Numerical Analysis - Part II

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Lecture 9

Partial differential equations of evolution

We consider the solution of the diffusion equation

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

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 $-\infty < x < \infty$?

Let us now assume a recurrence of the form

$$\sum_{k=r}^{s} a_{k} u_{m+k}^{n+1} = \sum_{k=r}^{s} b_{k} u_{m+k}^{n}, \qquad n \in \mathbb{Z}^{+},$$
(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!]

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

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

We equip sequences and functions with the norms

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

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Amplification factor

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

$$\sum_{m=-\infty}^{\infty} e^{-im\theta} \sum_{k=r}^{s} a_k u_{m+k}^{n+1} = \sum_{k=r}^{s} a_k \sum_{m=-\infty}^{\infty} e^{-im\theta} u_{m+k}^{n+1}$$
$$= \sum_{k=r}^{s} a_k \sum_{m=-\infty}^{\infty} e^{-i(m-k)\theta} u_m^{n+1} = \left(\sum_{k=r}^{s} a_k e^{ik\theta}\right) \widehat{u}^{n+1}(\theta).$$
(2)

Similarly manipulating the right-hand side, we deduce that

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

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

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

The advection and wave equations

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

$$u_t = u_x, \qquad t \ge 0, \qquad (4)$$

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

1) Downwind instability: Consider the discretization $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{h} [u_m(t) - u_{m-1}(t)]$, so coming to the ODE $u'_m(t) = \frac{1}{h} [u_m(t) - u_{m-1}(t)]$. 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 $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{h} [u_{m+1}(t) - u_m(t)]$, and solve the ODE again by Euler's method, then the result is

$$u_m^{n+1} = u_m^n + \mu (u_{m+1}^n - u_m^n), \quad n \in \mathbb{Z}_+$$
(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. We can again use Fourier analysis to analyze stability. The amplification factor is

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

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 (4) with the different methods provided
in the demonstration. Experience what can go wrong when "winding" in
the wrong direction!

The leapfrog method

Leap-frog method: We semidicretize (4) as $\frac{\partial u_m(t)}{\partial x} \approx \frac{1}{2h} [u_{m+1}(t) - u_{m-1}(t)]$, 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

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

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

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

$$\widehat{u}^{n+1}(\theta) = \mu \left(e^{i\theta} - e^{-i\theta} \right) \widehat{u}^n(\theta) + \widehat{u}^{n-1}(\theta)$$
(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 $|\hat{u}^n(\theta)|$ is uniformly bounded for all n, θ .

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

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

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

Consider the wave equation

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

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

The Fourier analysis (for Cauchy problem) provides

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

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

$$(1-2\mu\sin^2\frac{\theta}{2})^2 \le 1.$$

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

We are solving

$$\frac{\partial u}{\partial t} = \nabla^2 u, \qquad 0 \le x, y \le 1, \quad t \ge 0,$$
(8)

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

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 $u_{\ell,m}^n \approx u_{\ell,m}(nk)$ 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

$$\boldsymbol{u}' = rac{1}{h^2} A_* \boldsymbol{u}, \qquad \boldsymbol{u} = (u_{\ell,m}) \in \mathbb{R}^N,$$
 (9)

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

$$u_{\ell,m}^{n+1} = u_{\ell,m}^n + \mu (u_{\ell-1,m}^n + u_{\ell+1,m}^n + u_{\ell,m-1}^n + u_{\ell,m+1}^n - 4u_{\ell,m}^n),$$
(10)

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 $\eta = \mathcal{O}(k^2 + kh^2) = \mathcal{O}(h^4)$. 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,

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

Fourier analysis generalizes to two dimensions: of course, we now need to extend the range of (x, y) in (8) from $0 \le x, y \le 1$ to $x, y \in \mathbb{R}$. A 2D Fourier transform reads

$$\widehat{u}(\theta,\psi) = \sum_{\ell,m\in\mathbb{Z}} u_{\ell,m} \mathrm{e}^{-\mathrm{i}(\ell\theta+m\psi)}$$

and all our results readily generalize.

