Numerical Analysis - Part II

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Lecture 14

Spectral Methods

The Poisson equation

We consider the *Poisson equation*

$$\nabla^2 u = f, \quad -1 \leq x, y \leq 1, \tag{1}$$

where f is analytic and obeys the periodic boundary conditions

$$f(-1, y) = f(1, y), \quad -1 \leq y \leq 1, \quad f(x, -1) = f(x, 1), \quad -1 \leq x \leq 1.$$

Moreover, we add to (1) the following *periodic boundary conditions*

$$\begin{aligned} u(-1, y) = u(1, y), \quad u_x(-1, y) = u_x(1, y), \quad -1 \leq y \leq 1 \\ u(x, -1) = u(x, 1), \quad u_y(x, -1) = u_y(x, 1), \quad -1 \leq x \leq 1. \end{aligned} \tag{2}$$

With these boundary conditions alone, a solution of (1) is only defined up to an additive constant.

Hence, we add a *normalisation condition* to fix the constant:

$$\int_{-1}^{1}\int_{-1}^{1} u(x,y)\ dx\ dy = 0. \tag{3}$$

We have the spectrally convergent Fourier expansion

$$f(x,y) = \sum_{k,l=-\infty}^{\infty} \widehat{f}_{k,\ell} e^{i\pi(kx+\ell y)}$$

and seek the Fourier expansion of u

$$u(x,y) = \sum_{k,\ell=-\infty}^{\infty} \widehat{u}_{k,\ell} e^{i\pi(kx+\ell y)}.$$

Since

$$0 = \int_{-1}^{1}\int_{-1}^{1} u(x,y)\,dx\,dy = \sum_{k,\ell=-\infty}^{\infty} \widehat{u}_{k,\ell} \int_{-1}^{1}\int_{-1}^{1} e^{i\pi(kx+\ell y)}\,dx\,dy = \widehat{u}_{0,0},$$

and

$$\nabla^2 u(x,y) = -\pi^2 \sum_{k,\ell=-\infty}^{\infty} (k^2+\ell^2)\widehat{u}_{k,\ell} e^{i\pi(kx+\ell y)},$$

together with (1), we have

$$\begin{cases} \widehat{u}_{k,\ell} = -\dfrac{1}{(k^2+\ell^2)\pi^2}\widehat{f}_{k,\ell}, & k,\ell \in \mathbb{Z},\ (k,\ell) \neq (0,0) \\ \widehat{u}_{0,0} = 0. \end{cases}$$

Remark 1

Applying a spectral method to the Poisson equation is not representative for its application to other PDEs. The reason is the special structure of the Poisson equation. In fact, $\phi_{k,\ell} = e^{i\pi(kx+\ell y)}$ are the eigenfunctions of the Laplace operator with

$$\nabla^2 \phi_{k,\ell} = -\pi^2(k^2 + \ell^2)\phi_{k,\ell},$$

and they obey periodic boundary conditions.

General second-order linear elliptic PDE

We consider the more general second-order linear elliptic PDE

$$\nabla^\top (a\nabla u) = f, \quad -1 \le x, y \le 1,$$

with $a(x, y) > 0$, and a and f periodic. We again impose the periodic boundary conditions (2) and the normalisation condition (3). We rewrite

$$\nabla^\top (a\nabla u) = \frac{\partial}{\partial x}(a u_x) + \frac{\partial}{\partial y}(a u_y) = f\,.$$

Recall that for the Fourier expansions

$$g(x, y) = \sum_{k,\ell\in\mathbb{Z}} \widehat{g}_{k,\ell}\phi_{k,\ell}(x, y), \qquad h(x, y) = \sum_{m,n\in\mathbb{Z}} \widehat{h}_{m,n}\phi_{m,n}(x, y),$$

(here the $\phi_{k,\ell}$s are the complex exponentials) we have that

$$\widehat{(g\cdot h)}_{k,\ell} = \sum_{m,n\in\mathbb{Z}} \widehat{g}_{k-m,\ell-n}\widehat{h}_{m,n}, \qquad \widehat{(g_x)}_{k,\ell} = i\pi k\,\widehat{g}_{k,\ell}\,, \quad \widehat{(g_y)}_{k,\ell} = i\pi\ell\,\widehat{g}_{k,\ell}\,,$$

$$\widehat{(h_x)}_{m,n} = i\pi m\,\widehat{h}_{m,n}\,, \quad \widehat{(h_y)}_{m,n} = i\pi n\,\widehat{h}_{m,n}\,.$$

