Dr H. Fawzi

Mathematical Tripos Part II: Michaelmas Term 2021

Numerical Analysis – Lecture 12

Method 3.8 (The algebra of Fourier expansions) *Let $\mathcal{A}$ be the set of all functions $f : [-1,1] \to C$, which are analytic in $[-1,1]$, periodic with period 2, and that can be extended analytically into the complex plane.* Then $\mathcal{A}$ is a linear space, i.e., $f, g \in \mathcal{A}$ and $\alpha \in \mathbb{C}$ then $f+g \in \mathcal{A}$ and $af \in \mathcal{A}$. In particular, with f and g expressed in its Fourier series, i.e.,

$$f(x) = \sum_{n=-\infty}^{\infty} \widehat{f}_n e^{i\pi n x}, \quad g(x) = \sum_{n=-\infty}^{\infty} \widehat{g}_n e^{i\pi n x}$$

we have

$$f(x) + g(x) = \sum_{n=-\infty}^{\infty} (\widehat{f}_n + \widehat{g}_n) e^{i\pi n x}, \quad \alpha f(x) = \sum_{n=-\infty}^{\infty} \alpha \widehat{f}_n e^{i\pi n x} \tag{3.3}$$

and

$$f(x) \cdot g(x) = \sum_{n=-\infty}^{\infty} \left(\sum_{m=-\infty}^{\infty} \widehat{f}_{n-m} \widehat{g}_m \right) e^{i\pi n x} = \sum_{n=-\infty}^{\infty} \left(\widehat{f} * \widehat{g} \right)_n e^{i\pi n x}, \tag{3.4}$$

where $*$ denotes the convolution operator, hence $\widehat{(f \cdot g)}_n = (\widehat{f} * \widehat{g})_n$. Moreover, if $f \in \mathcal{A}$ then $f' \in \mathcal{A}$ and

$$f'(x) = i\pi \sum_{n=-\infty}^{\infty} n \cdot \widehat{f}_n e^{i\pi n x}. \tag{3.5}$$

Since $\{\widehat{f}_n\}$ decays faster than $\mathcal{O}(n^{-p})$ for any $p \in \mathbb{N}$, this provides that all derivatives of f have rapidly convergent Fourier expansions.

Example 3.9 (Application to differential equations) Consider the two-point boundary value problem: $y = y(x)$, $-1 \le x \le 1$, solves

$$y'' + a(x)y' + b(x)y = f(x), \quad y(-1) = y(1), \tag{3.6}$$

where $a, b, f \in \mathcal{A}$ and we seek a *periodic solution* $y \in \mathcal{A}$ for (3.6). Substituting y, a, b and f by their Fourier series and using (3.3)-(3.5) we obtain an infinite dimensional system of linear equations for the Fourier coefficients $\widehat{y}_n$:

$$-\pi^2 n^2 \widehat{y}_n + i\pi \sum_{m=-\infty}^{\infty} m \widehat{a}_{n-m} \widehat{y}_m + \sum_{m=-\infty}^{\infty} \widehat{b}_{n-m} \widehat{y}_m = \widehat{f}_n, \quad n \in \mathbb{Z}. \tag{3.7}$$

Since $a, b, f \in \mathcal{A}$, their Fourier coefficients decrease rapidly, like $\mathcal{O}(n^{-p})$ for every $p \in \mathbb{N}$. Hence, we can truncate (3.7) into the N-dimensional system

$$-\pi^2 n^2 \widehat{y}_n + i\pi \sum_{m=-N/2+1}^{N/2} m \widehat{a}_{n-m} \widehat{y}_m + \sum_{m=-N/2+1}^{N/2} \widehat{b}_{n-m} \widehat{y}_m = \widehat{f}_n, \qquad n = -N/2+1, \ldots, N/2. \tag{3.8}$$

Remark 3.10 The matrix of (3.8) is in general dense, but our theory predicts that fairly small values of N, hence very small matrices, are sufficient for high accuracy. For instance: choosing $a(x) = f(x) = \cos \pi x$, $b(x) = \sin 2\pi x$ (which incidentally even leads to a sparse matrix) we get

$N = 16$	error of size 10^{-10}
$N = 22$	error of size 10^{-15} (which is already hitting the accuracy of computer arithmetic)

Method 3.11 (Computation of Fourier coefficients (DFT)) We have to compute

$$\widehat{f}_n = \frac{1}{2}\int_{-1}^{1} f(t)e^{-i\pi nt}\,dt, \quad n \in \mathbb{Z}. \tag{3.9}$$

