Numerical Analysis - Part II

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Lecture 8

Partial differential equations of evolution

Solving the diffusion equation

We consider the solution of the *diffusion equation*

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

with *initial conditions* $u(x, 0) = u_0(x)$ for $t = 0$ and Dirichlet *boundary conditions* $u(0, t) = \phi_0(t)$ at $x = 0$ and $u(1, t) = \phi_1(t)$ at $x = 1$.

What if $-\infty < x < \infty$?

Fourier analysis of stability

Let us now assume a recurrence of the form

$$\sum_{k=r}^{s} a_k u_{m+k}^{n+1} = \sum_{k=r}^{s} b_k u_{m+k}^{n}, \qquad n \in \mathbb{Z}^+, \tag{1}$$

where m ranges over $\mathbb{Z}$. (Within our framework of discretizing PDEs of evolution, this corresponds to $-\infty < x < \infty$ in the undelying PDE and so there are no explicit boundary conditions, but the initial condition must be square-integrable in $(-\infty, \infty)$: this is known as a *Cauchy problem.*)

The coefficients a_k and b_k are independent of m, n, but typically depend upon μ. We investigate stability by *Fourier analysis.* [Note that it doesn't matter what is the underlying PDE: numerical stability is a feature of algebraic recurrences, not of PDEs!]

Fourier analysis of stability

Let $\mathbf{v} = (v_m)_{m\in\mathbb{Z}} \in \ell_2[\mathbb{Z}]$. Its *Fourier transform* is the function

$$\widehat{v}(\theta) = \sum_{m\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}m\theta} v_m, \qquad -\pi \le \theta \le \pi.$$

We equip sequences and functions with the norms

$$\|\mathbf{v}\| = \Big\{ \sum_{m\in\mathbb{Z}} |v_m|^2 \Big\}^{\frac{1}{2}} \qquad \text{and} \qquad \|\widehat{v}\|_* = \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} |\widehat{v}(\theta)|^2 d\theta \right\}^{\frac{1}{2}}.$$

Lemma 1 (Parseval's identity)

For any $\mathbf{v} \in \ell_2[\mathbb{Z}]$, *we have* $\|\mathbf{v}\| = \|\widehat{v}\|_*$.

Proof. By definition,

$$\begin{aligned} \|\widehat{v}\|_*^2 &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \Big|\sum_{m\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}m\theta} v_m\Big|^2 d\theta = \frac{1}{2\pi}\int_{-\pi}^{\pi} \sum_{m\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} v_m \bar{v}_k \mathrm{e}^{-\mathrm{i}(m-k)\theta} d\theta \\ &= \frac{1}{2\pi}\sum_{m\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} v_m\bar{v}_k \int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}(m-k)\theta} d\theta \overset{(*)}{=} \sum_{m\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} v_m \bar{v}_k \delta_{m-k} = \|\mathbf{v}\|^2, \end{aligned}$$

where equality $(*)$ is due to the fact that

$$\int_{-\pi}^{\pi} \mathrm{e}^{-\mathrm{i}\ell\theta} d\theta = \begin{cases} 2\pi, & \ell = 0, \\ 0, & \ell \in \mathbb{Z}\setminus\{0\}, \end{cases}$$

□

The implication of the lemma is that the Fourier transform is an *isometry* of the Euclidean norm. This is an important reason underlying its many applications in mathematics and beyond.

Amplification factor

For $\theta \in [-\pi, \pi]$, let $\widehat{u}^n(\theta) = \sum_{m\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}m\theta} u_m^n$ be the Fourier transform of the sequence $\mathbf{u}^n \in \ell_2[\mathbb{Z}]$. We multiply the discretized equations (1) by $\mathrm{e}^{-\mathrm{i}m\theta}$ and sum up for $m \in \mathbb{Z}$. Thus, the left-hand side yields

$$\begin{aligned}\sum_{m=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}m\theta} \sum_{k=r}^{s} a_k u_{m+k}^{n+1} &= \sum_{k=r}^{s} a_k \sum_{m=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}m\theta} u_{m+k}^{n+1} \\ &= \sum_{k=r}^{s} a_k \sum_{m=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}(m-k)\theta} u_m^{n+1} = \Big(\sum_{k=r}^{s} a_k \mathrm{e}^{\mathrm{i}k\theta}\Big)\widehat{u}^{n+1}(\theta).\end{aligned} \tag{2}$$

