KU LEUVEN

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Orthogonal systems with a skew-symmetric differentiation matrix

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Preprint available at both authors' websites.

Motivation

Time-dependent PDEs on the real line, $u(t,x)$, $t \in [0,\infty)$, $x \in \mathbb{R}$.

Diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(a(t,x,u)\frac{\partial u}{\partial x}\right), \qquad a \geq 0$$

Semi-classical Schrödinger

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\varepsilon^2\frac{\partial^2 u}{\partial x^2} + V(t,x,u)u, \qquad 0 < \varepsilon \ll 1, \quad \mathrm{Imag}(V) = 0$$

Nonlinear advection equation

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} + f(u), \qquad v \cdot f(v) \leq 0$$

For the solutions to these PDEs, the $\mathrm{L}_2(\mathbb{R})$ norm is nonincreasing or preserved:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty} |u(t,x)|^2\,\mathrm{d}x \leq 0, \text{ for all } t \geq 0.$$

Can we design numerical methods which respect this L_2 **stability property**?

The importance of being skew-symmetric

Spectral methods: Take an orthonormal basis $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+}$ of $\mathrm{L}_2(\mathbb{R})$, and represent the solution by

$$u(t,\cdot) = \sum_{n=0}^{\infty} u_n(t)\varphi_n$$

Semi-discretised equations: The PDE in question is equivalent to an ODE for the coefficients $\mathbf{u} = (u_0, u_1, \ldots)$,

$$\mathbf{u}'(t) = \mathcal{D}\mathcal{A}\mathcal{D}\mathbf{u}(t)$$

$$\mathrm{i}\varepsilon\mathbf{u}'(t) = -\varepsilon^2\mathcal{D}^2\mathbf{u}(t) + \mathcal{V}\mathbf{u}(t),$$

$$\mathbf{u}'(t) = \mathcal{D}\mathbf{u}(t) + \mathbf{f}(\mathbf{u}(t)) \qquad \text{(where } f_m(\mathbf{u}) = \langle\varphi_m, f(u(t,\cdot))\rangle\text{)}$$

Differentiation matrix: $\mathcal{D}$ is an infinite-dimensional matrix encoding differentiation, and $\mathcal{A}$ is this for multiplication by a,

$$\varphi_k'(x) = \sum_{j=0}^{\infty} D_{k,j}\varphi_j(x), \qquad a(x)\varphi_k(x) = \sum_{j=0}^{\infty} A_{k,j}\varphi_j(x).$$

Discrete stability: The orthonormality of Φ ensures $\|u(t,\cdot)\|_{\mathrm{L}_2(\mathbb{R})} = \|\mathbf{u}(t)\|_{\ell_2}$. For nonlinear advection, we have

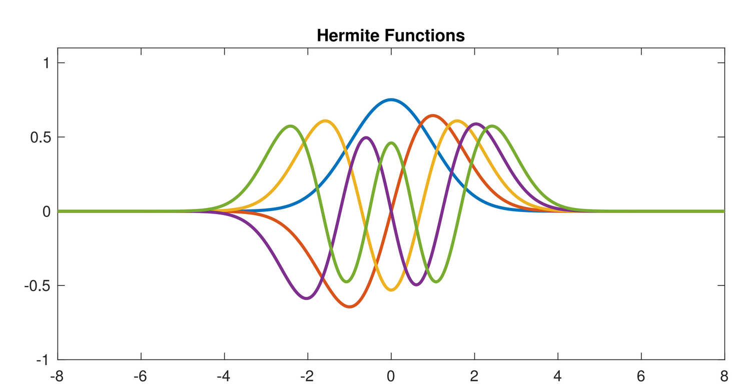
$$\frac{\mathrm{d}\|\mathbf{u}\|_{\ell^2}^2}{\mathrm{d}t} = 2\mathbf{u}^T\mathbf{u}' = 2\mathbf{u}^T\mathcal{D}\mathbf{u} + 2\mathbf{u}^T\mathbf{f}(\mathbf{u}) \leq 2\mathbf{u}^T\mathcal{D}\mathbf{u},$$

