$ and $\boldsymbol{r}_{N_t} = \boldsymbol{0}$,

$$\boldsymbol{w}_j\left(S_{jj}\boldsymbol{I}_x + T_{jj}\boldsymbol{A}\right) = \boldsymbol{G}_j - \boldsymbol{r}_j, \quad \boldsymbol{r}_j = \sum_{k=j+1}^{N_t} \boldsymbol{w}_k\left(S_{jk}\boldsymbol{I}_x + T_{jk}\boldsymbol{A}\right)$$

- **Pro:** Stable for large N_t, and can be assembled into a multiple domain approach. [Shen-Sheng'19, time-fractional]

Applications: Wave-type equation

- Consider the linear DE:

$$\partial_{xt}^2 u(x,t) + \sigma u(x,t) = 0, \quad x \in \mathbb{R}, \quad t > 0, \quad \sigma \neq 0. \tag{2}$$

Remark: It is related to the linear Kadomtsev-Petviashvili (KP) model:

$$\partial_x(\partial_t U(x,y,t) + \epsilon^2 \partial_x^3 U(x,y,t)) + \sigma \partial_y^2 U(x,y,t) = 0,$$

which can be interpreted as a linear KdV with (2) as input.

- **One-sided propagation**: If $\sigma > 0$ and $u_0(x)$ is compactly supported in (x_0, ∞), then $u(x,t) = 0, \forall\, x < x_0,\ t > 0$.

Space-time LDPG methods

- For $\sigma > 0$, we can set homogenous BC at left-side, leading to

$$\begin{cases} \partial_{xt}^2 u(x,t) + \sigma u(x,t) = 0, & x \in \Omega := (x_L, x_R), \;\; t \in (0,T], \\ u(x,0) = u_0(x), \;\; x \in \Omega; & u(x_L,t) = 0, \;\; t \in [0,T]. \end{cases}$$

- **Spectral scheme**:

$$\begin{cases} \text{Find } u_N(x,t) = u_0(x) + v_N(x,t) \text{ with } v_N \in {}_0X_N \text{ s.t.} \\ (\partial_{xt}^2 v_N, \psi) + \sigma(v_N, \psi) = -\sigma(u_0, \psi), \quad \forall \psi \in {}^0X_N, \end{cases}$$

where

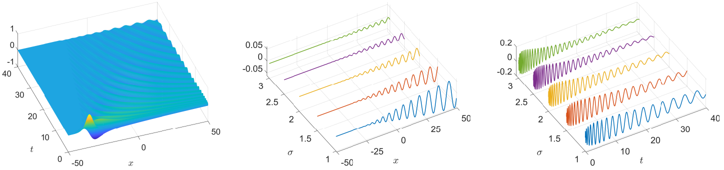
$${}_0X_N = {}_0\mathbb{P}_{N_t} \times {}_0\mathbb{P}_{N_x}, \quad {}^0X_N = {}^0\mathbb{P}_{N_t} \times {}^0\mathbb{P}_{N_x}, \quad N = (N_t, N_x).$$

- Use matrix diagonalization or QZ-decomposition in time.

Numerical results

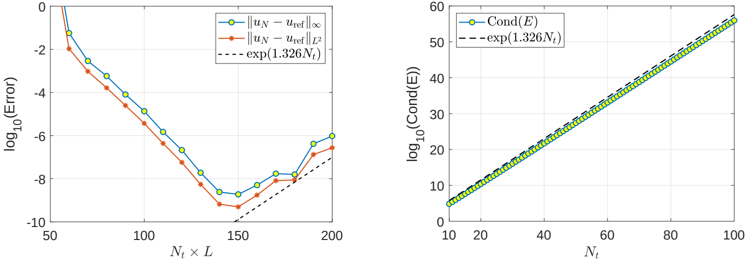
Choose the initial input

$$u_0(x) = \text{sech}^2\left(\sqrt{3}(x+35)/6\right) - \text{sech}^2(5\sqrt{3}/2), \quad x \in \Omega = (-50, 50).$$



(a) $u_N(x,t)$ with $\sigma = 1$ (b) $u_N(x,40)$ with different σ (c) $u_N(50,t)$ with different σ

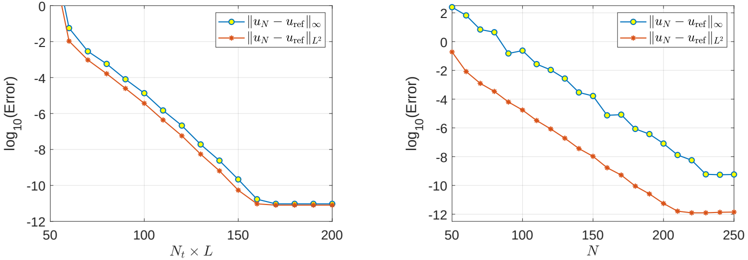
Figure 4: Numerical solutions $u_N(x,t)$ with $N_x = N_t = 400$ and different values of the parameter σ. (a) Numerical solution with $\sigma = 1$; (b)-(c) Profiles of the numerical solution at fixed t or x but with different σ.



