Numerical Solutions for Partial Differential Equations

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3.8 More general parabolic PDEs

The methods discussed in the previous sections apply to other parabolic PDEs, however the consistency and stability should be established for each case. In this section we consider more general parabolic PDEs.

3.8.1 Reaction-diffusion equation

Let us consider the model equation

$$u_t = \underbrace{\kappa u_{xx}}_{\text{diffusion}} + \underbrace{f(x,t,u)}_{\text{reaction}},$$

where f is a possibly nonlinear real function and κ is a positive real number. This equation is used to model predator-pray systems, disease models... We consider an example with a nonlinear function f given by

$$f(x,t,u) = u(1-u).$$

Any of the schemes described previously can be apply to equation (3.8.1), for example we consider a Crank-Nicolson method. Recall that the Crank-Nicolson method if the θ-method with $\theta = 1/2$, we have

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = \frac{1}{2}\left[\kappa \frac{\delta_x^2 U_{j,n}}{\Delta x^2} + U_{j,n}(1-U_{j,n})\right] + \frac{1}{2}\left[\kappa \frac{\delta_x^2 U_{j,n+1}}{\Delta x^2} + U_{j,n+1}(1-U_{j,n+1})\right]$$

which can be written as

$$U_{j,n+1} = U_{j,n} + \frac{s}{2}\delta_x^2 U_{j,n} + \frac{s}{2}\delta_x^2 U_{j,n+1} + \frac{\Delta t}{2} U_{j,n}(1-U_{j,n}) + \frac{\Delta t}{2} U_{j,n+1}(1-U_{j,n+1})$$

where $s = \kappa \Delta t/\Delta x^2$. As we said previously the above scheme is implicit. Implicit schemes are often difficult to use with nonlinear terms for it leads us to solve a nonlinear set of equations at each time step. We can alternatively use an explicit method, or mix an implicit method for the linear terms and an explicit method for the nonlinear terms. For example with equation (3.8.1) we obtain

$$U_{j,n+1} = U_{j,n} + \frac{s}{2}\delta_x^2 U_{j,n} + \frac{s}{2}\delta_x^2 U_{j,n+1} + U_{j,n}(1-U_{j,n})\Delta t.$$

3.8.2 Linear equation with variable coefficiants

Let us consider the PDE

$$u_t = A(x,t)u_{xx} + B(x,t)u_x + C(x,t)u,$$

where $A(x,t) > 0$. Again any of the schemes presented previously can be potentially apply to this equation, for example we consider a FTCS scheme

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} = A(x_j, t_n)\frac{\delta_x^2 U_{j,n}}{\Delta x^2} + B(x_j, t_n)\frac{D_x U_{j,n}}{2\Delta x} + C(x_j, t_n)U_{j,n}.$$

scheme	order	stability	comment
FTCS	$O(\Delta x^2, \Delta t)$	stable if $r \leq 1/2$	explicit, one-step
Crank-Nicolson	$O(\Delta x, \Delta t)$	unconditionally stable	implicit, one-step
Du Fort-Frankel	$O(\Delta x^2, \Delta t^2, r^2 \Delta x^2)$	need $\Delta t = O(\Delta x^2)$ for consistency	explicit, two-step

Table 1: summary

4 Hyperbolic equations

These equations typically model wave propagation. Let us consider the following 2nd order hyperbolic PDE, often called wave equation,

$$u_{tt} - a^2 u_{xx} = 0, \quad a \in \mathbb{R}, \tag{1}$$

together with the intitial condition $u(x, 0) = f(x)$ and the boundary condition $u_t = g(x)$. Consider the new variables $\zeta = x + at$ and $\eta = x - at$, the equation can be written as

$$u_{\eta\zeta} = 0. \tag{2}$$

D'Alembert's solution to this problem is given by

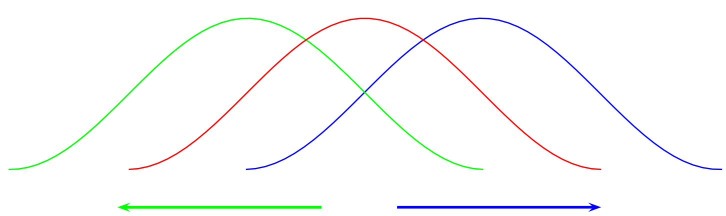
$$u(\eta, \zeta) = F(\eta) + G(\zeta), \tag{3}$$

in terms of the left travelling wave and the right travelling wave, which translate the shape of the initial condition to the left and to the right respectively. This result can be recovered by writing equation (1) as

$$\left(\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}\right)\left(\frac{\partial u}{\partial t} - a\frac{\partial u}{\partial x}\right) = 0, \tag{4}$$

which splits into the two first order hyperbolic equations

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0\ ,\ \frac{\partial u}{\partial t} - a\frac{\partial u}{\partial x} = 0. \tag{5}$$



