Numerical Analysis – Lecture 19[1]

5 Partial differential equations of evolution

Method 5.1 We consider the solution of the *diffusion equation*

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

where $u = u(x,t)$ is given for $0 \le x \le 1$, $t \ge 0$, with *initial conditions* for $t = 0$ and Dirichlet *boundary conditions* at $x = 0$ and $x = 1$. By Taylor's expansion

$$\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= \frac{1}{\Delta t}[u(x,t+\Delta t) - u(x,t)] + \mathcal{O}((\Delta t))\,, \\
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{(\Delta x)^2}[u(x-\Delta x,t) - 2u(x,t) + u(x+\Delta x,t)] + \mathcal{O}\big((\Delta x)^2\big)\,,
\end{aligned}$$

motivating the numerical scheme

$$u_m^{n+1} = u_m^n + \mu\left(u_{m-1}^n - 2u_m^n + u_{m+1}^n\right), \qquad m = 1,2,\ldots,M, \tag{5.1}$$

where $\Delta x = 1/(M+1)$, $u_m^n \approx u(m\Delta x, n\Delta t)$, while $\mu = \Delta t/(\Delta x)^2$ is the *Courant number.* Substituting whenever necessary initial conditions u_m^0 and boundary conditions u_0^n and u_M^n, we possess enough information to advance (5.1) from $\boldsymbol{u}^n$ to $\boldsymbol{u}^{n+1}$ for $n \in \mathbb{Z}^+$.

The question of *convergence* of the method (5.1) is of crucial importance. Specifically, *keeping μ fixed* and letting $\Delta x \to 0$,[2] we ask whether, for every $T > 0$, it is true that $u_m^n \to u(x,t)$ uniformly for $m\Delta x \to x \in [0,1]$, $n\Delta t \to t \in [0,T]$. Like for ODEs or for the Poisson equation, unless convergence takes place, the method should never be used! In the present case, however, a method has an extra parameter, μ. It is entirely possible for a method to converge for some choice of μ and diverge otherwise.

Theorem 5.2 *$\mu \le \frac{1}{2} \Rightarrow$ convergence.*

Proof Let $e_m^n := u_m^n - u(m\Delta x, n\Delta t)$, $m = 1,2,\ldots,M$, $n \ge 0$. Convergence is equivalent to

$$\lim_{\Delta x \downarrow 0} \max_{\substack{m=1,2,\ldots,M \\ 0 \le n \le T/\Delta t}} |e_m^n| = 0$$

for every constant $T > 0$. Since $\mathcal{O}(\Delta t) = \mathcal{O}\big((\Delta x)^2\big)$, it follows from (5.1) that there exists $C > 0$ such that $|e_m^{n+1} - e_m^n - \mu(e_{m-1}^n - 2e_m^n + e_{m+1}^n)| \le C(\Delta x)^4$. Let $\eta^n := \max_{m=1,\ldots,M} |e_m^n|$. Then

$$\begin{aligned}
|e_m^{n+1}| &\le |\mu e_{m-1}^n + (1-2\mu)e_m^n + \mu e_{m+1}^n| + C(\Delta x)^4 \le (2\mu + |1-2\mu|)\eta^n + C(\Delta x)^4 \\
&= \eta^n + C(\Delta x)^4,
\end{aligned}$$

by virtue of $\mu \le \frac{1}{2}$. Since $\eta^0 = 0$, induction yields

$$\eta^n \le Cn(\Delta x)^4 \le CT(\Delta x)^4/(\Delta t) = CT(\Delta x)^2/\mu \to 0$$

as $\Delta x \downarrow 0$. □

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[1] Please email all corrections and suggestions to these notes to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartII/Handouts.html`.

[2] Observe that Δt also tends to zero, since $\Delta t = \mu(\Delta x)^2$.

Discussion 5.3 In practice we wish to choose Δx and Δt of comparable size, therefore $\mu = (\Delta t)/(\Delta x)^2$ is likely to be large. Consequently, the restriction of the last theorem is disappointing: unless we are willing to advance with tiny time step Δt, the method (5.1) is of limited practical interest. The situation is similar to stiff ODEs: like the Euler method, the scheme (5.1) is simple, plausible, explicit, easy to execute and analyse – but of very limited utility….

Definition 5.4 *(Stability in the context of time-stepping methods for PDEs of evolution)* A numerical method for a PDE of evolution is *stable* if (for zero boundary conditions) it produces a uniformly bounded approximation of the solution in any bounded interval of the form $0 \le t \le T$ when $\Delta x \to 0$ and the Courant number (or a generalization thereof) is constant. This definition is relevant not just for the diffusion equation but for every PDE of evolution which is *well posed*, i.e. such that its exact solution depends (in a compact time interval) in a uniformly bounded manner on the initial conditions.[3] Most PDEs of practical interest are well posed.

