Numerical Solutions to PDEs

Lecture Notes #5 — Order of Accuracy of Finite Difference Schemes

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Outline

Previously...

Fourier Analysis — A Crash Course:

We introduced the Fourier transform, and its inverse

$$\widehat{u}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega x}\, u(x)\, dx, \quad u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x}\, \widehat{u}(\omega)\, d\omega.$$

Extended to grid functions (integration becomes summation). Introduced Parseval's equalities, *i.e.* $\|u(x)\|_2 = \|\widehat{u}(\omega)\|_2$.

Parseval's equalities $\rightarrow$ Well-posedness, and stability:

The energy conservation $\|u(x)\|_2 = \|\widehat{u}(\omega)\|_2$ gives us a powerful tool for showing well-posedness of IVPs, and stability of finite difference schemes.

Von Neumann Analysis — Stability of Finite Difference Schemes:

We set $v_m^n \rightarrow g^n\, e^{im\theta}$ in our finite difference schemes, and analyze the expression for g; if $|g| \leq 1 + Kk$, then the scheme is stable.

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Outstanding Question

"How do we deal with stability analysis for the Leapfrog scheme?"

or, more generally:

"How do we deal with stability analysis for multi step schemes?"

Fear not, answers are forthcoming [NOTES #7], [NOTES #8].

Consistency + Stability $\rightsquigarrow$ Convergence — "Not the Whole Truth"

So far we have only classified our finite difference schemes as convergent or non-convergent. This we deduce, using the **Lax-Richtmyer equivalence theorem**, from consistency and stability.

Convergence says that as $(h, k) \to 0$, the solution of the finite difference scheme will better and better approximate the solution of the PDE.

Convergence, however, **does not** tell us anything about the quality for a fixed grid (h^*, k^*) and nothing about how the solution would improve if we refined the grid to, say, $\left(\frac{1}{2}h^*, \frac{1}{2}k^*\right)$.

The missing piece of the puzzle is the **order of accuracy** of the scheme in question.

Before discussing the order of accuracy, we introduce two new schemes — the **Lax-Wendroff** and **Crank-Nicolson** schemes.

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The Lax-Wendroff Scheme

Consider the Taylor series expansion in time for $u(t+k,x)$, where u is the solution to the inhomogeneous one-way wave equation $u_t + au_x = f$:

$$u(t+k,x) = u(t,x) + ku_t(t,x) + \frac{k^2}{2}u_{tt}(t,x) + \mathcal{O}\left(k^3\right)$$

Now, since $u_t = -au_x + f$, and therefore (given enough smoothness)

$$\begin{aligned} u_{tt} &= -au_{xt} + f_t = a^2 u_{xx} - af_x + f_t \\ u_{xt} &= -au_{xx} + f_x \end{aligned}$$

we get (all quantities evaluated at (t,x), unless otherwise specified)

$$u(t+k,x) = u - aku_x + \frac{a^2k^2}{2}u_{xx} + kf - \frac{ak^2}{2}f_x + \frac{k^2}{2}f_t + \mathcal{O}\left(k^3\right).$$

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The Lax-Wendroff Scheme

Consider the Taylor series expansion in time for $u(t+k,x)$, where u is the solution to the inhomogeneous one-way wave equation $u_t + au_x = f$:

$$u(t+k,x) = u(t,x) + ku_t(t,x) + \frac{k^2}{2}\mathbf{u_{tt}(t,x)} + \mathcal{O}\left(k^3\right)$$

Now, since $u_t = -au_x + f$, and therefore (given enough smoothness)

$$\begin{aligned} \mathbf{u_{tt}} &= -a\mathbf{u_{xt}} + f_t = a^2 u_{xx} - af_x + f_t \\ \mathbf{u_{xt}} &= -au_{xx} + f_x \end{aligned}$$

we get (all quantities evaluated at (t,x), unless otherwise specified)

$$u(t+k,x) = u - aku_x + \frac{a^2k^2}{2}u_{xx} + kf - \frac{ak^2}{2}f_x + \frac{k^2}{2}f_t + \mathcal{O}\left(k^3\right).$$

The Lax-Wendroff Scheme

We now replace the derivatives in x by second order accurate differences, *i.e.*

$$u_x \approx \frac{u(t,x+h)-u(t,x-h)}{2h} = u_x + \frac{h^2}{6}u_{xxx} + \mathcal{O}\left(h^4\right)$$

$$u_{xx} \approx \frac{u(t,x+h)-2u(t,x)+u(t,x-h)}{h^2} = u_{xx} + \frac{h^2}{12}u_{xxxx} + \mathcal{O}\left(h^4\right),$$

and f_t by a forward difference, *i.e.*

$$f_t \approx \frac{f(t+k,x)-f(t,x)}{k} = f_t + \frac{k}{2}f_{tt} + \mathcal{O}\left(k^2\right).$$

The Lax-Wendroff Scheme

∃ Movie

With $v_m^n = u(t_n, x_m)$, we get the Lax-Wendroff Scheme

$$\begin{aligned} v_m^{n+1} &= v_m^n - \frac{a\lambda}{2}\left(v_{m+1}^n - v_{m-1}^n\right) + \frac{a^2\lambda^2}{2}\left(v_{m+1}^n - 2v_m^n + v_{m-1}^n\right) \\ &\quad + \frac{k}{2}\left(f_m^{n+1} + f_m^n\right) - \frac{ak\lambda}{4}\left(f_{m+1}^n - f_{m-1}^n\right) + \mathcal{O}\left(kh^2 + k^3\right). \end{aligned}$$