4.1 Upwind schemes for $u_t + au_x = 0$

We talk about upwind schemes for approximations for which a forward difference operator is used for u_t, that is

$$\frac{\partial u}{\partial t} \approx \frac{F_t u}{\Delta t}.$$

For the aprroximation of u_x we can use either

- a backward difference, $u_x \approx B_x u/\Delta x$,
- a central difference, $u_x \approx D_x u/2\Delta x$,
- a forward difference, $u_x \approx F_x u/\Delta x$.

We will study these three schemes, ie FTBS, FTCS and FTFS.

We start with the FTCS scheme

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} + a\frac{U_{j+1,n} - U_{j-1,n}}{2\Delta x} = 0, \tag{6}$$

which can be written as

$$U_{j,n+1} = U_{j,n} - \frac{p}{2}(U_{j+1,n} - U_{j-1,n}),$$

where $p = a\Delta t/\Delta x$ is known as the CFL number (Courant-Friedrich-Levy, 1928). We study the stability, applying the scheme to a solution of the form $U_{j,n} = A\mathrm{e}^{\mathrm{i}\omega j}\xi^n$, we obtain

$$A\mathrm{e}^{\mathrm{i}\omega j}\xi^{n+1} = A\mathrm{e}^{\mathrm{i}\omega j}\xi^n - \frac{p}{2}(\mathrm{e}^{\mathrm{i}\omega(j+1)} - \mathrm{e}^{\mathrm{i}\omega(j-1)})A\xi^n,$$

dividing through by $A\mathrm{e}^{\mathrm{i}\omega j}\xi^n$ gives

$$\xi = 1 - \frac{p}{2}\left(\mathrm{e}^{\mathrm{i}\omega} - \mathrm{e}^{-\mathrm{i}\omega}\right)$$

and from $\mathrm{e}^{\mathrm{i}\omega} - \mathrm{e}^{-\mathrm{i}\omega} = 2\mathrm{i}\sin\omega$ we can write

$$\xi = 1 - \mathrm{i}p\sin\omega,$$

and we have

$$|\xi|^2 = 1 + p^2\sin^2\omega,$$

therefore $|\xi| \geq 1, \ \forall\omega$, the method is unstable. Then although the scheme is consistant (exercise) it may not converge.

We now consider the FTBS scheme, that is

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} + a\frac{U_{j,n} - U_{j-1,n}}{\Delta x} = 0, \tag{7}$$

that is

$$U_{j,n+1} = U_{j,n} - p(U_{j,n} - U_{j-1,n}).$$

We use equation (7) to compute the LTE, we have

$$\mathcal{L}_\Delta u(x,t) = \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} + a\frac{u(x,t) - u(x-\Delta),t}{\Delta x},$$

then using Taylor's theorem, we have

$$\begin{aligned}
\mathcal{L}_\Delta u &= \frac{1}{\Delta t}\left[u + u_t\Delta t + u_{tt}\frac{\Delta t^{\,2}}{2!} + u_{ttt}\frac{\Delta t^{\,3}}{3!} + O(\Delta t^{\,4}) - u\right] \\
&\quad + \frac{a}{\Delta x}\left[u - \left(u - u_x\Delta x + u_{xx}\frac{\Delta x^{\,2}}{2!} - u_{xxx}\frac{\Delta x^{\,3}}{3!} + O(\Delta t^{\,4})\right)\right] \\
&= \frac{1}{2}\left(u_{tt}\Delta t - au_{xx}\Delta x\right) + \frac{1}{3!}\left(u_{ttt}\Delta t^{\,2} + au_{xxx}\Delta x^{\,2}\right) + O(\Delta t^{\,3}, \Delta t^{\,3})
\end{aligned}$$

and from

$$\begin{aligned}
u_t &= -au_x \\
u_{tt} &= -a(u_t)_x = a^2 u_{xx} \\
u_{ttt} &= -a(u_t)_{xx} = -a^3 u_{xxx} \\
\dots &= \dots
\end{aligned}$$

we obtain

$$\mathcal{L}_\Delta u(x,t) = \frac{1}{2}\left(a\Delta t - \Delta x\right) a u_{xx} + \frac{1}{3!}\left(-a^2\Delta t^{\,2} + \Delta x^{\,2}\right) a u_{xxx} + O(\Delta t^{\,3}, \Delta t^{\,3}).$$