General second-order linear elliptic PDE

This gives

$$-\pi^2 \sum_{k,\ell\in\mathbb{Z}} \sum_{m,n\in\mathbb{Z}} (km+\ell n)\,\widehat{a}_{k-m,\ell-n}\widehat{u}_{m,n}\phi_{k,\ell}(x,y) = \sum_{k,\ell\in\mathbb{Z}} \widehat{f}_{k,\ell}\phi_{k,\ell}(x,y)\,.$$

In the next steps, we truncate the expansions to $-N/2+1 \leq k,\ell,m,n \leq N/2$ and impose the normalisation condition $\widehat{u}_{0,0}=0$. This results in a system of N^2-1 linear algebraic equations in the unknowns $\widehat{u}_{m,n}$, where $m,n=-N/2+1\ldots N/2$, and $(m,n)\neq(0,0)$:

$$\sum_{m,n=-N/2+1}^{N/2} (km+\ell n)\,\widehat{a}_{k-m,\ell-n}\,\widehat{u}_{m,n} = -\frac{1}{\pi^2}\,\widehat{f}_{k,\ell}\,,\ \ k,\ell=-N/2+1\ldots N/2\,.$$

Analyticity and periodicity

The fast convergence of spectral methods rests on two properties of the underlying problem: analyticity and periodicity. If one is not satisfied the rate of convergence in general drops to polynomial. However, to a certain extent, we can relax these two assumptions while still retaining the substantive advantages of Fourier expansions.

Relaxing analyticity: In general, the speed of convergence of the truncated Fourier series of a function f depends on the smoothness of the function. In fact, the smoother the function the faster the truncated series converges, i.e., for $f \in C^p(-1,1)$ we receive an $\mathcal{O}(N^{-p})$ order of convergence.

Spectral convergence can be recovered, once analyticity is replaced by the requirement that $f \in C^\infty(-1,1)$, i.e., $f^{(m)}(x)$ exists for all $x \in (-1,1)$ and $m = 0, 1, 2, \ldots$. Consider, for instance, $f(x) = e^{-1/(1-x^2)}$. Then, $f \in C^\infty(-1,1)$ but cannot be extended analytically because of essential singularities at ± 1. Nevertheless, one can show that $|\widehat{f_n}| \sim \mathcal{O}(e^{-cn^\alpha})$, where $c > 0$ and $\alpha \approx 0.44$. While this is slower than exponential convergence in the analytic case, it is still faster than $\mathcal{O}(n^{-m})$ for any integer m and hence, we have spectral convergence.

Analyticity and periodicity – Relaxing periodicity

Relaxing periodicity: Disappointingly, periodicity is necessary for spectral convergence. Once this condition is dropped, we are back to the setting of Theorem 3.3, i.e., Fourier series converge as $\mathcal{O}(N^{-1})$ unless $f(-1) = f(1)$. One way around this is to change our set of basis functions, e.g., to Chebyshev polynomials.

Chebyshev polynomials

The Chebyshev polynomial of degree n is defined as

$$T_n(x) := \cos n \arccos x, \quad x \in [-1, 1],$$

or, in a more instructive form,

$$T_n(x) := \cos n\theta, \quad x = \cos\theta, \quad \theta \in [0, \pi]. \tag{4}$$

The three-term recurrence relation

1) The sequence (T_n) obeys the three-term recurrence relation

$$T_0(x) \equiv 1, \quad T_1(x) = x,$$
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n \geq 1,$$

in particular, T_n is indeed an algebraic polynomial of degree n, with the leading coefficient 2^{n-1}. (The recurrence is due to the equality $\cos(n+1)\theta + \cos(n-1)\theta = 2\cos\theta\cos n\theta$ via substitution $x = \cos\theta$, expressions for T_0 and T_1 are straightforward.)

The recurrence yields

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2-1, \quad T_3(x) = 4x^3-3x, \ \ldots,$$

and T_n is called the nth *Chebyshev polynomial* (of the first kind).

