Spectral methods for time-dependent PDEs

Summer Research in Mathematics

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Outline

What is a spectral method?

Consider the time-dependent problem

$$\frac{\partial u}{\partial t} = \mathcal{L}u + f, \quad t \geq 0, \quad x \in \Omega,$$

where $\mathcal{L}$ is a well-posed differential operator, with suitable initial and boundary conditions.

A spectral method is determined by an orthonormal basis $\Phi = \{\varphi_n\}_{n \in \mathbb{Z}_+}$ of the underlying Hilbert space. The solution of the PDE is expressed as

$$u(x,t) = \sum_{n=0}^{\infty} \hat{u}_n(t)\varphi_n(x),$$

where the evolution of the coefficients $\hat{u}_n(t)$ is obtained from the Galerkin conditions

$$\hat{u}_n' = \sum_{m=0}^{\infty} \langle \mathcal{L}\varphi_m, \varphi_n \rangle \hat{u}_m + \langle f, \varphi_n \rangle.$$

Desired properties of Φ

1. **Stability** The truncated ODE systems must be uniformly well posed as $N \to \infty$. This guarantees the convergence of the finite-dimensional solutions the solution of the PDE.
2. **Speed of convergence** We want $\hat{u}_n \to 0$ rapidly for all $n \gg 1$ as $n \to \infty$.
3. **Geometric numerical integration** The approximate solution must preserve qualitative features of the solution, in particular, dissipativity (diffusion equation, nonlinear advection equation) and mass conservation (linear Schrödinger equation).
4. **Low numerical cost** This largely depends on fast expansion in the basis Φ and fast linear algebra.

The differentiation matrix

Given a complete orthonormal system Φ, a differentiation matrix $\mathcal{D}$ is a linear map taking the vector $\boldsymbol{\varphi} = \{\varphi_n\}_{n\in\mathbb{Z}_+}$ to its derivative $\boldsymbol{\varphi'} = \{\varphi'_n\}_{n\in\mathbb{Z}_+}$. In other words,

$$\varphi'_m = \sum_{n=0}^{\infty} \mathcal{D}_{m,n}\varphi_n, \quad m \in \mathbb{Z}_+.$$

T-systems

An orthonormal system Φ is said to be a **T-system** if the differentiation matrix is skew-Hermitian and tridiagonal, in other words,

$$\varphi_n' = -b_{n-1}\varphi_{n-1} + ic_n\varphi_n + b_n\varphi_{n+1}, \quad n \in \mathbb{Z}_+,$$

where $c_n \in \mathbb{R}$, $b_n > 0$ for $n \in \mathbb{Z}_+$.
It is possible to map $\{\varphi_n\}_{n\in\mathbb{Z}_+}$ into a set $\{p_n\}_{n\in\mathbb{Z}_+}$ of polynomials which are orthogonal with respect to some symmetric measure $d\mu(x) = w(x)dx$.
We recover $\{\varphi_n\}_{n\in\mathbb{Z}_+}$ as follows.

Theorem (Iserles, Webb)

The system $\Phi = \{\varphi\}_{n=0}^{\infty}$ given by

$$\varphi_n = \frac{i^n}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p_n(\xi) g(\xi) e^{i\xi x} d\xi, \quad n \in \mathbb{Z}_+,$$

is a complete orthonormal system if $|g(\xi)| = \sqrt{w(\xi)}$ and $\operatorname{supp} w = \mathbb{R}$.

Example 1: Spherical Bessel functions

The Legendre measure $d\mu(\xi) = \chi_{(-1,1)}(\xi)d\xi$, $p_n(\xi) = \frac{P_n(\xi)}{\sqrt{n+\frac{1}{2}}}$, where $\{P_n(\xi)\}$ are the Legendre polynomials, and $g(\xi) \equiv 1$ give rise to

$$\varphi_n(x) = \frac{\sqrt{n+\frac{1}{2}}}{x} J_{n+\frac{1}{2}}(x), \quad n \in \mathbb{Z}_+,$$

the spherical Bessel functions.

Example 2: Hermite functions

The Hermite measure $d\mu(\xi) = e^{-\xi^2} d\xi$, scaled Hermite polynomials $p_n(\xi) = \frac{H_n(\xi)}{\sqrt{2^n n! \sqrt{\pi}}}$ and $g(\xi) = e^{-\xi^2/2}$ give rise to

$$\varphi_n(x) = \frac{H_n(x)}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2}, \quad n \in \mathbb{Z}_+,$$

the Hermite functions.