Thus we have $\mathcal{L}_\Delta u \to 0$ as $\Delta x \to 0$ and $\Delta t \to 0$, that is the scheme is consistent withe the PDE. The scheme is 1st order in time and first order in space. Moreover if $p = 1$, that is $a\Delta t = \Delta x$, and then $a^2\Delta t^{\,2} = \Delta x^{\,2}$, $a^2\Delta t^{\,3} = \Delta x^{\,3}$, $\ldots$, we have $\mathcal{L}_\Delta u = 0$, and we say that the scheme is exact. In this case the scheme reduces to

$$U_{j,n+1} = U_{j-1,n}.$$

We now study the stability of the FTBS scheme for $u_t + a u_x = 0$. The scheme is given by

$$U_{j,n+1} = (1-p)U_{j,n} + U_{j-1,n},$$

applying it to a solution of the form $A\mathrm{e}^{\mathrm{i}\omega j}\xi^n$ gives

$$A\mathrm{e}^{\mathrm{i}\omega j}\xi^{n+1} = (1-p)A\mathrm{e}^{\mathrm{i}\omega j}\xi^n + A\mathrm{e}^{\mathrm{i}\omega(j-1)}\xi^n,$$

by dividing through by $A\mathrm{e}^{\mathrm{i}\omega j}\xi^n$ we obtain

$$\xi = 1 - p + p\mathrm{e}^{-\mathrm{i}\omega}.$$

Using the relation $\mathrm{e}^{-\mathrm{i}\omega} = \cos\omega - \mathrm{i}\sin\omega$, the above expression can be written as

$$\xi = 1 - p + p(\cos\omega - \mathrm{i}\sin\omega),$$

and then

$$\begin{aligned} |\xi|^2 &= (1-p+p\cos\omega)^2 + \sin^2\omega \\ &= (1-p)^2 + 2p(1-p)\cos\omega + p^2 \\ &= 1 - 2p(1-p)(1-\cos\omega). \end{aligned}$$

For stability we require $|\xi|^2 \le 1$, that is

$$1 - 1 \ge 2p(1-p)(1-\cos\omega) \le 1.$$

Since $0 \le 1 - \cos\omega$ we then need

$$0 \le 2p(1-p). \tag{8}$$

Studying the graph of the function $x \mapsto 2x(1-x)$ is we see that the inequality (8) requires $0 \le p \le 1$, and since $p = a\Delta t/\Delta\, x$, the scheme is stable if $a > 0$ and $\Delta t \le \Delta x/a$.

The analysis of the FTFS scheme is similar, we find similar results for the LTE: consistent for all p and exact for $p = -1$ (exercise); and the scheme is stable if $-1 \le p \le 0$, that is $a < 0$ and $\Delta t \le \Delta x/a$ (exercise).

4.2 Other schemes for $u_t + a u_x = 0$

4.2.1 Leapfrog scheme

The Leapfrog scheme is a CTCS scheme, that is

$$\frac{U_{j,n+1} - U_{j,n-1}}{2\Delta t} + a\frac{U_{j+1,n} - U_{j-1,n}}{2\Delta x} = 0, \tag{9}$$

that is

$$U_{j,n+1} = U_{j,n-1} - p(U_{j,n} - U_{j-1,n}).$$

This is a consistent (exercise) two-step method, 2nd order in space and time. It is stable for $-1 \leq p \leq 1$ (exercise), it works equally well for $a > 0$ and $a < 0$. By definition the Leapfrog scheme requires the two previous timesteps to compute the current time step, but at the first time step t_1 we only have the values at the previous timestep t_0 therefore to compute $U_{j,1}$ we need to use a single timestep scheme, either a FTBS or a FTCS depending on the sign of a.