Similarly manipulating the right-hand side, we deduce that

$$\widehat{u}^{n+1}(\theta) = H(\theta)\widehat{u}^n(\theta)\,, \quad \text{where} \quad H(\theta) = \frac{\sum_{k=r}^{s} b_k \mathrm{e}^{\mathrm{i}k\theta}}{\sum_{k=r}^{s} a_k \mathrm{e}^{\mathrm{i}k\theta}}\,. \tag{3}$$

The function H is sometimes called the *amplification factor* of the recurrence (1)

Fourier analysis of stability

Theorem 2

The method (1) is stable $\Leftrightarrow$ $|H(\theta)| \leq 1$ *for all* $\theta \in [-\pi, \pi]$.

Stability: Euler and the diffusion equation

Consider the Cauchy problem for the diffusion equation.

1) For the Euler method

$$u_m^{n+1} = u_m^n + \mu(u_{m-1}^n - 2u_m^n + u_{m+1}^n)\,,$$

we obtain

$$H(\theta) = 1 + \mu\left(\mathrm{e}^{-\mathrm{i}\theta} - 2 + \mathrm{e}^{\mathrm{i}\theta}\right) = 1 - 4\mu\sin^2\tfrac{\theta}{2} \;\in\; [1-4\mu, 1]\,,$$

thus the method is stable iff $\mu \le \frac{1}{2}$.

Stability: Backward Euler and the diffusion equation

2) For the backward Euler method

$$u_m^{n+1} - \mu(u_{m-1}^{n+1} - 2u_m^{n+1} + u_{m+1}^{n+1}) = u_m^n\,,$$

we have

$$H(\theta) = \left[1 - \mu\left(\mathrm{e}^{-\mathrm{i}\theta} - 2 + \mathrm{e}^{\mathrm{i}\theta}\right)\right]^{-1} = \left[1 + 4\mu\sin^2\tfrac{\theta}{2}\right]^{-1} \in (0, 1]\,.$$

thus stability for all μ.

Stability: Crank–Nicolson and the diffusion equation

3) The Crank–Nicolson scheme

$$u_m^{n+1} - \tfrac{1}{2}\mu(u_{m-1}^{n+1} - 2u_m^{n+1} + u_{m+1}^{n+1}) = u_m^n + \tfrac{1}{2}\mu(u_{m-1}^n - 2u_m^n + u_{m+1}^n),$$

results in

$$H(\theta) = \frac{1 + \frac{1}{2}\mu(\mathrm{e}^{-\mathrm{i}\theta} - 2 + \mathrm{e}^{\mathrm{i}\theta})}{1 - \frac{1}{2}\mu(\mathrm{e}^{-\mathrm{i}\theta} - 2 + \mathrm{e}^{\mathrm{i}\theta})} = \frac{1 - 2\mu \sin^2 \frac{\theta}{2}}{1 + 2\mu \sin^2 \frac{\theta}{2}} \in (-1, 1]$$

Hence stability for all $\mu > 0$.

The advection and wave equations

Problem 3 (The advection equation)

A useful paradigm for hyperbolic PDEs is the *advection equation*

$$u_t = u_x, \qquad 0 \le x \le 1, \qquad t \ge 0, \tag{4}$$

where $u = u(x,t)$. It is given with the initial condition $u(x,0) = \varphi(x)$, $x \in [0,1]$ and (for simplicity) the boundary condition $u(1,t) = \varphi(t+1)$. The exact solution of (4) is simply $u(x,t) = \varphi(x+t)$, a unilateral shift leftwards. This, however, does not mean that its numerical modelling is easy.

