Mat1062: Introductory Numerical Methods for PDE

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1 Ownership

These notes are the joint property of Rob Almgren and Mary Pugh.

2 Convergence rate for the explicit upwind and Lax-Friedrichs schemes

When doing the convergence study for step-function initial data

$$u_0(x) = \begin{cases} 1 & \text{for } x < 0 \\ 0 & \text{otherwise} \end{cases}$$

we observed that if one computed the L^1 norm of the error and then took the ratios of the errors while refining h and k, that if the refinements were done by halving h and k then the ratios of the errors appeared to be converging to $\sqrt{2}$. This suggests that the convergence rate (for such initial data) is $\mathcal{O}(\sqrt{h})$.

Here I will try to make a suggestive argument as to why the convergence rate for the shock wave solution is $\mathcal{O}(\sqrt{h})$. If we have the discrete solution computed up to a fixed time T and the exact solution $u_0(x - aT)$, we want to see that the L^1 norm of their difference goes to zero as h and k go to zero along a fixed refinement path (μ fixed).

From the modified equation analysis, we see that both Explicit Upwind and Lax-Friedrichs result in approximate solutions that are close to solutions of

$$u_t + au_x = Du_{xx}.$$

For the step function initial data this equation has the solution

$$u(x,t) = 1 - \operatorname{erf}\left(\frac{x - at}{\sqrt{4Dt}}\right) \tag{1}$$

where

$$\operatorname{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x} e^{-t^2}\, dt.$$

And so rather than trying to control the L^1 norm of the discrete solution minus the travelling wave solution of $u_t + au_x = 0$, I'll try to control the L^1 norm of the solution (1) minus the travelling wave solution. In short, I want to understand

$$||u(\cdot,T) - v(\cdot,T)||_{L^1(\mathbb{R})} = \int_{-\infty}^{\infty} |u(x,T) - v(x,T)|\, dx$$

where

$$u(x,T) = 1 - \operatorname{erf}\left(\frac{x - aT}{\sqrt{4DT}}\right), \qquad v(x,T) = \begin{cases} 1 & \text{if } x - aT < 0 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

The L^1 norm is translation invariant and both profiles are moving with the same speed a, and so I can go into a moving frame and take

$$u(x,T) = 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4DT}}\right), \qquad v(x,T) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{otherwise} \end{cases}$$

Next, write $u(x,T)$ as $u(x,T) = 1/2 + \tilde{u}(x,T)$ and $v(x,T) = 1/2 + \tilde{v}(x,T)$:

$$\tilde{u}(x,T) = \frac{1}{2} - \operatorname{erf}\left(\frac{x - aT}{\sqrt{4DT}}\right), \qquad v(x,T) = \begin{cases} \frac{1}{2} & \text{if } x - aT < 0 \\ -\frac{1}{2} & \text{otherwise} \end{cases}$$

Note that $\tilde{u}$ and $\tilde{v}$ are both odd about $x = 0$ and both go to $1/2$ (at $-\infty$) and $1/2$ (at ∞). Hence, $|u(x,T) - v(x,T)| = |\tilde{u}(x,T) - \tilde{v}(x,T)|$ is an even function and so

$$\begin{aligned} \int_{-\infty}^{\infty} |u(x,t) - v(x,t)|\, dx &= 2\int_{-\infty}^{0} |\tilde{u}(x,T) - \tilde{v}(x,T)|\, dx \\ &= 2\int_{-\infty}^{0} \operatorname{erf}\left(\frac{x}{\sqrt{4DT}}\right)\, dx = 4\sqrt{DT}\int_{-\infty}^{0} \operatorname{erf}(\tilde{x})\, d\tilde{x} = C\sqrt{DT} \end{aligned}$$

where C is a constant that depends on the error function.

We are now ready to look for the convergence rate. We have just shown that the L^1 norm of the error is close to a constant times $\sqrt{D}$:

$$\|u^n - v(\cdot, T)\|_{L^1(\mathbb{R})} \approx \|u(\cdot, T) - v(\cdot, T)\|_{L^1(\mathbb{R})} = C\sqrt{DT}.$$

where u and v are given by (2). Consider Explicit Upwind first. For this scheme,

$$C\sqrt{D_{\text{EU}}T} = C\sqrt{h\frac{a}{2}(1-\mu)\ T} = \mathcal{O}(\sqrt{h})$$

As a result, the L^1 norm of the error decreases like $\sqrt{h}$, as desired. Similarly, for Lax-Friedrichs,

$$C\sqrt{D_{\text{LF}}T} = C\sqrt{h\frac{a}{2\mu}(1-\mu^2)\ T} = \mathcal{O}(\sqrt{h})$$

and the L^1 norm of the error also decreases like $\sqrt{h}$.