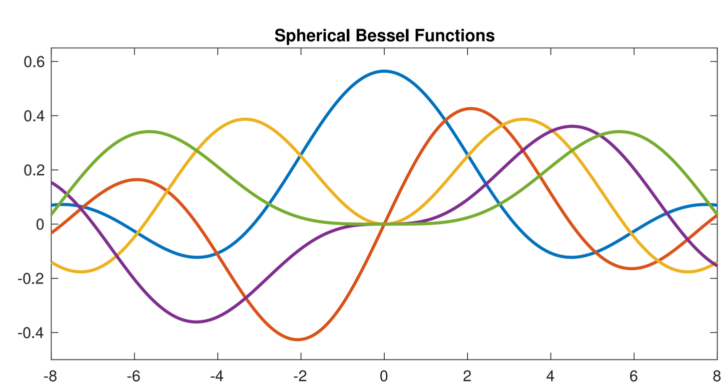
and similar for diffusion and Schrödinger. We see, ℓ_2 **stability is achieved if** $\mathcal{D}$ **is skew-symmetric**, mimicking the differentiation operator itself.

Finite difference methods with skew-symmetric differentiation matrices yield analogous applications to Dirichlet problems on an interval, see Iserles 2014, 2016 and Hairer-Iserles 2015, 2016.

Previously known examples

- For periodic boundary conditions, the humble **Fourier basis** works perfectly: $\varphi_0(x) \equiv \frac{1}{(2\pi)^{1/2}}$, $\varphi_{2n}(x) = \frac{\cos nx}{\pi^{1/2}}$, $\varphi_{2n+1}(x) = \frac{\sin nx}{\pi^{1/2}}$
- The **Hermite functions**, $\varphi_n(x) = \frac{(-1)^n}{(2^n n!)^{1/2}\pi^{1/4}}\mathrm{e}^{-x^2/2}\mathrm{H}_n(x)$ are well-known to satisfy $\varphi_n'(x) = \sqrt{\frac{n}{2}}\varphi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\varphi_{n+1}(x)$
- Scaled **spherical Bessel functions** $\varphi_n(x) = (n+1/2)^{1/2}\,\mathrm{j}_n(x)$ also meet our requirements





Main theorems

Theorem 1 (Iserles-Webb 2018) A sequence $\Phi = \{\varphi_n\}_{n\in\mathbb{Z}_+}$ has a real, skew-symmetric, tridiagonal, irreducible, differentiation matrix if and only if

$$\varphi_n(x) = \frac{(-\mathrm{i})^n}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}x\xi}\,p_n(\xi)\,g(\xi)\,\mathrm{d}\xi,$$

where $P = \{p_n\}_{n\in\mathbb{Z}_+}$ is an orthonormal polynomial system on the real line with respect to a symmetric probability measure $\mathrm{d}\mu$, and $g(\xi) = \frac{1}{\sqrt{2\pi}}\int \mathrm{e}^{-\mathrm{i}x\xi}\,\varphi_0(x)\,\mathrm{d}x$.

Sketch of proof: Since $\mathcal{F}[\varphi'](\xi) = -\mathrm{i}\xi\mathcal{F}[\varphi]$,

$$\begin{aligned} \xi p_n(\xi) &= b_{n-1}p_{n-1}(\xi) + b_n p_{n+1}(\xi) \\ \Longleftrightarrow \quad \varphi_n'(x) &= -b_{n-1}\varphi_{n-1}(x) + b_n\varphi_{n+1}(x). \end{aligned}$$

Theorem 2 (Iserles-Webb 2018) Such sequences Φ are orthonormal in $\mathrm{L}_2(\mathbb{R})$ if and only if $\mathrm{d}\mu(\xi) = |g(\xi)|^2\,\mathrm{d}\xi$.