In particular, the Fourier transform is an isometry from $\ell_2[\mathbb{Z}^2]$ to $L_2([-\pi,\pi]^2)$, i.e.

$$\Big(\sum_{\ell,m\in\mathbb{Z}}|u_{\ell,m}|^2\Big)^{1/2}=:\|\boldsymbol{u}\|=\|\widehat{u}\|_*:=\Big(\frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}|\widehat{u}(\theta,\psi)|^2\,d\theta\,d\psi\Big)^{1/2},$$

and the method is stable iff $|H(\theta, \psi)| \leq 1$ for all $\theta, \psi \in [-\pi, \pi]$. The proofs are an easy elaboration on the one-dimensional theory. Insofar as the Euler method (10) is concerned,

$$H(\theta,\psi) = 1 + \mu \left(e^{-i\theta} + e^{i\theta} + e^{-i\psi} + e^{i\psi} - 4 \right) = 1 - 4\mu \left(\sin^2 \frac{\theta}{2} + \sin^2 \frac{\psi}{2} \right),$$

and we again deduce stability if and only if $\mu \leq \frac{1}{4}$.

Parseval's identity

Lemma 2 (Parseval's identity)

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

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

where equality (*) is due to the fact that

$$\int_{-\pi}^{\pi}\mathrm{e}^{-\mathrm{i}\ell heta}d heta= \left\{egin{array}{cc} 2\pi, & \ell=0, \ 0, & \ell\in\mathbb{Z}\setminus\{0\}, \end{array}
ight.$$

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.

Applying the trapezoidal rule to our semi-dicretization (9) we obtain the two-dimensional Crank-Nicolson method:

$$(I - \frac{1}{2}\mu A_*) \boldsymbol{u}^{n+1} = (I + \frac{1}{2}\mu A_*) \boldsymbol{u}^n, \qquad (11)$$

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

$$\lambda(A) = rac{\lambda(\mathcal{C})}{\lambda(B)} = rac{1+rac{1}{2}\mu\lambda(A_*)}{1-rac{1}{2}\mu\lambda(A_*)} \hspace{3mm} \Rightarrow \hspace{3mm} |\lambda(A)| < 1 ext{ as } \lambda(A_*) < 0$$

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

We would like to find a fast solver to the system (11). The matrix $B = I - \frac{1}{2}\mu A_*$ has a structure similar to that of A_* , where

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

so we may apply the Hockney method.

The total computational cost per iteration is $\mathcal{O}(M^2 \log M)$ for a $M \times M$ discretization grid.

Matlab demo: Download the Matlab GUI for *Solving the Wave* and *Diffusion Equations in 2D* from http://www.damtp.cam.ac. uk/user/hf323/M21-II-NA/demos/pdes_2d/pdes_2d.html and solve the diffusion equation (8) for different initial conditions. For the numerical solution of the equation you can choose from the Euler method and the Crank-Nicolson scheme. The GUI allows you to solve the wave equation as well. Compare the behaviour of solutions!

Splitting

In all the examples of semi-discretization we have seen so far, we always reach a linear system of ODE of the form:

$$\boldsymbol{u}' = A\boldsymbol{u}, \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0. \tag{12}$$

The solution of this linear system of ODE is given by

$$\boldsymbol{u}(t) = \mathrm{e}^{tA} \boldsymbol{u}_0 \tag{13}$$

where the *matrix exponential* function is defined by $e^B := \sum_{k=0}^{\infty} \frac{1}{k!} B^k$. It is easily verified that $de^{tA}/dt = Ae^{tA}$, therefore (13) is indeed a solution of (12).

If A can be diagonalized $A = VDV^{-1}$, then $e^{tA} = Ve^{tD}V^{-1}$ where e^{tD} is the diagonal matrix consisting diag $(e^{tD_{ii}})$. As such one can compute the solution of (12) exactly. However computing an eigenvalue decomposition can be costly, and so one would like to consider more efficient methods, based on the solution of sparse linear systems instead. Observe that one-step methods for solving (12) are approximating a matrix exponential. Indeed, with $k = \Delta t$, we have:

Euler:
$$\boldsymbol{u}^{n+1} = (l + kA)\boldsymbol{u}^n$$
, $e^z = 1 + z + \mathcal{O}(z^2)$;
Implicit Euler: $\boldsymbol{u}^{n+1} = (l - kA)^{-1}\boldsymbol{u}^n$, $e^z = (1 - z)^{-1} + \mathcal{O}(z^2)$;
Trapezoidal: $\boldsymbol{u}^{n+1} = (l - \frac{1}{2}kA)^{-1}(l + \frac{1}{2}kA)\boldsymbol{u}^n$, $e^z = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z} + \mathcal{O}(z^3)$.