3 Second-order schemes and dispersion

We now turn to the Law-Wendroff and Beam-Warming schemes. For the step function initial data, both schemes produced approximate solutions that had ripples in them. We want to understand the source of these ripples. First, we'll do this via the modified equations and then we'll do this via a direct study of the discrete schemes.

3.1 Modified equations and group velocities

Both the Law-Wendroff and Beam-Warming schemes have modified equations of the form:

$$u_t + au_x = Du_{xxx}$$

where

$$D_{\text{LW}} = \frac{h^2 a}{6}\left(\mu^2 - 1\right) \qquad \text{(Lax-Wendroff)} \qquad (3)$$

$$D_{\text{BW}} = \frac{h^2 a}{6}(\mu - 1)(\mu - 2) \qquad \text{(Beam-Warming)} \qquad (4)$$

The equation $u_t + au_x = Du_{xxx}$ is the advection equation $u_t + au_x = 0$ with dispersive smoothing. As with the first-order schemes, we see immediately that if one chooses the usual "refinement path" of fixed μ then as $h \to 0$ the dispersive smoothing gets smaller and smaller. Again, one could use this as a method to construct solutions of the underlying hyperbolic problem.

We find solutions of $u_t + au_x = Du_{xxx}$ via Fourier methods. Specifically, we take $u(x,t)$ of the form

$$u(x,t) = \int_{-\infty}^{\infty} \widehat{u}(\xi,t) e^{i\xi x}\, d\xi.$$

To find $\widehat{u}(\xi,t)$ we look at a single frequency in isolation and seek $c(\xi)$ such that

$$e^{i(\xi x - c(\xi)t)}$$

solves $u_t + au_x = Du_{xxx}$. This results in

$$c(\xi) = a\xi + D\xi^3.$$

And so we see that this particular oscillating wave moves with speed $a + D\xi^2$:

$$u(x,t) = e^{i\xi(x-(a+D\xi^2)t)}$$

is a travelling wave solution of $u_t + au_x = Du_{xxx}$. Because the speed depends on ξ, different frequencies travel with different speeds: the equation is dispersive. And so the solution of the initial value problem is

$$u(x,t) = \int_{-\infty}^{\infty} \widehat{u_0}(\xi) e^{i(\xi x - (a\xi + D\xi^3)t)}\, d\xi \text{ where } u_0(x) = \int_{-\infty}^{\infty} \widehat{u_0}(\xi) e^{i\xi x}\, d\xi.$$

Because the equation is dispersive, each frequency travels with different speed and the only travelling wave solutions must be made of a single frequency. Any other type of initial data will lose its shape as the different frequencies that make it up travel at different speeds. For example, if one took initial data $u_0 = e^{i\xi_0 x} + e^{i\xi_1 x}$ then there is no speed c such that $u(x,t) = u_0(x - ct)$ is a solution of $u_t + au_x = Du_{xx}$ because if you find a c which works for the ξ_0 frequency, it won't work for the ξ_1 frequency.

For dispersive equations, one considers the *group velocity*

$$c_g(\xi) = c'(\xi) = a + 3D\xi^2.$$

For Lax-Wendroff, if $\mu \in (-1,1)$ the dispersive coefficient $D_{LW} < 0$ and so $c_g(\xi) < a$. That is, the group velocity is smaller than the advection speed a. This is related to why the ripples in Figure 2 of the February 14 notes occur *behind* the shock, but I am not presenting a rigorous explanation here. On the other hand, for Beam-Warming if $\mu \in (0,1)$ then $D_{BW} > 0$ and so $c_g(\xi) > a$. This is related to why the ripples occur *ahead* of the shock in Figure 2 (again claimed without rigorous proof).

3.2 Discrete Schemes and Phase error

Another way to understand the error in the discrete scheme is to return to the original equation

$$u_t + a u_x = 0$$

and consider solutions of the form $u(x,t) = U(t)\exp(i\xi x)$, for $\xi \in \mathbb{R}$. The true solution has $U(t) = \exp(-ia\xi t)$, so that $u(x,t) = \exp(i\xi(x - at))$. To relate these waves to the solutions of the discrete formula, we identify $x_j = jh$ and $t_n = nk$, and revisit the von Neumann stability analysis. This relied on exact solutions of the discrete scheme $u_j^n = \eta^n \omega^j$. If

$$\omega = e^{i\xi h}, \qquad \eta = e^{-i\kappa k}$$

then

$$u_j^n = \eta^n \omega^j = e^{-i\kappa n k} e^{i\xi j h} = e^{i(\xi x_j - \kappa t_n)} = e^{i\xi(x_j - \frac{\kappa}{\xi} t_n)}.$$