Theorem 5.5 *(The Lax equivalence theorem). Suppose that the underlying PDE is well posed and that it is solved by a numerical method with an error of $\mathcal{O}\big((\Delta x)^{p+1}\big)$, $p \ge 1$. Then stability $\Leftrightarrow$ convergence.*

Problem 5.6 *(Stability of (5.1)* Although we can deduce from the theorem that $\mu \le \frac{1}{2} \Rightarrow$ stability, we will prove directly that stability $\Leftrightarrow \mu \le \frac{1}{2}$. Let $\boldsymbol{u}^n = [u_1^n, u_2^n, \ldots, u_M^n]^\top$. We can express the recurrence (5.1) as $\boldsymbol{u}^{n+1} = A\boldsymbol{u}^n$, where A is TST, with $1-2\mu$ along the diagonal and μ in the subdiagonal. Hence $\sigma(A) = \{(1-2\mu) + 2\mu\cos\frac{\pi k}{M+1} \,:\, k = 1,\ldots,M\} = \{1 - 4\mu\sin^2\frac{\pi k}{2M+2} \,:\, k=1,\ldots,M\}$ and (A being symmetric)

$$\|A\|_2 = \rho(A) = \begin{cases} |1-4\mu\left(\sin\frac{\pi M}{2M+2}\right)^2| \le 1, & \mu \le \frac{1}{2}, \\ 4\mu\left(\sin\frac{\pi M}{2M+2}\right)^2 - 1 > 1, & \frac{1}{2} < \mu. \end{cases}$$

We distinguish between two cases.

(i) $\mu \le \frac{1}{2}$: $\|\boldsymbol{u}^{n+1}\| \le \|A\| \cdot \|\boldsymbol{u}^n\| \le \cdots \le \|A\|^{n+1}\|\boldsymbol{u}^0\| \le \|\boldsymbol{u}^0\|$ as $n \to \infty$, for every $\boldsymbol{u}^0$.

(ii) $\mu > \frac{1}{2}$: Choose $\boldsymbol{u}^0$ as the eigenvector corresponding to the largest (in modulus) eigenvalue, λ, say. Hence, by induction, $\boldsymbol{u}^n = \lambda^n\boldsymbol{u}^0$, becoming unbounded as $n \to \infty$.

Technique 5.7 *(The method of lines)* Let $u_m(t) = u(m\Delta x, t)$, $m = 0, 1, \ldots, M+1$, $t \ge 0$. Approximating $\partial^2/\partial x^2$ as before, we deduce from the PDE that the *semidiscretization*

$$\frac{\mathrm{d}u_m}{\mathrm{d}t} = \frac{1}{(\Delta x)^2}(u_{m-1} - 2u_m + u_{m+1}), \qquad m = 1, 2, \ldots, M \tag{5.2}$$

carries an error of $\mathcal{O}\big((\Delta x)^2\big)$. This is an *ODE system*, and we can solve it by any ODE solver. Thus, Euler's method yields (5.1), while backward Euler results in

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

This approach is commonly known as *the method of lines.* Much (although not all!) of the theory of finite-difference methods for PDEs of evolution can be presented as a two-stage task: first semidiscretize, getting rid of space variables, then use an ODE solver. Typically, each stage is conceptually easier than the process of discretizing in unison in both time and in space (so-called *full discretization*).

Method 5.8 *(The Crank–Nicolson scheme)* Discretizing the ODE (5.2) with the trapezoidal rule, we obtain

$$u_m^{n+1} - \tfrac{1}{2}\mu(u_{m-1}^{n+1} - 2u_m^{n+1} + u_{m+1}^{n+1}) = u_m^n + \tfrac{1}{2}\mu(u_{m-1}^n - 2u_m^n + u_{m-1}^n), \qquad m = 1, 2, \ldots, M. \tag{5.3}$$

Thus, each step requires the solution of an $M \times M$ TST system. The error is still $\mathcal{O}\big((\Delta x)^2\big)$ (inherited from space discretization). However, as we will see, Crank–Nicolson enjoys superior stability features, as compared with the method (5.1).

Note further that (5.3) is an *implicit* method: advancing each time step requires to solve a linear algebraic system. However, the matrix of the system is TST and its solution by sparse Cholesky factorization can be done in $\mathcal{O}(M)$ operations.

[3] Thus, "stability" is nothing but the statement that well posedness is retained under discretization, uniformly for $\Delta x \to 0$.