Numerical Analysis - Part II

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Lecture 11

The diffusion equation in two space dimensions

The diffusion equation in two space dimensions

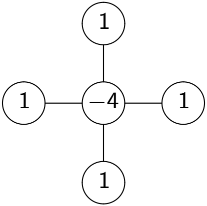
We are solving

$$\frac{\partial u}{\partial t} = \nabla^2 u, \qquad 0 \leq x, y \leq 1, \quad t \geq 0, \tag{1}$$

where $u = u(x, y, t)$, together with initial conditions at $t = 0$ and Dirichlet boundary conditions at $\partial\Omega$, where $\Omega = [0, 1]^2 \times [0, \infty)$. It is straightforward to generalize our derivation of numerical algorithms, e.g. by the method of lines.

Recall the five point formula

We have the *five-point method*



$$u_{i,j} = u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}\ ,$$

discretising the two dimensional Laplacian.

The diffusion equation in two space dimensions

Thus, let $u_{\ell,m}(t) \approx u(\ell h, mh, t)$, where $h = \Delta x = \Delta y$, and let $u^n_{\ell,m} \approx u_{\ell,m}(nk)$ where $k = \Delta t$. The five-point formula results in

$$u'_{\ell,m} = \tfrac{1}{h^2}(u_{\ell-1,m} + u_{\ell+1,m} + u_{\ell,m-1} + u_{\ell,m+1} - 4u_{\ell,m}),$$

or in the matrix form

$$\boldsymbol{u}' = \tfrac{1}{h^2} A_* \boldsymbol{u}, \qquad \boldsymbol{u} = (u_{\ell,m}) \in \mathbb{R}^N, \tag{2}$$

where A_* is the block TST matrix of the five-point scheme:

$$A_* = \begin{bmatrix} H & I & & \\ I & \ddots & \ddots & \\ & \ddots & \ddots & I \\ & & I & H \end{bmatrix}, \quad H = \begin{bmatrix} -4 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -4 \end{bmatrix}.$$

Crank-Nicolson for 2D

Applying the trapezoidal rule to our semi-dicretization (2) we obtain the two-dimensional Crank-Nicolson method:

$$(I - \tfrac{1}{2}\mu A_*)\,\boldsymbol{u}^{n+1} = (I + \tfrac{1}{2}\mu A_*)\,\boldsymbol{u}^{n}\,, \tag{3}$$

in which we move from the n-th to the $(n+1)$-st level by solving the system of linear equations $B\boldsymbol{u}^{n+1} = C\boldsymbol{u}^{n}$, or $\boldsymbol{u}^{n+1} = B^{-1}C\boldsymbol{u}^{n}$. For stability, similarly to the one-dimensional case, the eigenvalue analysis implies that $A = B^{-1}C$ is normal and shares the same eigenvectors with B and C, hence

$$\lambda(A) = \frac{\lambda(C)}{\lambda(B)} = \frac{1 + \frac{1}{2}\mu\lambda(A_*)}{1 - \frac{1}{2}\mu\lambda(A_*)} \quad \Rightarrow \quad |\lambda(A)| < 1 \text{ as } \lambda(A_*) < 0$$

and the method is stable for all μ. The same result can be obtained through the Fourier analysis.

Spectral Methods

Large matrices versus small matrices

Finite difference schemes rest upon the replacement of derivatives by a linear combination of function values. This leads to the solution of a system of algebraic equations, which on the one hand tends to be large (due to the slow convergence properties of the approximation) but on the other hand is highly structured and sparse, leading itself to effective algorithms for its solution. We will get to know some of these algorithms in Section 4.

However, an enticing alternative to this strategy are methods that produce small matrices in the first place. Although, these matrices will usually not be sparse anymore, the much smaller the size of the matrices renders its solution affordable. The key point for such approximations are better convergence properties requiring much smaller number of parameters.

General idea of spectral methods

The basic idea of spectral methods is simple. Consider a PDE of the form

$$\mathcal{L}u = f \tag{4}$$

where $\mathcal{L}$ is a differential operator (e.g., $\mathcal{L} = \frac{\partial^2}{\partial x^2}$, or $\mathcal{L} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, etc.) and f is a right-hand side function. We consider a finite-dimensional subspace of functions V spanned by a basis $\psi_1, \ldots, \psi_N$. A typical choice for V is a space of (trigonometric) polynomials of finite degree. We seek an approximate solution to the PDE by a linear combination of the ψ_n, i.e., $u_N(x) = \sum_{n=1}^N c_n \psi_n(x)$. Plugging $u_N(x)$ in the PDE we get the following linear equation in the unknowns (c_n):

$$\sum_{n=1}^{N} c_n \mathcal{L}\psi_n = f. \tag{5}$$

In general the equation will not have a solution, as there is no reason to expect that the original PDE has a solution in the subspace V. However, we can seek to satisfy equation (5) approximately. Assume that the $(\psi_n)_{1 \le n \le N}$ are an orthonormal family of functions, with respect to some inner product $\langle \cdot, \cdot \rangle$. Then instead of looking for (c_n) that satisfy (5), we will require only that the projection of $\mathcal{L}u_N - f$ on the subspace V is zero. This is the same as requiring that

$$\sum_{n=1}^{N} c_n \langle \mathcal{L}\psi_n, \psi_m \rangle = \langle f, \psi_m \rangle \qquad \forall m = 1, \ldots, N. \tag{6}$$