4.2.2 Lax-Wendroff scheme

This scheme is a modification of the FTCS scheme, it can be derived by considering a Taylor expansion of $u(x, t + \Delta t)$ and replacing time derivatives with space derivatives since $u_t = -au_x$. The space derivatives are then approximated using a central difference operator. We have

$$u(x, t + \Delta t) = u + u_t \Delta t + u_{tt} \frac{\Delta t^2}{2!} + O(\Delta t^3),$$

but since $u_t = -au_x$, $u_{tt} = a^2 u_{xx}$, ..., we can write

$$u(x, t + \Delta t) = u - au_x \Delta t + a^2 u_{xx} \frac{\Delta t^2}{2!} + O(\Delta t^3).$$

The Lax-Wendroff scheme consists in approximating the above expression using central difference operators, we obtain

$$U_{j,n+1} = U_{j,n} - a \frac{D_x U_{j,n}}{2\Delta x} \Delta t + \frac{a^2}{2} \frac{\delta_x^2 U_{j,n}}{\Delta x^2} \Delta t^2$$

which can be written as

$$U_{j,n+1} = (1 - p^2) U_{j,n} + \frac{p}{2}(p - 1) U_{j+1,n} + \frac{p}{2}(1 + p) U_{j-1,n}.$$

The leading order term of the LTE is given by (exercise)

$$\frac{1}{6} \left(\Delta t^2 u_{ttt} + a \Delta x^2 u_{xxx} \right),$$

therefore the scheme is consistent with the PDE, it is 2nd order in space and time. The amplification factor ξ is given by

$$\xi = 1 - 2p^2 \sin^2 \frac{\omega}{2} - 2\mathrm{i} p \sin \frac{\omega}{2} \cos \frac{\omega}{2},$$

therefore it is stable $-1 \leq p \leq 1$.

4.2.3 Crank-Nicolson scheme

The Crank-Nicolson scheme consists in using a forward difference operator (upwind) for the time derivative, and the average of central difference operators in space evaluated at t and $t + \Delta t$ for the space derivative, it gives

$$\frac{U_{j,n+1} - U_{j,n}}{\Delta t} + \frac{a}{2} \frac{D_x U_{j,n}}{2\Delta x} + \frac{a}{2} \frac{D_x U_{j,n+1}}{2\Delta x} = 0,$$

which can be written as

$$U_{j,n+1} = U_{j,n} - \frac{p}{4}\left(U_{j+1,n} - U_{j-1,n}\right) - \frac{p}{4}\left(U_{j+1,n+1} - U_{j-1,n+1}\right),$$

This is a one-step implicit scheme. The LTE is given by (exercise)

$$\mathcal{L}_\Delta u = a u_{xxx}\left(\frac{1}{6} + \frac{p^2}{12}\right)\Delta x^{\,2} + O(\Delta x^{\,3}, \Delta t^{\,3})$$

The amplification factor is given by (exercise)

$$\xi = \frac{1 - \frac{1}{2}\mathrm{i}p\sin\omega}{1 + \frac{1}{2}\mathrm{i}p\sin\omega},$$

therefore it is stable for all p.

scheme	order	stability	comment
FTCS	$O(\Delta x^{\,2}, \Delta t)$	unstable	explicit, one step
FTBS	$O(\Delta x, \Delta t)$	stable if $a > 0$ and $\lvert p\rvert \leq 1$	explicit, one step
FTFS	$O(\Delta x^{\,2}, \Delta t)$	stable if $a < 0$ and $\lvert p\rvert \leq 1$	explicit, one step
Leapfrog	$O(\Delta x^{\,2}, \Delta t^{\,2})$	stable if $-1 \leq p \leq 1$	explicit, two-step tendency to get oscillations
Lax-Wendroff	$O(\Delta x^{\,2}, \Delta t^{\,2})$	stable if $-1 \leq p \leq 1$	explicit, one-step fewer oscillations
Crank-Nicolson	$O(\Delta x^{\,2}, \Delta t^{\,2})$	stable $\forall p$	implicit, one-step

