Mathematical Tripos Part II: Michaelmas Term 2023

Numerical Analysis – Lecture 12

Computation of Fourier coefficients (DFT) When applying spectral methods, we often need to compute the Fourier coefficients of the problem data, i.e., we need to compute integrals of the form:

$$\widehat{f}_n = \frac{1}{2}\int_{-1}^{1} f(t)e^{-i\pi n t}\,dt, \quad n \in \mathbb{Z}. \tag{3.3}$$

Call $h(t) = f(t)e^{-i\pi n t}$. One simple way to approximate the integral of h on $[-1, 1]$ is using the *rectangle rule*:

$$\int_{-1}^{1} h(t)\,dt \approx \frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right). \tag{3.4}$$

This approximation happens to be exponentially convergent in N.

Theorem 3.8 *Let h be a 2-periodic function such that its Fourier series is absolutely convergent. Let $I(h) = \int_{-1}^{1} h(t)dt$, and for an even integer N, let $I_N(h) = \frac{2}{N}\sum_{k=-N/2+1}^{N/2} h\left(\frac{2k}{N}\right)$. Then*

$$I_N(h) - I(h) = 2\sum_{r\in\mathbb{Z},|r|\geq 1} \hat{h}_{Nr}. \tag{3.5}$$

As a consequence, if h is analytic on the horizontal strip $\{z \in \mathbb{C} : |\operatorname{Im} z| < a\}$ and $|h(z)| \leq M$ for $|\operatorname{Im} z| < a$, then by letting $c = e^{-a\pi} \in (0, 1)$, we have $|I_N(h) - I(h)| \leq 4Mc^N/(1 - c^N)$.

Remark 3.9 *Another consequence of the expression* (3.5) *is that $I_N(h) = I(h)$ if h is a trigonometric polynomial of degree $< N$, i.e., if $\hat{h}_n = 0$ for $|n| \geq N$. This is reminiscent of Gaussian quadrature rules which are exact for polynomials up to degree $2N - 1$. For more on the exponential convergence of the rectangle rule for periodic analytic functions, we refer the interested reader to the following review article The Exponentially Convergent Trapezoidal Rule, SIAM Review, 2014 by L. N. Trefethen, and J. A. C. Weideman.*

Proof. Let $\omega_N = e^{2\pi i/N}$. Then we have

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

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

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

Since $I(h) = 2\hat{h}_0$, we immediately obtain the expression (3.5).

For the second part of the theorem, the analyticity assumption guarantees, that the Fourier coefficients $|\hat{h}_n|$ decay exponentially fast, namely $|\hat{h}_n| \leq Mc^{|N|}$ (see Lecture 11). In this case we have

$$2\sum_{r\in\mathbb{Z},|r|\geq 1}|\hat{h}_{Nr}| \leq 4M\sum_{r=1}^{\infty}c^{Nr} = 4Mc^N/(1-c^N)$$

as desired.

Remark 3.10 Applying the rectangle rule to the integral in (3.3) corresponds to the approximation

$$\hat{f}_n \approx \frac{1}{N} \sum_{k=-N/2+1}^{N/2} f\left(\frac{2k}{N}\right) e^{-2ik\pi n/N}.$$

We recognize that the right-hand side, for $n = -N/2+1, \ldots, N/2$, corresponds to the discrete Fourier transform of the sequence $(y_k) = \left(f(\frac{2k}{N})\right)$. Thus, one can compute the approximations to $\hat{f}_n$ using the FFT algorithm.

The Poisson equation We consider the *Poisson equation*

$$\nabla^2 u = f, \quad -1 \le x, y \le 1, \tag{3.6}$$

for which we are looking a periodic solution $u(x+2, y) = u(x, y) = u(x, y+2)$. We assume f is analytic and periodic. We have the Fourier expansion of f

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

and seek the Fourier expansion of u

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

Since

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

equating the Fourier coefficients gives us

$$-\pi^2 (k^2 + l^2) \widehat{u}_{k,l} = \widehat{f}_{k,l}, \qquad k, l \in \mathbb{Z}.$$

A necessary condition for the above to have a solution is that $\widehat{f}_{0,0} = 0$. In this case, we have the simple closed-form solution for the PDE:

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

Remark 3.11 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, $\phi_{k,l} = e^{i\pi(kx+ly)}$ are the eigenfunctions of the Laplace operator with

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

and they obey periodic boundary conditions.

General 2D diffusion equation We consider the more general diffusion PDE

$$\frac{\partial}{\partial x}\left(a(x, y) \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(a(x, y) \frac{\partial u}{\partial y}\right) = f, \quad -1 \le x, y \le 1,$$

with $a(x, y) > 0$, and a and f periodic, and we are looking for a periodic solution. If

$$u(x, y) = \sum_{k,l \in \mathbb{Z}} \widehat{u}_{k,l} e^{i\pi(kx+ly)}$$

is the Fourier expansion of u, the bivariate versions of the algebra of Fourier expansions gives (denoting $u_x = \partial u/\partial x$ and $u_y = \partial u/\partial y$):

$$\begin{aligned} \widehat{(u_x)}_{k,l} &= i\pi k \widehat{u}_{k,l} \\ \widehat{a \cdot (u_x)}_{m,n} &= \sum_{k,l\in\mathbb{Z}} \widehat{a}_{m-k,n-l}(i\pi k)\widehat{u}_{k,l}, \end{aligned} \tag{3.7}$$

and similarly

$$\begin{aligned} \widehat{(u_y)}_{k,l} &= i\pi l \widehat{u}_{k,l} \\ \widehat{a \cdot (u_y)}_{m,n} &= \sum_{k,l\in\mathbb{Z}} \widehat{a}_{m-k,n-l}(i\pi l)\widehat{u}_{k,l}. \end{aligned} \tag{3.8}$$

This gives

$$-\pi^2 \sum_{m,n\in\mathbb{Z}} \sum_{k,l\in\mathbb{Z}} (mk+nl)\,\widehat{a}_{m-k,n-l}\widehat{u}_{k,l} e^{i\pi(mx+ny)} = \sum_{m,n\in\mathbb{Z}} \widehat{f}_{m,n} e^{i\pi(mx+ny)}\,.$$

We look for an approximate solution where $\widehat{u}_{k,l} = 0$ for $|k|,|l| > N/2$. This means that the inner sum can be restricted to $|k|,|l| \le N/2$. Then, we impose equality of the Fourier terms corresponding to $|n|,|m| \le N/2$ only. This results in a linear system of $(N+1)^2$ equations in the unknowns $\widehat{u}_{m,n}$, where $m,n = -N/2...N/2$:

$$\sum_{k,l=-N/2}^{N/2} (mk+nl)\,\widehat{a}_{m-k,n-l}\,\widehat{u}_{k,l} = -\frac{1}{\pi^2}\,\widehat{f}_{m,n}\,, \qquad m,n = -N/2...N/2\,. \tag{3.9}$$

By looking at the equation corresponding to $(m,n) = (0,0)$ we see that a necessary condition for (3.9) to have a solution is that $\widehat{f}_{0,0} = 0$. We also see that $\widehat{u}_{0,0}$ does not play a role in the linear system above. Thus (3.9) really consists of $(N+1)^2 - 1$ equations in $(N+1)^2 - 1$ unknowns.

Discussion 3.12 (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.

- *Relaxing periodicity*: Disappointingly, periodicity is necessary for spectral convergence. One way around this is to change our set of basis functions, e.g., to Chebyshev polynomials.