Example 3: Malmquist-Takenaka functions

We begin with the Laguerre measure $d\mu(\xi) = e^{-\xi}\chi_{[0,\infty)}d\xi$, Laguerre polynomials $p_n(\xi) = L_n(\xi)$ and $g(\xi) = e^{-\xi/2}$. To extend the closure of $\{\varphi_n\}_{n\in\mathbb{Z}_+}$ to $L_2(\mathbb{R})$, we combine it with the mirror weight $e^{\xi}\chi_{(-\infty,0]}$, which corresponds to $p_n(\xi) = L_n(-\xi)$. This gives the Malmquist-Takenaka functions

$$\varphi_n(x) = \sqrt{\frac{2}{\pi}} i^n \frac{(1+2ix)^2}{(1-2ix)^{n+1}}, \quad n \in \mathbb{Z},$$

where $b_n = n+1$ and $c_n = 2n+1$, $n \in \mathbb{Z}$.
An appealing feature of MT functions is that the coefficients can be computed fast with FFT

$$\hat{f}_n = \int_{-\infty}^{\infty} f(x)\overline{\varphi_n(x)}dx = \frac{(-i)^n}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \left(1 - i\tan\frac{\theta}{2}\right) f\left(\frac{1}{2}\tan\frac{\theta}{2}\right) e^{-in\theta} d\theta.$$

Speed of convergence

Convergence of orthogonal polynomials to an analytic function in a compact interval, say $[-1, 1]$, is well understood.

Theorem (Bernstein)

If f can be analytically extended from $[-1, 1]$ to the Bernstein ellipse $\{\rho e^{i\theta} + \rho^{-1} e^{-i\theta} : \theta \in [-\pi, \pi)\}$ for some $\rho > 1$, then

$$\hat{f}_n = \mathcal{O}(\rho^{-n}), \quad n \gg 1.$$

Corollary

Suppose f is analytic at infinity and in the strip

$$\mathscr{S}_\gamma = \{z \in \mathbb{C} : |\mathrm{Im}\, z| \leq \gamma\}.$$

Then the MT expansion coefficients $\hat{f}_n$ exhibit geometric convergence.

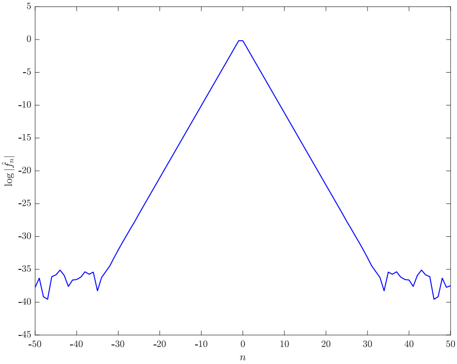
However, this does not generally work in the application of T-systems to the real line.

Convergence of Malmquist-Takenaka

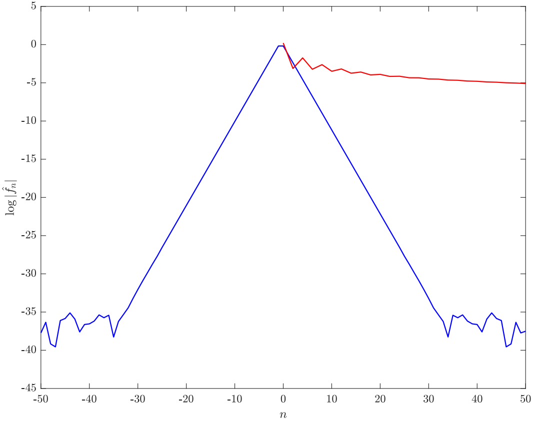
Consider $f(x) = \frac{1}{1+x^2}$. We can expand it explicitly in the MT basis as

$$\frac{1}{1+x^2} = -\sqrt{2\pi}\sum_{n=0}^{\infty} \frac{i^{-n-1}}{3^{n+1}}\varphi_{-n-1}(x) + \sqrt{2\pi}\sum_{n=0}^{\infty} \frac{i^{n}}{3^{n+1}}\varphi_{n}(x),$$

and we have geometric convergence with $\rho = 3$.

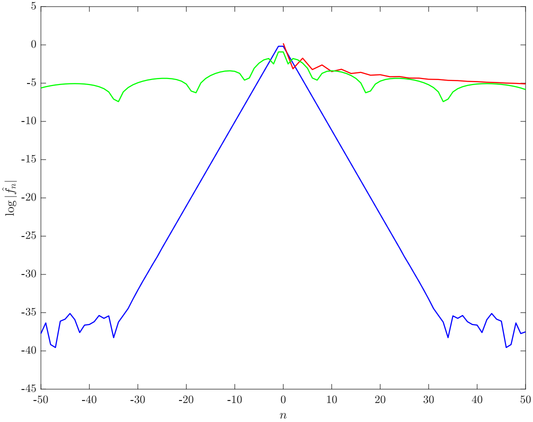


The same f expanded in the Hermite basis gives the following.