For this, suppose we wish to compute the integral on $[-1,1]$ of a function $h \in \mathcal{A}$ by means of the Riemann sums on the uniform partition

$$\int_{-1}^{1} h(t)\,dt \approx \frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right). \tag{3.10}$$

This is known as a *rectangle rule*. We want to know how good this approximation is. Let $\omega_N = e^{2\pi i/N}$. Then we have

$$\frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right) \;=\; \frac{2}{N}\sum_{k=-N/2+1}^{N/2}\sum_{n=-\infty}^{\infty}\widehat{h}_n e^{2\pi i nk/N} = \frac{2}{N}\sum_{n=-\infty}^{\infty}\widehat{h}_n \sum_{k=-N/2+1}^{N/2}\omega_N^{nk}\,.$$

Since $\omega_N^N = 1$ we have

$$\sum_{k=-N/2+1}^{N/2}\omega_N^{nk} = \omega_N^{-n(N/2-1)}\sum_{k=0}^{N-1}\omega_N^{nk} = \begin{cases} N, & n \equiv 0 \pmod{N}, \\ 0, & n \not\equiv 0 \pmod{N}, \end{cases}$$

and we deduce that

$$\frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right) = 2\sum_{r=-\infty}^{\infty}\widehat{h}_{Nr}\,.$$

Hence, the error committed by the Riemann approximation is

$$\begin{aligned} e_N(h) \;&:=\; \frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right) - \int_{-1}^{1} h(t)\,dt \;=\; 2\sum_{r=-\infty}^{\infty}\widehat{h}_{Nr} - 2\widehat{h}_0 \\ &=\; 2\sum_{r=1}^{\infty}\left(\widehat{h}_{Nr} + \widehat{h}_{-Nr}\right). \end{aligned}$$

Since $h \in \mathcal{A}$, its Fourier coefficients decay at spectral rate, namely $\widehat{h}_{Nr} = \mathcal{O}((Nr)^{-p})$, and hence the error of the Riemann sums approximation (3.10) decays spectrally as a function of N,

$$e_N(h) = \mathcal{O}(N^{-p}) \quad \forall p \in \mathbb{N}\,.$$

Going back to the computation of the Fourier coefficients (3.9), we see that we may compute the integral of $h(x) = \frac{1}{2}f(x)e^{-i\pi nx}$ by means of the Riemann sums, and this gives a spectral method for calculating the Fourier coefficients of f:

$$\widehat{f}_n \approx \frac{1}{N}\sum_{k=-N/2+1}^{N/2} f\left(\frac{2k}{N}\right)\omega_N^{-nk}, \qquad n = -N/2+1,\ldots,N/2\,. \tag{3.11}$$

Remark 3.12 One can recognise that formula (3.11) is the *discrete Fourier transform (DFT)* of the sequence $(y_k) = \big(f(\frac{2k}{N})\big)$, see previous definition, hence not only have we a spectral rate of convergence, but also a fast algorithm (FFT) of computing the Fourier coefficients.

Problem 3.13 (The Poisson equation) We consider the *Poisson equation*

$$\nabla^2 u = f, \quad -1 \le x, y \le 1, \tag{3.12}$$

where f is analytic and obeys the periodic boundary conditions

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

Moreover, we add to (3.12) the following *periodic boundary conditions*

$$\begin{aligned} u(-1,y) &= u(1,y), \quad u_x(-1,y) = u_x(1,y), \quad -1 \le y \le 1 \\ u(x,-1) &= u(x,1), \quad u_y(x,-1) = u_y(x,1), \quad -1 \le x \le 1. \end{aligned} \tag{3.13}$$

With these boundary conditions alone, a solution of (3.12) is only defined up to an additive constant. Hence, we add a *normalisation condition* to fix the constant:

$$\int_{-1}^{1}\int_{-1}^{1} u(x,y)\,dx\,dy = 0. \tag{3.14}$$

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 (3.12), we have

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

Remark 3.14 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.

Problem 3.15 (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 (3.13) and the normalisation condition (3.14). We rewrite

$$\nabla^\top(a\nabla u) = \frac{\partial}{\partial x}(au_x) + \frac{\partial}{\partial y}(au_y) = f\,,$$

and use the Fourier expansions

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

together with the bivariate versions of (3.4)-(3.5)

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

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

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 $-N/2+1 \le k,\ell,m,n \le N/2$ 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 $m,n = -N/2+1...N/2$, and $(m,n) \neq (0,0)$:

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

Discussion 3.16 (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 (cf. Remark 3.7), it is still faster than $\mathcal{O}(n^{-m})$ for any integer m and hence, we have spectral convergence.

- *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.