If we call A the matrix $A_{m,n} = \langle \mathcal{L}\psi_n, \psi_m \rangle$, we end up with a $N \times N$ linear system $Ac = \tilde{f}$, where $\tilde{f}_m = \langle f, \psi_m \rangle$.

Fourier approximation of functions

We consider the *truncated Fourier approximation* of a function f on the interval $[-1,1]$:

$$f(x) \approx \phi_N(x) = \sum_{n=-N/2+1}^{N/2} \widehat{f}_n e^{i\pi nx}, \quad x \in [-1,1], \tag{7}$$

where here and elsewhere in this section $N \geq 2$ is an even integer and

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

are the (Fourier) coefficients of this approximation. We want to analyse the approximation properties of (7).

Theorem 1 (The de la Valleé Poussin theorem)

If the function f is Riemann integrable and $\widehat{f_n} = \mathcal{O}(n^{-1})$ for $|n| \gg 1$, then $\phi_N(x) = f(x) + \mathcal{O}(N^{-1})$ as $N \to \infty$ for every point $x \in (-1, 1)$ where f is Lipschitz.

Carleson's Theorem

Let f be an L^2 periodic function with Fourier coefficients $\widehat{f}(n)$. Then

$$\lim_{N\to\infty} \sum_{|n|\leq N} \widehat{f}(n)e^{inx} = f(x)$$

for almost every x.

There exists a L^1 periodic function where the Fourier series diverges everywhere (Kolmogorov), however, the above result can be extended to L^p functions for $p > 1$.

Remark 2 (The Gibbs effect at the end points)

Note that if f is smoothly differentiable then, integrating by parts,

$$\widehat{f}_n = \frac{(-1)^{n+1}}{2\pi in}[f(1) - f(-1)] + \frac{1}{\pi in}\widehat{f'_n} = \mathcal{O}(n^{-1}) \text{ for } |n| \gg 1.$$

Since such an f is Lipschitz on $(-1, 1)$, we deduce from Theorem 1 that ϕ_N converges to f there with speed $\mathcal{O}(N^{-1})$. However, convergence with speed $\mathcal{O}(N^{-1})$ is very slow and moreover, we cannot guarantee convergence at the endpoints -1 and 1. In fact, it is possible to show that

$$\phi_N(\pm 1) \to \frac{1}{2}[f(-1) + f(1)] \text{ as } n \to \infty$$

and hence, unless f is periodic we fail to converge.

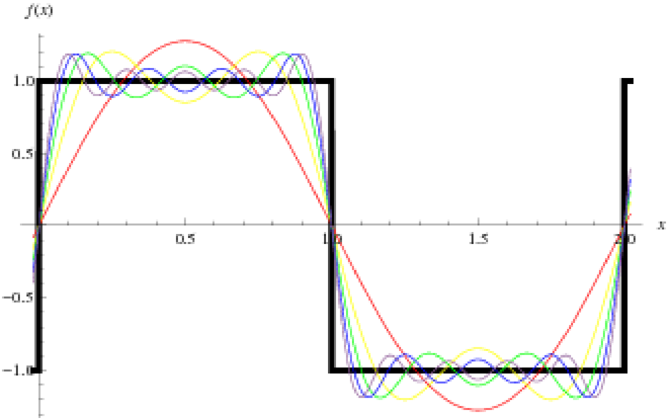


Figure: Convergence of the Fourier series

Fourier approximation for periodic functions

Suppose f is an analytic function in $[-1,1]$, that can be extended analytically to a closed complex domain Ω. In addition let f be periodic with period 2. In particular, $f^{(m)}(-1) = f^{(m)}(1)$ for all $m \in \mathbb{Z}_+$. Then, by multiple integration by parts, we get

$$\widehat{f}_n = \frac{1}{\pi i n}\widehat{f'_n} = \frac{1}{(\pi i n)^2}\widehat{f''_n} = \frac{1}{(\pi i n)^3}\widehat{f'''_n} = \dots .$$

Thus, we have

$$\widehat{f}_n = \frac{1}{(\pi i n)^m}\widehat{f_n^{(m)}}, \quad m = 0, 1, \dots . \tag{8}$$

But, how large is $\left|\widehat{f_n^{(m)}}\right|$?