(a) Diagonalisation (multi-domain in t)

(b) Conditioning of $\boldsymbol{E}$

Figure 5: Convergence of space-time spectral methods (a) Diagonalisation technique with $L = 10$ sub-domains for $t \in [0, 40]$; and conditioning of the eigenvector matrix (in (b)).



(a) QZ (multi-domain in t)

(b) QZ (single domain in t)

Figure 6: (a) QZ decomposition with a multi-domain implementation: $L = 10$ subintervals of $t \in [0, 40]$ with various $N_t \in [5, 20]$ and $N_x = 400$. (b) Single domain space-time spectral method with various $N = N_t = N_x$.

Well-conditioned system in space

Table 1: Conditioning and eigenvalues of $\boldsymbol{A} = \boldsymbol{I}_{N_x} + \boldsymbol{M}_x$.

N_x	20	30	40	50	100	200
Cond($\boldsymbol{A}$)	1.8730	1.8730	1.8730	1.8730	1.8730	1.8730
$\min_j \lvert\lambda_j^{\boldsymbol{A}}\rvert$	1.0143	1.0071	1.0043	1.0029	1.0009	1.0003
$\max_j \lvert\lambda_j^{\boldsymbol{A}}\rvert$	1.0708	1.0513	1.0539	1.0533	1.0513	1.0514

Application: KdV-type equation

As a second example, we apply the space-time LDPG method to the KdV-type equation:

$$\begin{cases} \partial_t U + \alpha U \partial_x U + \epsilon^2 \partial_x^3 U + \sigma \partial_x^{-1} U = 0, & x \in \Omega := (x_L, x_R), \quad t > 0, \\ U(x_L, t) = U(x_R, t) = \partial_x U(x_R, t) = 0, & t \geq 0, \\ U(x, 0) = U_0(x), & x \in \bar{\Omega}, \end{cases} \tag{3}$$

where $\alpha \geq 0, \epsilon > 0$ and $\sigma \neq 0$ are constants, and

$$\partial_x^{-1} U(x,t) = \frac{1}{2}\Big(\int_{x_L}^{x} U(y,t)\mathrm{d}y - \int_{x}^{x_R} U(y,t)\mathrm{d}y \Big).$$

Note: It is resulted from integrating the nonlinear KP-equation:

$$\partial_x\big(\partial_t U(x,t) + \alpha U \partial_x U + \epsilon^2 \partial_x^3 U(x,t)\big) + \sigma U(x,t) = 0.$$

Numerical results

Choose the initial condition given by

$$U_0(x) = \text{sech}^2\big(\sqrt{3}(x+5)/6\big), \quad x \in \Omega = (-50, 50), \tag{4}$$

taken from the exact soliton solution of the KdV equation:

$$U(x,t) = \text{sech}^2\big(\sqrt{3}(x - t/3 + 5)/6\big).$$

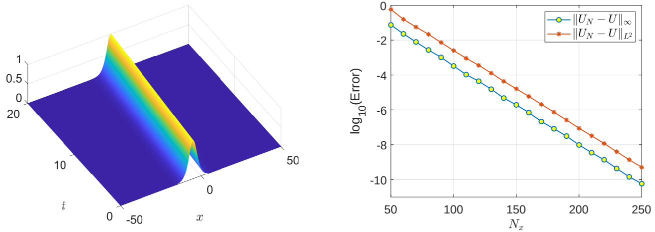
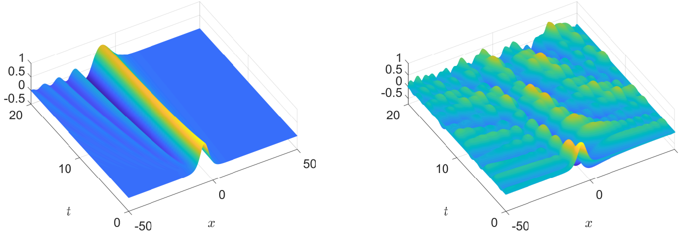


Figure 7: Left: numerical solution $u_N(x,t)$ (with $N_x = 250, N_t = 80$) of the KdV equation. Right: Errors against $N_x = 50:10:250$ and fixed $N_t = 80$ in semi-log scale.



(a) Linear KdV (b) KdV with a nonlocal term

Figure 8: Numerical solution with $N_x = 250, N_t = 80$ and the initial input $U_0(x)$ given in (4). (a) Linear KdV equation (i.e.„ (3) with $\epsilon = 1$ and $\alpha = \sigma = 0$). (b) KdV-type equation with a nonlocal term (i.e., (3) with $\alpha = 0, \epsilon = 1$ and $\sigma = 0.1$).

Summary

- We showed for the first time that the eigen-pairs of spectral matrix resulted from the LDPG methods for IVPs cab be exactly or approximately characterized by the GBPs.
- The findings provided fundamental insights into spectral methods in time. PinT may not be practical in the context of spectral methods, but QZ decomposition is the method of choice.

THANK YOU!