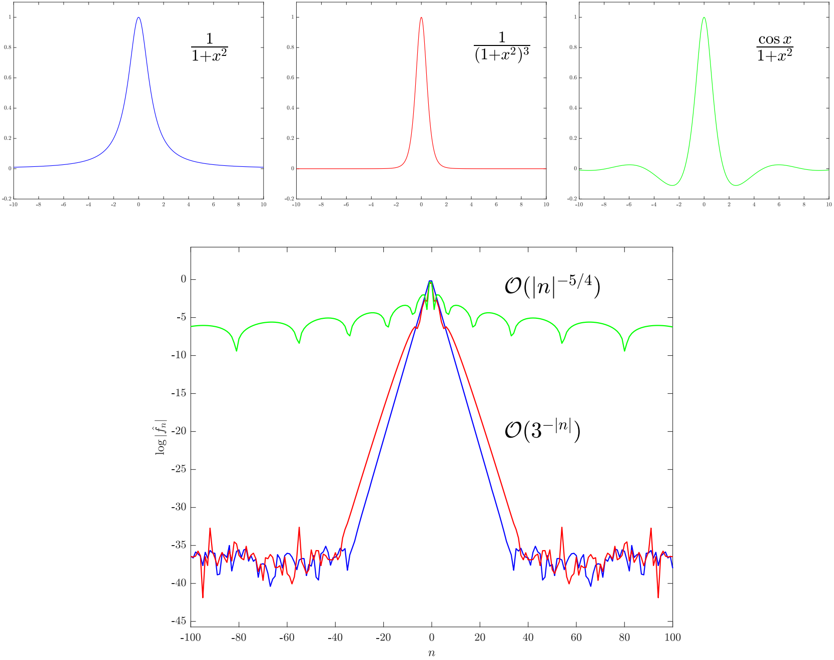


Very slow decay, little better than linear.

Now, instead consider $f(x) = \frac{\sin x}{1+x^2}$.



Just as bad as Hermite.



$\frac{1}{1+x^2}$
$\frac{1}{(1+x^2)^3}$
$\frac{\cos x}{1+x^2}$
$\mathcal{O}(|n|^{-5/4})$
$\mathcal{O}(3^{-|n|})$
$\log|\hat{f}_n|$
n

Convergence of MT

Theorem (Boyd, Weideman)

Let $f \in L_2(\mathbb{R})$. The MT expansion coefficients satisfy $\hat{f}_n = \mathcal{O}(\rho^{-|n|})$ for some $\rho > 1$ if and only if the function $z \mapsto (1 - 2iz)f(z)$ can be analytically extended to the set

$$C_\rho = \overline{\mathbb{C}} \setminus \left(\mathbb{D}_{r_\rho}(a_\rho) \cup \mathbb{D}_{r_\rho}(\overline{a}_\rho)\right),$$
$$a_\rho = \frac{i}{2}\frac{\rho + \rho^{-1}}{\rho - \rho^{-1}}, \quad r_\rho = \frac{1}{\rho - \rho^{-1}}.$$

Note that is necessary that $\lim_{|z|\to\infty} f(z) = 0$.

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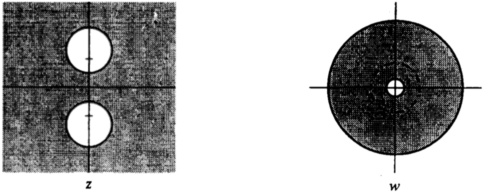

Steepest descent for Malmquist-Takenaka (Weideman)

$f(x)$	$\hat{f}_n$
e^{-x^2}	$\mathcal{O}\left(e^{-\frac{3^{3/2}}{2}\lvert n\rvert^{2/3}}\right)$
$\operatorname{sech} x$	$\mathcal{O}(e^{-2\lvert n\rvert^{1/2}})$
$\frac{\sin x}{1+x^2}$	$\mathcal{O}(\lvert n\rvert^{-5/4})$
$\frac{\sin x}{1+x^4}$	$\mathcal{O}(\lvert n\rvert^{-9/4})$

The general pattern is unknown.

Hermite

$f(x)$	$\hat{f}_n$
$e^{-\alpha x^2}$, $\mathrm{Re}\,\alpha > 0$	$\mathcal{O}(c^n n^{-1/4})$, $\lvert c\rvert < 1$
$e^{-\alpha(x-x_0)^2}\cos\omega x$, $\mathrm{Re}\,\alpha > 0$	$\mathcal{O}(c^{n/2} n^{-1/4})$, $\lvert c\rvert < 1$
$\frac{1}{1+x^2}$	$\mathcal{O}(n^{-1/4})$
$\frac{\sin x}{x}$	$\mathcal{O}(n^{-3/4})$
$\chi_{[-1,1]}$	$\mathcal{O}(n^{-3/4})$

Malmquist-Takenaka

$f(x)$	$\hat{f}_n$
$e^{-\alpha x^2}$, $\mathrm{Re}\,\alpha > 0$	$\mathcal{O}(e^{-(-2\alpha)^{1/3} n^{2/3}})$
$\frac{1}{1+x^2}$	$\mathcal{O}(3^{-\lvert n \rvert})$
$\frac{1}{1+x^4}$	$\mathcal{O}\left((1+\sqrt{2})^{-\lvert n \rvert}\right)$
$\frac{1}{1+x^2} \log \frac{1+x}{1+2x}$	$\mathcal{O}(2^{-\lvert n \rvert})$
$\frac{\sin x}{x}$	$\mathcal{O}(n^{-3/4})$

General theory

There is no viable convergence theory, even for orthogonal polynomials on the real line, although some preliminary results on the convergence of MT and Hermite functions have been achieved by taking the problem to the Fourier space.

Generally, the rate of convergence must be calculated separately for each and every f. This can be done with steepest descent analysis, computation or by (tricky) algebra, where working in the Fourier space is, again, often a useful technique.