The scheme would give the exact solution $\exp(i\xi(x - at))$ if $\kappa = a\xi$:

$$\kappa = a\xi \quad \Longrightarrow \quad \eta^n \omega^j = e^{i\xi(x_j - a t_n)}.$$

Returning to

$$u_j^n = e^{i\xi(x_j - \frac{\kappa}{\xi} t_n)} = e^{i\xi\left(x_j - \frac{\mathrm{Re}\,\kappa}{\xi} t_n\right)} e^{\mathrm{Im}\,\kappa\, t_n}$$

we see that if κ has an imaginary part then this will cause growth or decay of the Fourier modes due to the discretization. For a stable scheme we will always have $|\eta| \le 1$ so $\mathrm{Im}\,\kappa \le 0$. If $\mathrm{Re}\,\kappa > a\xi$ (for $\xi > 0$) then the mode with wavenumber ξ is traveling too *quickly* and if $\mathrm{Re}\,\kappa < a\xi$ then the mode is traveling too *slowly*. Bearing all this in mind, we now revisit the four schemes, find their ηs, and examine their real and imaginary parts.

For the explicit upwind scheme we know η from the von Neumann stability analysis

$$\eta = 1 - \mu(1 - \overline{\omega}) = 1 - \mu(1 - e^{-i\xi h})$$

and so

$$\kappa = \frac{i}{k}\ln(\eta) \quad \Longrightarrow \quad \kappa = a\xi - i\frac{a}{2}h(\mu-1)\xi^2 + \mathcal{O}(h^2) = a\xi - iD_{\text{EU}}\xi^2 + \mathcal{O}(h^2)$$

where the diffusion constant $D_{\text{EU}} = h\,a/2\,(1-\mu)$. And so, the $\mathcal{O}(h)$ term is purely imaginary with $\operatorname{Im}\kappa < 0$ resulting in a diffusive effect with diffusion coefficient D_{EU}.

For the Lax-Friedrichs scheme,

$$\eta = \cos(\xi h) - i\mu \sin(\xi h)$$

hence

$$\kappa = a\xi - i\frac{h^2}{2k}(1-\mu^2)\xi^2 + \mathcal{O}(h^2) = a\xi - iD_{\text{LF}}\xi^2 + \mathcal{O}(h^2).$$

Again, we see the diffusive effect with the diffusion coefficient D_{LF}.

For the Lax-Wendroff scheme,

$$\eta = 1 - \mu^2 + \mu^2\cos(\xi h) - i\mu\sin(\xi h)$$

hence

$$\kappa = a\xi + h^2\frac{a}{6}\left(\mu^2 - 1\right)\xi^3 + \mathcal{O}(h^3) = a\xi + D_{\text{LW}}\xi^3 + \mathcal{O}(h^3).$$

Bearing in mind that we take $|\mu|^2 \le 1$ in order to ensure stability, we see that modes with $\xi \ne 0$ travel slightly too *slowly* (because $D_{\text{LW}} < 0$ implies $\kappa < a\xi$ for small h), by an amount that is second-order in h (because D_{LW} is $\mathcal{O}(h^2)$), but are not damped ($\operatorname{Im}\kappa = 0$). The errors are *dispersive*. In practice, this can be even worse than dissipation since the maximum principle is not maintained. The modes travelling too slowly is related to the ripples we observed behind the advancing sharp transition for step-function initial data (this is stated without a rigorous proof).

Finally, for the Beam-Warming scheme,

$$\eta = 1 + \frac{\mu}{2}\left(-\overline{\omega}^2 + 4\overline{\omega} - 3\right) + \frac{\mu^2}{2}\left(\overline{\omega}^2 - 2\overline{\omega} + 1\right)$$

hence

$$\kappa = a\xi + \frac{a}{6}h^2(\mu-1)(\mu-2)\xi^3 + \mathcal{O}(h^3) = a\xi + D_{\text{BW}}\xi^3 + \mathcal{O}(h^3).$$

Bearing in mind that we take $0 \leq \mu \leq 2$ in order to ensure stability, we see that for $0 \leq \mu < 1$ modes with $\xi \neq 0$ travel slightly too *quickly* by an amount which is second-order in h. And if $1 < \mu < 2$ then modes travel slightly too slowly. Because the parameters in the February 5 notes resulted in $0 < \mu < 1$, this is related to why we saw the ripples ahead of the advancing sharp transition for step-function initial data (this is stated without a rigorous proof).

In this way we see that phase analysis produces a number of the qualitative observations we made based on the modified equations.