Chebyshev polynomials - How they look

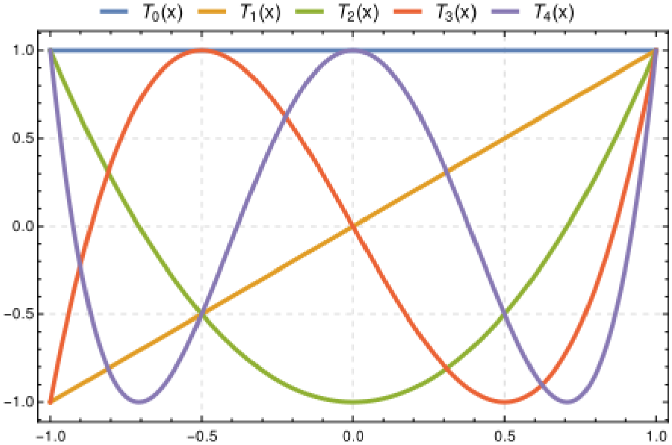

Figure: Chebyshev polynomials

Chebyshev polynomials are orthogonal

2) Also, (T_n) form a sequence of orthogonal polynomials with respect to the inner product $(f,g)_w := \int_{-1}^{1} f(x)g(x)w(x)dx$, with the weight function $w(x) := (1-x^2)^{-1/2}$. Namely, we have

$$(T_n, T_m)_w = \int_{-1}^{1} T_m(x)T_n(x)\,\frac{dx}{\sqrt{1-x^2}} = \int_0^{\pi} \cos m\theta \cos n\theta \, d\theta$$

$$= \begin{cases} \pi, & m = n = 0\,, \\ \frac{\pi}{2}, & m = n \geq 1\,, \\ 0, & m \neq n\,. \end{cases} \qquad (5)$$

Chebyshev expansion

Since $(T_n)_{n=0}^{\infty}$ form an orthogonal sequence, a function f such that $\int_{-1}^{1} |f(x)|^2 w(x)\, dx < \infty$ can be expanded in the series

$$f(x) = \sum_{n=0}^{\infty} \breve{f}_n T_n(x),$$

with the Chebyshev coefficients $\breve{f}_n$. Making inner product of both sides with T_n and using orthogonality yields

$$\begin{aligned}(f, T_n)_w = \breve{f}_n (T_n, T_n)_w \quad \Rightarrow \quad \breve{f}_n &= \frac{(f, T_n)_w}{(T_n, T_n)_w} \\ &= \frac{c_n}{\pi} \int_{-1}^{1} f(x) T_n(x) \frac{dx}{\sqrt{1-x^2}}\,,\end{aligned} \tag{6}$$

where $c_0 = 1$ and $c_n = 2$ for $n \geq 1$.

https://en.wikipedia.org/wiki/Stone-Weierstrass_theorem
https://en.wikipedia.org/wiki/Chebyshev_polynomials

Connection to the Fourier expansion

Letting $x = \cos\theta$ and $g(\theta) = f(\cos\theta)$, we obtain

$$\int_{-1}^{1} f(x)\,T_n(x)\,\frac{dx}{\sqrt{1-x^2}} = \int_0^{\pi} f(\cos\theta)\,T_n(\cos\theta)\,d\theta = \frac{1}{2}\int_{-\pi}^{\pi} g(\theta)\cos n\theta\,d\theta\,. \tag{7}$$

Given that $\cos n\theta = \frac{1}{2}(e^{in\theta} + e^{-in\theta})$, and using the Fourier expansion of the 2π-periodic function g,

$$g(\theta) = \sum_{n\in\mathbb{Z}} \widehat{g}_n \mathrm{e}^{in\theta}, \quad \text{where} \quad \widehat{g}_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(t)e^{-int}\,dt, \quad n \in \mathbb{Z}\,,$$

we continue (7) as

$$\int_{-1}^{1} f(x)\,T_n(x)\frac{dx}{\sqrt{1-x^2}} = \frac{\pi}{2}(\widehat{g}_{-n} + \widehat{g}_n)\,,$$

and from (6) we deduce that

$$\breve{f}_n = \begin{cases} \widehat{g}_0, & n = 0\,, \\ \widehat{g}_{-n} + \widehat{g}_n, & n \geq 1\,. \end{cases}$$

Properties of the Chebyshev expansion

As we have seen, for a general integrable function f, the computation of its Chebyshev expansion is equivalent to the Fourier expansion of the function $g(\theta) = f(\cos\theta)$. Since the latter is periodic with period 2π, we can use a discrete Fourier transform (DFT) to compute the Chebyshev coefficients $\check{f}_n$. [Actually, based on this connection, one can perform a direct fast Chebyshev transform].