Table 2: summary

4.3 Second order hyperbolic equation

We return to the second order wave equation $u_{tt} = a^2 u_{xx}$, we use a CSCT scheme to discretize this equation, we have

$$\frac{\delta_t^2 U_{j,n}}{\Delta t^2} = a^2 \frac{\delta_x^2 U_{j,n}}{\Delta x^2}, \tag{10}$$

that is

$$U_{j,n+1} = -U_{j,n-1} + p^2 U_{j+1,n} + 2(1-p^2)U_{j,n} + p^2 U_{j-1,n}.$$

This is an explicit two-step scheme, the LTE is given by (exercise)

$$\mathcal{L}_\Delta u = \frac{a^2}{12}(p^2-1)u_{4x}\Delta x^2 + O(\Delta x^4, \Delta t^4),$$

the scheme is consistent and of order 2 in space, as before it is exact for $p = 1$. The scheme is stable if $-1 \leq p \leq 1$ (exercise). Since it is a two-step scheme, we need $U_{j,0}$ and $U_{j,1}$ to calculate $U_{j,2}$, where $U_{j,0}$ and $U_{j,0}$ are given by two boundary conditions: $u(x,0) = f(x)$ and $u_t(x,0) = g(x)$. We use $u(x,0) = f(x)$ to calculate $U_{j,0}$, $j = 0,\ldots,N$, we use $u_t(x,0) = g(x)$ to calculate $U_{j,1}$, $j = 0,\ldots,N$ using a forward operator, that is

$$\frac{U_{j,1} - U_{j,0}}{\Delta t} = g(x_j), \quad j = 0,\ldots,N,$$

which gives

$$U_{j,1} = U_{j,0} + g(x_j)\Delta t, \quad j = 0,\ldots,N.$$

Now we can use the two-step scheme to calculate $U_{j,n}$, $n = 0,\ldots,K$.

5 Elliptic equations

We consider the following 2nd order elliptic equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y), \quad (x,y) \in [0,1]^2, \tag{11}$$

together with boundary conditions at $u(0,y)$, $u(1,y)$, $u(x,0)$ and $u(x,1)$.

We choose $(N,K) \in \mathbb{N}^2$ and we discretize the domain as follows

$$x_j = j\Delta x, \quad j = 0,\ldots,N, \tag{12}$$

$$y_k = k\Delta y, \quad k = 0,\ldots,K, \tag{13}$$

where $\Delta x = 1/N$, $\Delta y = 1/K$. We use 2nd order central difference operator for the space derivatives, we have

$$\frac{\delta_x^2 U_{j,k}}{\Delta x^2} + \frac{\delta_y^2 U_{j,k}}{\Delta y^2} = f(x_j, y_k), \tag{14}$$

for all interior points, that is

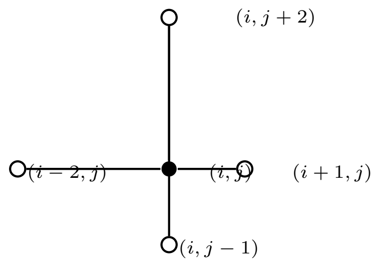
$$\frac{U_{j+1,k} - 2U_{j,k} + U_{j-1,k}}{\Delta x^2} + \frac{U_{j,k+1} - 2U_{j,k} + U_{j,k+1}}{\Delta y^2} = f(x_j, y_k). \tag{15}$$

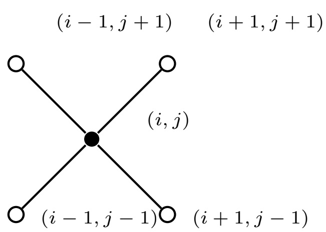
Considering for simplicity that $\Delta x^2 = \Delta y^2$, ie that $K = N$, the above equation can be rewritten as

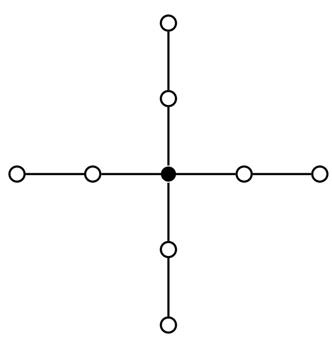
$$U_{j+1,k} + U_{j-1,k} - 4U_{j,k} + U_{j,k+1} + U_{j,k-1} = \Delta x^2 f(x_j, y_k).$$

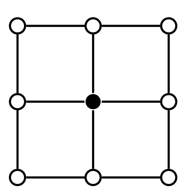
For Dirichlet boundary conditions, we thus have a linear system in $(N-1)^2$ unknowns (exercise). For each node requires input from four oher nodes, the scheme is called a five point scheme, the computational molecule can be represented as

Other approximations can derived by choosing other nodes, or by considering nine points schemes, we can for example consider the following the computational molecules









For each graph the plain node can be expressed as a weighted combination of the other nodes, the weights are determined by Taylor series expansions (see tutorial).