To answer this question we use Cauchy's theorem of complex analysis, which states that

$$f^{(m)}(x) = \frac{m!}{2\pi i} \int_\gamma \frac{f(z)\, dz}{(z-x)^{m+1}}, \quad x \in [-1,1],$$

where γ is the positively oriented boundary of Ω. Therefore, with $\alpha^{-1} > 0$ being the minimal distance between γ and $[-1,1]$ and $M = \max\{|f(z)| : \ z \in \gamma\} < \infty$, it follows that

$$|f^{(m)}(x)| \leq \frac{m!}{2\pi} \int_\gamma \frac{|f(z)|\ |dz|}{|z-x|^{m+1}} \leq \frac{M \text{ length } \gamma}{2\pi} m!\, \alpha^{m+1},$$

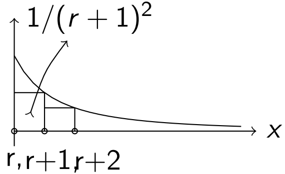
and hence, we can bound $\left|\widehat{f_n^{(m)}}\right| \leq c\, m!\, \alpha^{m+1}$ for some $c > 0$.

Now, using (8) and the above upper bound,

$$
\begin{aligned}
|\phi_N(x) - f(x)| &= \Big| \sum_{n=-N/2+1}^{N/2} \widehat{f}_n e^{i\pi n x} - \sum_{n=-\infty}^{\infty} \widehat{f}_n e^{i\pi n x} \Big| \\
&\leq \sum_{|n|\geq N/2} |\widehat{f}_n| = \sum_{|n|\geq N/2} \frac{|\widehat{f_n^{(m)}}|}{|\pi n|^m} \leq \frac{c m! \alpha^{m+1}}{\pi^m} \sum_{n=N/2}^{+\infty} \frac{1}{n^m} \, .
\end{aligned}
$$

Using, that for any $r \in \mathbb{N}$, and $m > 1$

$$\sum_{n=r+1}^{+\infty} \frac{1}{n^m} \leq \int_r^\infty \frac{dt}{t^m} = \frac{1}{m-1} r^{-m+1},$$



we deduce that

$$|\phi_N(x) - f(x)| \leq c' m! \left(\frac{\alpha}{\pi N}\right)^{m-1}, \quad m \geq 2.$$

Finally, we have a competition between $(\alpha/(\pi N))^{m-1}$ and $m!$ for large m. Because of Stirling's formula

$$m! \approx \sqrt{2\pi}\, m^{m+1/2} e^{-m}$$

we have

$$m! \Big(\frac{\alpha}{\pi N}\Big)^{m-1} \approx \sqrt{2\pi m}\, \frac{m}{e} \Big(\frac{\alpha m}{\pi e N}\Big)^{m-1}$$

which becomes very small for large N. Hence, $|\phi_N - f| = \mathcal{O}(N^{-p})$ for any $p \in \mathbb{N}$ and we deduce that the Fourier approximation of an analytic periodic function is of infinite order.

Definition 3 (Convergence at spectral speed)

An N-term approximation ϕ_N of a function f converges to f at *spectral* speed if $\|\phi_N - f\|$ decays faster than $\mathcal{O}(N^{-p})$ for any $p = 1, 2, \ldots$.

Remark 4

It is possible to prove that there exist constants $c_1, w > 0$ such that $\|\phi_N - f\| \leq c_1 e^{-wN}$ for all $N \in \mathbb{N}$ uniformly in $[-1, 1]$. Thus, convergence is at least at an exponential rate.

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.,

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

we have

$$f(x) + g(x) = \sum_{n=-\infty}^{\infty} (\widehat{f}_n + \widehat{g}_n) e^{i\pi nx}, \quad \alpha f(x) = \sum_{n=-\infty}^{\infty} \alpha \widehat{f}_n e^{i\pi nx}. \quad (9)$$

Moreover,

$$f(x)\cdot g(x)=\sum_{n=-\infty}^{\infty}\left(\sum_{m=-\infty}^{\infty}\widehat{f}_{n-m}\widehat{g}_m\right)e^{i\pi nx}=\sum_{n=-\infty}^{\infty}\left(\widehat{f}*\widehat{g}\right)_n e^{i\pi nx}, \tag{10}$$

where $*$ denotes the convolution operator (recall `https://en.wikipedia.org/wiki/Convolution`), hence $\widehat{(f\cdot g)}_n=(\widehat{f}*\widehat{g})_n$.
Moreover, if $f\in\mathcal{A}$ then $f'\in\mathcal{A}$ and

$$f'(x)=i\pi\sum_{n=-\infty}^{\infty}n\cdot\widehat{f}_n e^{i\pi nx}. \tag{11}$$

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.