Also, if f can be analytically extended from $[-1, 1]$ (to the so-called Bernstein ellipse), then $\check{f}_n$ decays spectrally fast for $n \gg 1$ (with the rate depending on the size of the ellipse). Hence, the Chebyshev expansion inherits the rapid convergence of spectral methods without assuming that f is periodic.

The algebra of Chebyshev expansions

Let $\mathcal{B}$ be the set of analytic functions in $[-1,1]$ that can be extended analytically into the complex plane. We identify each such function with its Chebyshev expansion. Like the set $\mathcal{A}$, the set $\mathcal{B}$ is a linear space and is closed under multiplication. In particular, we have

$$\begin{aligned} T_m(x)\,T_n(x) &= \cos(m\theta)\cos(n\theta) \\ &= \tfrac{1}{2}\left[\cos((m-n)\theta)+\cos((m+n)\theta)\right] \\ &= \tfrac{1}{2}\left[\,T_{|m-n|}(x)+T_{m+n}(x)\right] \end{aligned}$$

and hence,

$$\begin{aligned} f(x)g(x) &= \sum_{m=0}^{\infty}\breve{f}_m T_m(x)\cdot\sum_{n=0}^{\infty}\breve{g}_n T_n(x) \\ &= \frac{1}{2}\sum_{m,n=0}^{\infty}\breve{f}_m\breve{g}_n\left[T_{|m-n|}(x)+T_{m+n}(x)\right] \\ &= \frac{1}{2}\sum_{m,n=0}^{\infty}\breve{f}_m\Big(\breve{g}_{|m-n|}+\breve{g}_{m+n}\Big)\,T_n(x). \end{aligned}$$

Lemma 2 (Derivatives of Chebyshev polynomials)

We can express derivatives T_n' in terms of (T_k) as follows,

$$T_{2n}'(x) = (2n) \cdot 2 \sum_{k=1}^{n} T_{2k-1}(x), \tag{8}$$

$$T_{2n+1}'(x) = (2n+1)\left[T_0(x) + 2 \sum_{k=1}^{n} T_{2k}(x)\right]. \tag{9}$$

Proof. From (4), we deduce

$$T_m(x) = \cos m\theta \quad \Rightarrow \quad T_m'(x) = \frac{m \sin m\theta}{\sin\theta} \qquad x = \cos\theta\,.$$

So, for $m = 2n$, (8) follows from the identity

$$\frac{\sin 2n\theta}{\sin\theta} = 2\sum_{k=1}^{n} \cos(2k-1)\theta,$$

which is verified as
https:
//en.wikipedia.org/wiki/List_of_trigonometric_identities

$$\begin{aligned} 2\sin\theta \sum_{k=1}^{n} \cos\,(2k-1)\theta &= \sum_{k=1}^{n} 2\cos\,(2k-1)\theta\sin\theta \\ &= \sum_{k=1}^{n} \left[\,\sin 2k\theta - \sin\,(2k-1)\theta\right] = \sin 2n\theta. \end{aligned}$$

Derivatives of Chebyshev polynomials

Proof. Cont. For $m = 2n + 1$, (9) turns into identity

$$\frac{\sin(2n+1)\theta}{\sin\theta} = 1 + 2\sum_{k=1}^{n}\cos 2k\theta,$$

and that follows from

$$\begin{aligned}\sin\theta\Big(1 + 2\sum_{k=1}^{n}\cos 2k\theta\Big) &= \sin\theta + \sum_{k=1}^{n}\big[\sin(2k{+}1)\theta - \sin(2k-1)\theta\big]\\ &= \sin(2n+1)\theta.\end{aligned}$$

□

Remark 3 (Application to PDEs)

With Lemma 2 all derivatives of u can be expressed in an explicit form as a Chebyshev expansion (cf. Exercise 19 on Example Sheets). For the computation of the Chebyshev coefficients the function f has to be sampled at the so-called Chebyshev points $\cos(2\pi k/N)$, $k = -N/2 + 1, \ldots, N/2$. This results into a grid, which is denser towards the edges. For elliptic problems this is not problematic, however for initial value PDEs such grids can cause numerical instabilities.