Instability and the advection equation

We commence by semidiscretizing $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{2h}\left[u_{m+1}(t) - u_{m-1}(t)\right]$, so coming to the ODE $u_m'(t) = \frac{1}{2h}\left[u_{m+1}(t) - u_{m-1}(t)\right]$. For the Euler method, the outcome is

$$u_m^{n+1} = u_m^n + \tfrac{1}{2}\mu(u_{m+1}^n - u_{m-1}^n), \qquad m = 0...M, \quad n \in \mathbb{Z}_+,$$

with $u_0^n = 0$ for all n. In matrix form this reads

$$\mathbf{u}^{n+1} = A\mathbf{u}^n, \qquad A = \begin{bmatrix} 1 & \frac{1}{2}\mu & & \\ -\frac{1}{2}\mu & 1 & \ddots & \\ & \ddots & \ddots & \frac{1}{2}\mu \\ & & -\frac{1}{2}\mu & 1 \end{bmatrix}.$$

The matrix A is normal, with the eigenvalues $\lambda_\ell = 1 + i\mu\cos\ell\pi h$ (see Example 2.15), so that $\|A\|^2 = 1 + \mu^2$, hence instability for any μ.

The upwind method

If we semidiscretize $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{h}\left[u_{m+1}(t) - u_m(t)\right]$, and solve the ODE again by Euler's method, then the result is

$$u_m^{n+1} = u_m^n + \mu(u_{m+1}^n - u_m^n), \qquad m = 0 \ldots M, \quad n \in \mathbb{Z}_+ \qquad (5)$$

The local error is $\mathcal{O}(k^2 + kh)$ which is $\mathcal{O}(h^2)$ for a fixed μ, hence convergence if the method is stable.

The upwind method

The eigenvalue analysis of stability does not apply here, since the matrix A in $\mathbf{u}^{n+1} = A\mathbf{u}^n$ is no longer normal (see Example 2.16), so we do it directly (as in Lecture 5). We let the boundary condition at $x = 1$ be zero and define $\|\mathbf{u}^n\| = \max_m |u_m^n|$. It follows at once from (5) that

$$\|\mathbf{u}^{n+1}\| = \max_m |u_m^{n+1}| \le \max_m \{|1-\mu|\,|u_m^n| + \mu\,|u_{m+1}^n|\} \le (|1-\mu| + \mu)\|\mathbf{u}^n\|,$$

Therefore, $\mu \in (0,1]$ means that $\|\mathbf{u}^{n+1}\| \le \|\mathbf{u}^n\| \le \cdots \le \|\mathbf{u}^0\|$, hence stability.

The leapfrog method

We semidicretize (4) as $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{2h}\left[u_{m+1}(t) - u_{m-1}(t)\right]$, but now solve the ODE with the second-order *midpoint rule*

$$\mathbf{y}_{n+1} = \mathbf{y}_{n-1} + 2k\mathbf{f}(t_n, \mathbf{y}_n), \qquad n \in \mathbb{Z}_+ .$$

The outcome is the two-step *leapfrog* method

$$u_m^{n+1} = \mu\left(u_{m+1}^n - u_{m-1}^n\right) + u_m^{n-1}. \tag{6}$$

The error is now $\mathcal{O}(k^3 + kh^2) = \mathcal{O}(h^3)$.

Stability of the leapfrog method with Fourier analysis

We analyse stability by the Fourier technique, assuming that we are solving a Cauchy problem. Thus, proceeding as before,

$$\widehat{u}^{n+1}(\theta) = \mu\left(\mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{-\mathrm{i}\theta}\right)\widehat{u}^{n}(\theta) + \widehat{u}^{n-1}(\theta) \tag{7}$$

whence

$$\widehat{u}^{n+1}(\theta) - 2\mathrm{i}\mu\,\sin\theta\,\widehat{u}^{n}(\theta) - \widehat{u}^{n-1}(\theta) = 0, \qquad n \in \mathbb{Z}_+\,,$$

and our goal is to determine values of μ such that $|\widehat{u}^{n}(\theta)|$ is uniformly bounded for all n, θ.