In practice the matrix A is very sparse, and this can be exploited when solving linear systems e.g., for the implicit Euler or Trapezoidal Rule.

Splitting

In many cases, the matrix A is naturally expressed as a sum of two matrices, A = B + C. For example, when discretizing the diffusion equation in 2D with zero boundary conditions, we have $A = \frac{1}{h^2}(A_x + A_y)$ where $\frac{1}{h^2}A_x \in \mathbb{R}^{M^2 \times M^2}$ corresponds to the 3-point discretization of $\frac{\partial^2}{\partial x^2}$, and $\frac{1}{h^2}A_y \in \mathbb{R}^{M^2 \times M^2}$ corresponds to the 3-point discretization of $\frac{\partial^2}{\partial y^2}$. In matrix notations, if the grid points are ordered by columns, then we have:

$$A_{x} = \begin{bmatrix} -2I & I \\ I & \ddots & \ddots \\ & \ddots & \ddots & I \\ & I & -2I \end{bmatrix}, A_{y} = \begin{bmatrix} G \\ G \\ & \ddots \\ & G \end{bmatrix}, G = \begin{bmatrix} -2 & 1 \\ 1 & \ddots & \ddots \\ & \ddots & 1 \\ & 1 & -2 \end{bmatrix} \in \mathbb{R}^{M \times M}$$
(14)

Remark: It is convenient to note that $A_x = G \otimes I$ and $A_y = I \otimes G$, where \otimes is the Kronecker product of matrices (kron in Matlab) defined by

$$A \otimes B = \begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1m_A}B \\ A_{21}B & A_{22}B & \dots & A_{2m_A}B \\ \vdots & & & \\ A_{n_A1}B & \dots & \dots & A_{n_Am_A}B \end{bmatrix} \in \mathbb{R}^{n_A n_B \times m_A m_B}$$

where $A \in \mathbb{R}^{n_A \times m_A}$ and $B \in \mathbb{R}^{n_B \times m_B}$.

In general, $\exp(t(B + C)) \neq \exp(tB) \exp(tC)$. Equality holds however when *B* and *C* commute.

Proposition 3

For any matrices B, C,

$$e^{t(B+C)} = e^{tB}e^{tC} + \frac{1}{2}t^2(CB - BC) + O(t^3).$$
 (15)

If B and C commute, then $\mathrm{e}^{B+C}=\mathrm{e}^{B}\mathrm{e}^{C}.$

Proof. We Taylor-expand both expressions $e^{tB}e^{tC}$ and $e^{t(B+C)}$:

$$e^{tB}e^{tC} = (I + tB + t^2B^2/2 + \mathcal{O}(t^3))(I + tC + t^2C^2/2 + \mathcal{O}(t^3))$$
$$= I + t(B + C) + \frac{t^2}{2}(B^2 + C^2 + 2BC) + \mathcal{O}(t^3)$$

and

$$e^{t(B+C)} = I + t(B+C) + \frac{t^2}{2}(B+C)^2 + \mathcal{O}(t^3)$$
$$= I + t(B+C) + \frac{t^2}{2}(B^2 + C^2 + BC + CB) + \mathcal{O}(t^3)$$

Equation (15) follows.

Splitting the exponential

Proof.

When B and C commute, we can write:

$$\exp(B+C) = \sum_{n=0}^{\infty} \frac{1}{n!} (B+C)^n = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\sum_{k=0}^n \binom{n}{k} B^{n-k} C^k \right) = \sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \frac{1}{n!} \binom{n}{k} B^{n-k} C^k$$

Recall that $\binom{n}{k} = \frac{n!}{k!(n-k)!}$, so
$$\exp(B+C) = \sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \frac{1}{k!(n-k)!} B^{n-k} C^k = \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{k!m!} B^m C^k = e^B e^C.$$