Chebyshev expansion for the derivatives

The lemma above allows us to express the Chebyshev coefficients of the derivative of a function f, in terms of those of f.
We get

$$\begin{cases} \breve{f'}_0 & = \breve{f}_1 + 3\breve{f}_3 + 5\breve{f}_5 + \cdots \\ \breve{f'}_1 & = 2(2\breve{f}_2 + 4\breve{f}_4 + 6\breve{f}_6 + \cdots) \\ \breve{f'}_2 & = 2(3\breve{f}_3 + 5\breve{f}_5 + \cdots) \\ \breve{f'}_3 & = 2(4\breve{f}_4 + 6\breve{f}_6 + \cdots) \\ \vdots \end{cases}$$

In general, for the k'th derivative we get:

$$\breve{f^{(k)}}_n = c_n \sum_{\substack{m=n+1 \\ n+m \text{ odd}}}^{\infty} m \, \breve{f^{(k-1)}}_m, \quad \forall\, k \geq 1,$$

where $c_0 = 1$ and $c_n = 2$ for $n \geq 1$.

The spectral method for evolutionary PDEs

We consider the problem

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t} = \mathcal{L}u(x,t), & x \in [-1,1], \quad t \geq 0\,, \\ u(x,0) = g(x), & x \in [-1,1], \end{cases} \tag{10}$$

with appropriate boundary conditions on $\{-1,1\} \times \mathbb{R}_+$ and where $\mathcal{L}$ is a linear operator, e.g. a differential operator (acting on the x variable). We want to solve this problem by the method of lines (semi-discretization), using a spectral method for the approximation of u and its derivatives in the spatial variable x. Then, in a general spectral method, we seek solutions $u_N(x,t)$ with

$$u_N(x,t) = \sum_{n=-N/2+1}^{N/2} c_n(t)\,\varphi_n(x), \tag{11}$$

where $c_n(t)$ are expansion coefficients and φ_n are basis functions chosen according to the specific structure of (10).

The spectral method for evolutionary PDEs

For example, we may take:

1) the *Fourier expansion* with $c_n(t) = \widehat{u}_n(t)$, $\varphi_n(x) = e^{i\pi nx}$ for periodic boundary conditions,

2) a polynomial expansion such as the *Chebyshev expansion* with $c_n(t) = \breve{u}_n(t)$, $\varphi_n(x) = T_n(x)$ for other boundary conditions.

The spectral approximation in space (11) results into a $N \times N$ system of ODEs for the expansion coefficients $\{c_n(t)\}$:

$$\boldsymbol{c}' = B\boldsymbol{c}\,, \tag{12}$$

where $B \in \mathbb{R}^{N\times N}$, and $\boldsymbol{c} = \{c_n(t)\} \in \mathbb{R}^N$. We can solve it with standard ODE solvers (Euler, Crank-Nikolson, etc.) which as we have seen are approximations to the matrix exponent in the exact solution $\boldsymbol{c}(t) = \mathrm{e}^{tB}\boldsymbol{c}(0)$.

The diffusion equation

Consider the diffusion equation for a function $u = u(x,t)$,

$$\begin{cases} u_t = u_{xx}, & (x,t) \in [-1,1] \times \mathbb{R}_+ \,, \\ u(x,0) = g(x), & x \in [-1,1]\,. \end{cases} \tag{13}$$

with the periodic boundary conditions $u(-1,t) = u(1,t)$, $u_x(-1,t) = u_x(1,t)$, and standard normalisation $\int_{-1}^{1} u(x,t)\,dx = 0$, both imposed for all values $t \geq 0$.

For each t, we approximate $u(x,t)$ by its N-th order partial Fourier sum in x,

$$u(x,t) \approx u_N(x,t) \; = \sum_{n \in \Gamma_N} \widehat{u}_n(t)\, e^{i\pi n x}\,, \qquad \Gamma_N := \{-N/2{+}1, ..., N/2\}\,.$$