Proof: Parseval's Theorem implies $\langle\varphi_m, \varphi_n\rangle = (-\mathrm{i})^{n-m}\int p_n(\xi)p_m(\xi)|g(\xi)|^2\,\mathrm{d}\xi$.

Theorem 3 (Iserles-Webb 2018) If polynomials are dense in $\mathrm{L}_2(\mathbb{R},\mathrm{d}\mu)$, then such orthonormal sequences are complete in the Paley-Wiener space $\mathrm{PW}_\Omega(\mathbb{R})$, where $\Omega = \mathrm{supp}(\mathrm{d}\mu)$.

Remark: **Spherical Bessel functions** and **Hermite functions** are derived by Fourier transforms of **Legendre polynomials** and **Hermite functions** (resp.)!

New examples

Chebyshev polynomials (2nd kind)

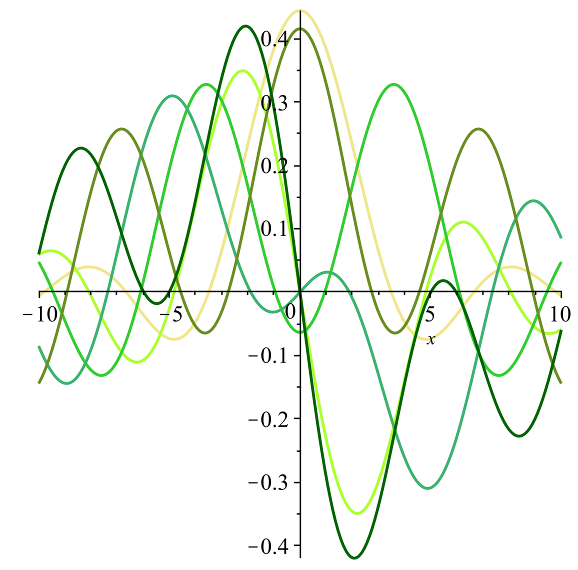
$\mathrm{d}\mu(\xi) = \chi_{[-1,1]}(\xi)\sqrt{1-\xi^2}\mathrm{d}\xi$

$b_n = \frac{1}{2}$ for all $n \in \mathbb{Z}_+$

$\varphi_0(x) \propto \int_{-1}^{1}(1-\xi^2)^{1/4}\,\mathrm{e}^{\mathrm{i}x\xi}\mathrm{d}\xi \propto \frac{\mathrm{J}_1(x)}{x}$

$\varphi_1(x) \propto \int_{-1}^{1}\xi\,(1-\xi^2)^{1/4}\,\mathrm{e}^{\mathrm{i}x\xi}\mathrm{d}\xi \propto \frac{\mathrm{J}_2(x)}{x}$

φ_2 is more complicated...



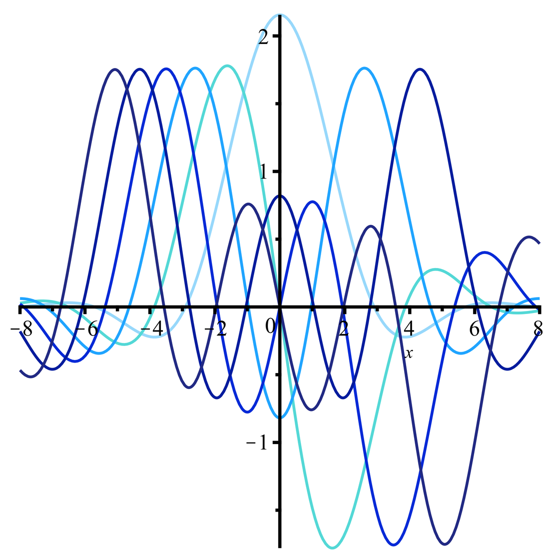
Freud polynomials (basic)

$\mathrm{d}\mu(\xi) = e^{-t^4}\,\mathrm{d}\mu(\xi)$

Recursion for b_n known

$$\varphi_0(x) \propto 2\pi\,{}_0F_2\left[\begin{matrix} -; \\ \frac{1}{2}, \frac{3}{4}; \end{matrix}\ \frac{x^4}{128}\right] - x^2\Gamma^2\left(\tfrac{3}{4}\right){}_0F_2\left[\begin{matrix} -; \\ \frac{5}{4}, \frac{3}{2}; \end{matrix}\ \frac{x^4}{128}\right]$$

φ_1 is more complicated...



