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 $\boldsymbol{v} = (v_m)_{m\in\mathbb{Z}} \in \ell_2[\mathbb{Z}]$. 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

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

Parseval's identity

Lemma 1 (Parseval's identity)

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

Proof. By definition,

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

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 $\boldsymbol{u}^n \in \ell_2[\mathbb{Z}]$. 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 $\quad \Leftrightarrow \quad |H(\theta)| \leq 1$ *for all* $\theta \in [-\pi, \pi]$.

Proof. The definition of stability is equivalent to the statement that there exists $c > 0$ such that $\|\boldsymbol{u}^n\| \leq c$ for all $n \in \mathbb{Z}^+$. [Because we are solving a Cauchy problem, equations are identical for all $h = \Delta x$, and this simplifies our analysis and eliminates a major difficulty: there is no need to insist explicitly that $\|\boldsymbol{u}^n\|$ remains uniformly bounded when $h \to 0$]. The Fourier transform being an isometry, stability is thus equivalent to $\|\widehat{u}^n\|_* \leq c$ for all $n \in \mathbb{Z}^+$. Iterating (3), we obtain

$$\widehat{u}^n(\theta) = [H(\theta)]^n \widehat{u}^0(\theta), \qquad |\theta| \leq \pi, \quad n \in \mathbb{Z}^+. \tag{4}$$

Proof. (Continuing)
1) Assume first that $|H(\theta)| \leq 1$ for all $|\theta| \leq \pi$. Then, by (4),

$$|\widehat{u}^n(\theta)| \leq |\widehat{u}^0(\theta)|$$
$$\Rightarrow \quad \|\widehat{u}^n\|_*^2 = \frac{1}{2\pi}\int_{-\pi}^{\pi} |\widehat{u}^n(\theta)|^2 \mathrm{d}\theta \leq \frac{1}{2\pi}\int_{-\pi}^{\pi} |\widehat{u}^0(\theta)|^2 \mathrm{d}\theta = \|\widehat{u}^0\|_*^2. \tag{5}$$

Hence stability.

Fourier analysis of stability (proof)

Proof. (Continuing) 2) Suppose, on the other hand, that there exists $\theta_0 \in [-\pi, \pi]$ such that $|H(\theta_0)| = 1 + 2\epsilon > 1$, say. Since H is continuous, there exist $-\pi \le \theta_1 < \theta_2 \le \pi$ such that $|H(\theta)| \ge 1 + \epsilon$ for all $\theta \in [\theta_1, \theta_2]$. We set $\eta = \theta_2 - \theta_1$ and choose as our initial condition the function (or the $\ell_2[\mathbb{Z}]$-sequence)

$$\widehat{u}^0(\theta) = \begin{cases} \sqrt{\frac{2\pi}{\eta}}, & \theta_1 \le \theta \le \theta_2, \\ 0, & \text{otherwise}, \end{cases}$$

Then

$$\begin{aligned} \|\widehat{u}^n\|_*^2 &= \frac{1}{2\pi}\int_{-\pi}^{\pi} |H(\theta)|^{2n} |\widehat{u}^0(\theta)|^2 \mathrm{d}\theta = \frac{1}{2\pi}\int_{\theta_1}^{\theta_2} |H(\theta)|^{2n} |\widehat{u}^0(\theta)|^2 \mathrm{d}\theta \\ &\ge \frac{1}{2\pi}(1+\epsilon)^{2n} \int_{\theta_1}^{\theta_2} \frac{2\pi}{\eta} \mathrm{d}\theta = (1+\epsilon)^{2n} \to \infty \quad (n \to \infty). \end{aligned}$$

We deduce that the method is unstable. □

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.

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

We look at the *advection equation* which we already considered in Lecture 6.

$$u_t = u_x, \qquad t \geq 0, \tag{6}$$

where $u = u(x,t)$. It is given with the initial condition $u(x,0) = \varphi(x)$. The exact solution of (6) 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

1) *Downwind instability*: Consider the discretization $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{2h}\left[u_m(t) - u_{m-1}(t)\right]$, so coming to the ODE $u_m'(t) = \frac{1}{2h}\left[u_m(t) - u_{m-1}(t)\right]$. For the Euler method, the outcome is

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

We can analyze the stability of this method using Fourier analysis. The amplification factor is

$$H(\theta) = 1 + \mu - \mu e^{-\mathrm{i}\theta}.$$

We see that for $\theta = \pi/2$, $|H(\theta)|^2 = (1+\mu)^2 + \mu^2 > 1$, and so the method is unstable for all $\mu > 0$.