Stability of the leapfrog method with Fourier analysis

This is a difference equation $w_{n+1} + bw_n + cw_{n-1} = 0$ with the general solution $w_n = c_1\lambda_1^n + c_2\lambda_2^n$, where λ_1, λ_2 are the roots of the characteristic equation $\lambda^2 + b\lambda + c = 0$, and c_1, c_2 are constants, dependent on the initial values w_0 and w_1. If $\lambda_1 = \lambda_2$, then solution is $w_n = (c_1 + c_2 n)\lambda^n$. In our case, we obtain

$$\lambda_{1,2}(\theta) = \mathrm{i}\mu \sin\theta \pm \sqrt{1 - \mu^2 \sin^2\theta}\,.$$

Stability is equivalent to $|\lambda_{1,2}(\theta)| \leq 1$ for all θ and this is true if and only if $\mu \leq 1$.

Stability in the presence of boundaries

It is easy to extend Fourier analysis for the Euler method $u_m^{n+1} = u_m^n + \mu(u_{m+1}^n - u_m^n)$, with the initial condition $u(x,0) = \phi(x)$, $x \in [0,1)$, and zero boundary condition along $x = 1$.

Consider the Cauchy problem for the advection equation with the initial condition $u(x,0) = \phi(x)$ for $x \in [0,1)$, and $u(x,0) = 0$ otherwise (it isn't differentiable, but this is not much of a problem). Solving the Cauchy problem with Euler, we recover $\mathbf{u}^n$ that is identical to the solution obtained from the zero boundary condition.

Stability in the presence of boundaries

This justifies using Fourier analysis for the problem with a boundary, and we obtain

$$\widehat{u}^{n+1}(\theta) = H(\theta)\,\widehat{u}^{n}(\theta)\,, \qquad H(\theta) = (1-\mu) + \mu e^{\mathrm{i}\theta}\,,$$

so that $\max|H(\theta)| = |1-\mu| + |\mu|$, hence stability if and only if $\mu \leq 1$.

Unfortunately, this is no longer true for leapfrog. Closer examination reveals that we cannot use leapfrog at $m = 0$, since u^n_{-1} is unknown. The naive remedy, setting $u^n_{-1} = 0$, leads to instability, which propagates from the boundary inwards. We can recover stability letting, for example, $u_0^{n+1} = u_1^n$ (the proof is *very* difficult).

The wave equation

Consider the wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \qquad x \in [0,1], \qquad t \geq 0,$$

given with initial (for u and u_t) and boundary conditions. The usual approximation looks as follows

$$u_m^{n+1} - 2u_m^n + u_m^{n-1} = \mu(u_{m+1}^n - 2u_m^n + u_{m-1}^n),$$

with the Courant number being now $\mu = k^2/h^2$.

Discretising the wave equation

To advance in time we have to pick up the numbers $u_m^1 = u(x_m, k)$ (of course they should depend on the initial derivative $u_t(x, 0)$. Euler's method provides the obvious choice $u(x_m, k) = u(x_m, 0) + ku_t(x_m, 0)$, but the following technique enjoys better accuracy. Specifically, we set u_m^1 to the right-hand side of the formula

$$\begin{aligned} u(x_m, k) &\approx u(x_m, 0) + ku_t(x_m, 0) + \tfrac{1}{2}k^2 u_{tt}(x_m, 0) \\ &= u(x_m, 0) + ku_t(x_m, 0) + \tfrac{1}{2}k^2 u_{xx}(x_m, 0) \\ &\approx u_m^0 + \tfrac{1}{2}\mu(u_{m-1}^0 - 2u_m^0 + u_{m+1}^0) + ku_t(x_m, 0)\,. \end{aligned}$$

Stability using Fourier analysis

The Fourier analysis (for Cauchy problem) provides

$$\widehat{u}^{n+1}(\theta) - 2\widehat{u}^{n}(\theta) + \widehat{u}^{n-1}(\theta) = -4\mu \sin^2 \tfrac{\theta}{2}\, \widehat{u}^{n}(\theta)\,,$$

with the characteristic equation $\lambda^2 - 2(1 - 2\mu \sin^2 \frac{\theta}{2})\lambda + 1 = 0$. The product of the roots is one, therefore stability (that requires the moduli of both λ to be at most one) is equivalent to the roots being complex conjugate, so we require

$$(1 - 2\mu \sin^2 \tfrac{\theta}{2})^2 \leq 1.$$

This condition is achieved if and only if $\mu = k^2/h^2 \leq 1$.