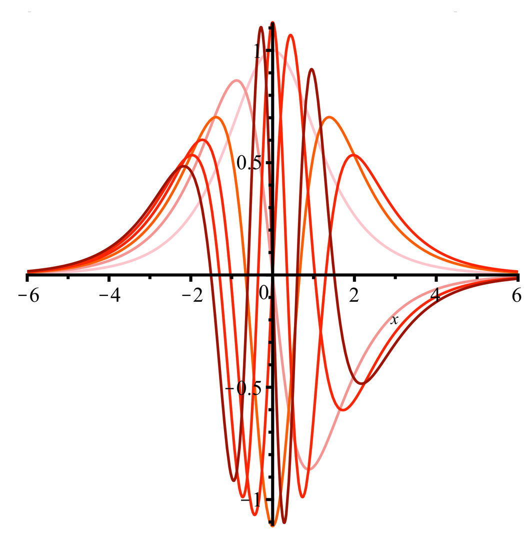
Carlitz polynomials (modified)

$\mathrm{d}\mu = \mathrm{sech}^2(\pi\xi)\,\mathrm{d}\xi$

$\varphi_0(x) = \mathrm{sech}(x)$

$\varphi_1(x) = -\sqrt{3}\tanh(x)\mathrm{sech}(x)$

$\varphi_2(x) = \frac{\sqrt{5}}{2}\left(2\mathrm{sech}(x) - 3\mathrm{sech}^3(x)\right)$



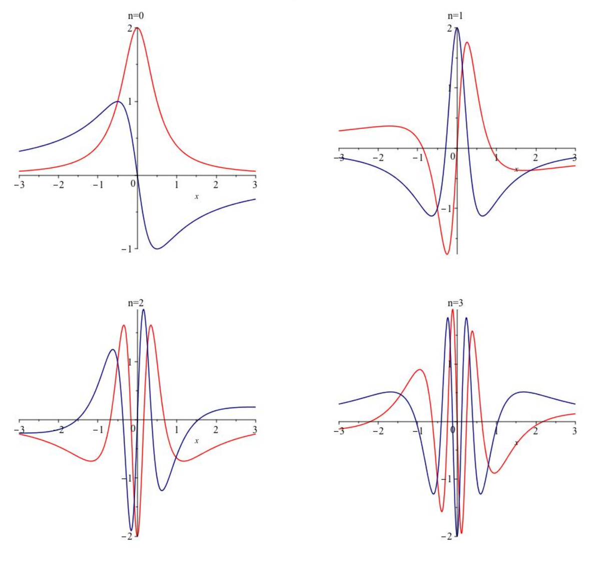
Laguerre polynomials

$\mathrm{d}\mu(\xi) = \chi_{[0,\infty)}(\xi)\mathrm{e}^{-\xi}\,\mathrm{d}\xi$

$\varphi_n(x) = \mathrm{i}^n\frac{(1-2\mathrm{i}x)^n}{(1+2\mathrm{i}x)^{n+1}}$

$\varphi_n' = -n\varphi_{n-1} + \mathrm{i}(2n+1)\varphi_n + (n+1)\varphi_{n+1}$

Nonsymmetric $\mu \implies$ skew-Hermitian $\mathcal{D}$



Directions for this research

- Computation and convergence for approximating functions in Φ bases
- Interesting special features of $\varphi_n(x)$? E.g. interlacing roots
- Can functions of $\mathcal{D}$ be effectively approximated?
- Can new, improved, practical, L_2 stable spectral methods for time-dependent PDEs be developed following this work?

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