Spectral methods for time-dependent PDEs

Xane Miles

We want to approximate partial differential equations of the form

$$\frac{\partial u}{\partial t} = \mathcal{L}u + f, \quad (\boldsymbol{x}, t) \in \Omega \times \mathbb{R}_+$$

given a well-posed differentiable operator $\mathcal{L}$ and suitable initial and boundary conditions. Let φ be a sufficiently smooth, orthonormal system of functions in $L_2(\Omega)$, such that $\langle \varphi_m, \varphi_n \rangle = \int_\Omega \varphi_m(\boldsymbol{x})\varphi_n(\boldsymbol{y}) d\boldsymbol{x} = \delta_{m,n}, m, n \in \mathbb{Z}_+$.

Then, a spectral method is an approximation of the solution to this equation in the form $u(\boldsymbol{x}, t) \approx u_N(\boldsymbol{x}, t) = \sum_{n=0}^{N} \hat{u}_n(t)\varphi_n(\boldsymbol{x})$, where the coefficients $\hat{u}$ are obtained by imposing *Galerkin conditions* on the equation and solving ODEs of the form

$$\frac{d\hat{u}_m}{dt} = \sum_{n=0}^{N} \hat{u}\langle \mathcal{L}\varphi_n, \varphi_m \rangle + \langle f, \varphi_m \rangle, \quad m = 0, \ldots, N$$

How do we pick an appropriate orthonormal system? The solution to our equation must be *stable*, which is to say that it must converge as N tends to infinity, this convergence must be *quick* enough to be usable, with $\hat{u_n} \to 0$ for each $n \gg 1$ as $n \to \infty$, and finally each extra step from $k\Delta t$ to $(k+1)\Delta t$ should have a *low cost.*

We guarantee this by studying an orthonormal system $\Phi = \{\varphi_n\}_{n=0}^{\infty} \in C^1(\Omega)$ *differentiation matrix.* This is a natural linear map $\Phi \to \Phi^{'}$ produced by it, defined by $\varphi_n^{'} = \sum_{k=0}^{\infty} \mathcal{D}_{n,k}\varphi_k, \quad n \in \mathbb{Z}_+$.

If we consider the function u as a vector of each of its coefficients. As u can be written as an infinite sum of the components of φ, the differentiation matrix $\mathcal{D}$ will send u to its derivative u'.

Lemma. *If every ϕ_n obeys zero Dirichlet conditions, $\mathcal{D}$ is skew-Hermitian.*

An orthonormal system with a skew-Hermitian differentiation matrix is a stable orthonormal system.

There are two approaches to finding spectral solutions, T-systems and W-functions. When defining T-systems, we impose a requirement that the differentiation matrix is tridiagonal. However, in my research we exclusively inspected W-functions.

A function w is a weight function if it is non-negative, if each of its moments $\int_{-\infty}^{\infty} x^n w(x) dx$ are bounded and if the zeroth moment is positive.

An orthogonal polynomial sequence (OPS) is a sequence of polynomials which obey the equation: $\langle P_n, P_m \rangle = \int_a^b w(x)P_n(x)P_n(x)dx = \delta_{m,n}$.

If we have a weight function which generates an OPS, we can define the n-th W-function by $\phi_n(x) = \sqrt{w(x)p_n(x)}, \quad n \in \mathbb{N}_0$.

As this results in the same equation on the standard functional inner product as an OPS does on its weighted inner product, we immediately have an orthonormal system.

Additionally, we have the following lemma,

Lemma. *$\mathcal{D}$ is skew symmetric if and only if $w(a) = w(b) =$* 0.

In one dimension, intervals either have zero finite endpoints, in which case they do not have a boundary that conditions can be imposed on, one finite endpoint or two finite endpoints. We solve PDEs with one finite endpoints using the Laguerre W-function, orthogonal on $(0, \infty)$ with weight function $x^\alpha e^{-x}$ and the Jacobi W-function, orthogonal on $(-1, 1)$ with weight function $(1-x)^\alpha(1+x)^\beta$. Specifically, we use the ultraspherical W-function, where $\alpha = \beta$. Closed form expressions for these W-functions can be found in Iserles and Webb.

As the W-function system is formed by multiplying the weight function by an orthogonal polynomial, we can use properties of the weight function to observe properties of the W-function. See that Laguerre and ultraspherical functions obey Dirichlet conditions on their endpoints, and therefore have a skew-symmetric differentiation matrix. In general, if we set boundary conditions on the k-th derivative, then we find the Laguerre W-function with $\alpha = k$ and the ultraspherical W-function with $\alpha = \beta = k$ fulfill these conditions.

What if we have general Dirichlet conditions, instead of zero or constant Dirichlet conditions?

On a line, this is easy. Take the PDE $\frac{\partial u}{\partial t} = \mathcal{L}u + f(u, t), \quad t \geq 0, x \in [-1, 1]$. Then, apply the initial condition $u(x, 0) = u_0(x)$ and the boundary conditions $u(-1, t) = a_-(t)$, $u(1, t) = a_+(t)$. We can construct the appropriate linear interpolation $\mu(x, t) = \frac{1}{2}(1-x)a_-(t) + \frac{1}{2}(1+x)a_+(t)$, set $v(x, t) = u(x, t) - \mu(x, t)$, producing the equation

$$\frac{\partial v}{\partial t} = \mathcal{L}v + f(t, v + \mu) + \mathcal{L}\mu - \frac{\partial \mu}{\partial t}$$

with initial condition and zero Dirichlet conditions, which we can solve using a spectral method.

We can use the method of Hermite interpolation to expand to higher order conditions on a line. However, in two or more dimensions, general boundary conditions become more tricky. For Dirichlet conditions in two dimensions this is already solved, and we can interpolate within a triangle: see a forthcoming paper from Iserles. Higher dimensions and higher order conditions remain an open problem.

References

[1] Chihara, T.S. (1978) *An introduction to orthogonal polynomials*, New York: Gordon and Breach.

[2] Iserles, A. & Webb, M. (2024), Orthogonal systems for time-dependent spectral methods, arXiv:2302.04217

[3] D. Huybrechs, A. Iserles & S.P. Nørsett (2011), *From high oscillation to rapid approximation V: The equilateral triangle*, IMA J. Num. Anal. 31 (2011), 755–785.

[4] Ismail, M.E.H. (2005) *Classical and quantum orthogonal polynomials in one variable*, Cambridge: Cambridge University Press.