The upwind method

Upwind scheme: 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

$$u_m^{n+1} = u_m^n + \mu(u_{m+1}^n - u_m^n), \quad n \in \mathbb{Z}_+ \tag{7}$$

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. We can again use Fourier analysis to analyze stability. The amplification factor is

$$H(\theta) = 1 - \mu + \mu e^{i\theta}$$

and we see that $|H(\theta)| = |1 - \mu + \mu e^{i\theta}| \le |1 - \mu| + \mu = 1$ for $\mu \in [0, 1]$. Hence we have stability for $\mu \le 1$. If $\mu > 1$, then note that $|H(\pi)| = |1 - 2\mu| > 1$, and so we have instability for $\mu > 1$.

Matlab demo: Download the Matlab GUI for *Solving the Advection Equation, Upwinding and Stability* from `https://www.damtp.cam.ac.uk/user/hf323/M21-II-NA/demos/index.html` and solve the advection equation (6) with the different methods provided in the demonstration. Experience what can go wrong when "winding" in the wrong direction!

Euler for advection equation – Upwind method

What about the case when $0 \leq x \leq 1$ (bounded domain)?

Recall from Lecture 6 when we considerd the Euler method for the advection equation

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

We have $\boldsymbol{u}^{n+1} = A\boldsymbol{u}^n$, where

$$A = \begin{bmatrix} 1-\mu & \mu & & \\ & 1-\mu & \ddots & \\ & & \ddots & \mu \\ & & & 1-\mu \end{bmatrix},$$

but A is *not* normal, and although its eigenvalues are bounded by 1 for $\mu \leq 2$ (note $1-\mu$ is the only eigenvalue of A), it is the matrix induced norm of A that matters. For this example, it is easier to work with $\|A\|_{\infty\to\infty}$ which we see is given by $|1-\mu| + \mu$ (by the formula in Lecture 5), and this is smaller than 1 precisely when $\mu \leq 1$.

The leapfrog method

Leap-frog method: We semidicretize (6) 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*

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

The outcome is the two-step *leapfrog* method

$$u_m^{n+1} = \mu\,(u_{m+1}^n - u_{m-1}^n) + u_m^{n-1}. \tag{8}$$

The local 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,

$$\widehat{u}^{n+1}(\theta) = \mu\left(e^{i\theta} - e^{-i\theta}\right)\widehat{u}^{n}(\theta) + \widehat{u}^{n-1}(\theta) \qquad (9)$$

whence

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

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 $\mu \leq 1$.

The wave equation

Consider the wave equation

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

given with initial conditions $u(x, 0)$ and $u_t(x, 0) = \frac{\partial u}{\partial t}(x, 0)$. 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 $\mu = k^2/h^2$.

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 $\mu = k^2/h^2 \leq 1$.

Recall: For any quadratic equation $ax^2 + bx + c = 0$ whose roots are α and β, the sum of the roots, $\alpha + \beta = -\frac{b}{a}$. The product of the roots, $\alpha \times \beta = \frac{c}{a}$.

The diffusion equation in two space dimensions

The diffusion equation in two space dimensions

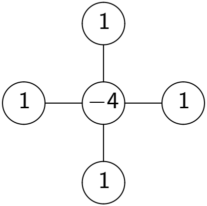
We are solving

$$\frac{\partial u}{\partial t} = \nabla^2 u, \qquad 0 \leq x, y \leq 1, \quad t \geq 0, \tag{10}$$

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

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

or in the matrix form

$$\boldsymbol{u}' = \frac{1}{h^2}A_*\boldsymbol{u}, \qquad \boldsymbol{u} = (u_{\ell,m}) \in \mathbb{R}^N, \tag{11}$$

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

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

The diffusion equation in two space dimensions

Thus, the Euler method yields

$$u_{\ell,m}^{n+1} = u_{\ell,m}^{n} + \mu(u_{\ell-1,m}^{n} + u_{\ell+1,m}^{n} + u_{\ell,m-1}^{n} + u_{\ell,m+1}^{n} - 4u_{\ell,m}^{n}), \quad (12)$$

or in the matrix form

$$\boldsymbol{u}^{n+1} = A\boldsymbol{u}^{n}, \qquad A = I + \mu A_*$$

where, as before, $\mu = \frac{k}{h^2} = \frac{\Delta t}{(\Delta x)^2}$. The local error is $\boldsymbol{\eta} = \mathcal{O}(k^2 + kh^2) = \mathcal{O}(h^4)$. To analyse stability, we notice that A is symmetric, hence normal, and its eigenvalues are related to those of A_* by the rule

$$\lambda_{k,\ell}(A) = 1 + \mu\lambda_{k,\ell}(A_*) \stackrel{\text{Prop. 1.12}}{=} 1 - 4\mu\left(\sin^2\frac{\pi kh}{2} + \sin^2\frac{\pi\ell h}{2}\right).$$

Consequently,

$$\sup_{h>0}\rho(A) = \max\{1, |1-8\mu|\}, \qquad \text{hence} \qquad \mu \le \tfrac{1}{4} \quad \Leftrightarrow \quad \text{stability.}$$