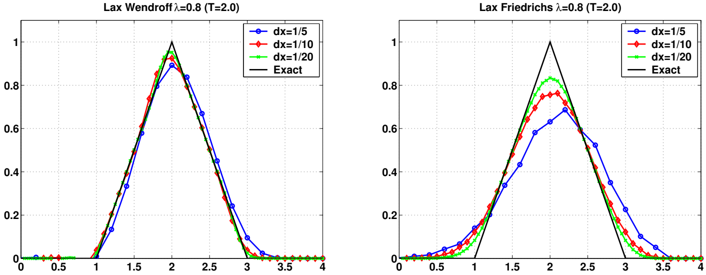

Figure: Comparison of the Lax-Wendroff (left) and Lax-Friedrichs schemes. Clearly, the solutions produced by the L-W scheme is of better quality (for the same grid spacing).

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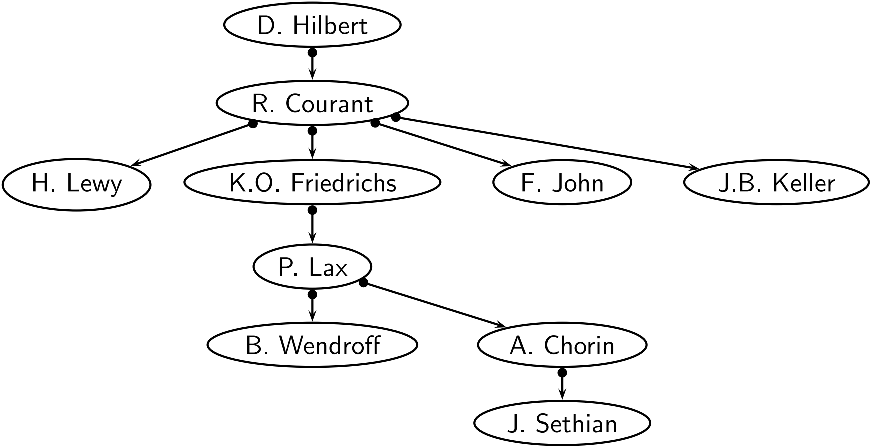

The Crank-Nicolson Scheme

Formally, the Crank-Nicolson scheme is obtained by differencing the one-way wave equation about the point $(t+k/2, x)$, using central differencing in time to get second-order accuracy:

$$u_t\left(t+\frac{k}{2}, x\right) = \frac{u(t+k,x)-u(t,x)}{k} + \frac{k^2}{24}u_{ttt}\left(t+\frac{k}{2}, x\right) + \mathcal{O}\left(k^4\right).$$

Then we use

$$\begin{aligned} u_x\left(t+\frac{k}{2}, x\right) &= \frac{u_x(t+k,x)+u_x(t,x)}{2} + \mathcal{O}\left(k^2\right) \\ &= \frac{1}{2}\left[\frac{u(t+k,x+h)-u(t+k,x-h)}{2h} + \frac{u(t,x+h)-u(t,x-h)}{2h}\right] \\ &\quad +\mathcal{O}\left(k^2+h^2\right). \end{aligned}$$

With this we can write down the Crank-Nicolson scheme...

$$\frac{v_m^{n+1}-v_m^n}{k} + a\frac{v_{m+1}^{n+1}-v_{m-1}^{n+1}+v_{m+1}^n-v_{m-1}^n}{4h} = \frac{f_m^{n+1}+f_m^n}{2} + \mathcal{O}\left(k^2+h^2\right)$$

The Crank-Nicolson Scheme

Since the Crank-Nicolson scheme is **implicit**

$$\frac{\mathbf{v}_{\mathbf{m}}^{\mathbf{n+1}} - v_m^n}{k} + a\frac{\mathbf{v}_{\mathbf{m+1}}^{\mathbf{n+1}} - \mathbf{v}_{\mathbf{m-1}}^{\mathbf{n+1}} + v_{m+1}^n - v_{m-1}^n}{4h} = \frac{\mathbf{f}_{\mathbf{m}}^{\mathbf{n+1}} + f_m^n}{2}$$

we are going to have to develop some more "technology" in order to compute the solution.

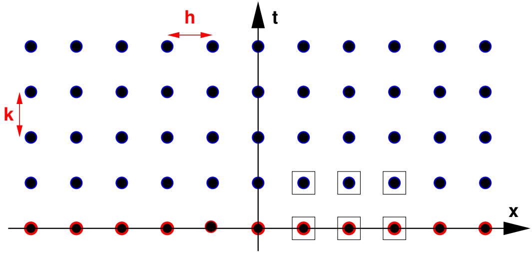

Figure: Illustration of the stencil for the Crank-Nicolson finite difference schemes; it contains three points on the previous (known) time-level, and three points on the new (to-be-determined) time-level.

Order of Accuracy

Both the Lax-Wendroff, and the Crank-Nicolson schemes can be written as $P_{k,h}v = R_{k,h}f$ evaluated at a grid point (t_n, x_m); and the expression involves a finite sum of terms involving $v_{m'}^{n'}$ and $f_{m'}^{n'}$. With this in mind, we can now give the definition of the order of accuracy of a scheme:

Definition (Order of Accuracy (version 0.99))

A scheme $P_{k,h}v = R_{k,h}f$ that is consistent with the differential equation $Pu = f$ is accurate of order p in time and order q in space if for any smooth function $\Phi(t,x)$,

$$P_{k,h}\Phi - R_{k,h}P\Phi = \mathcal{O}\left(k^p + h^q\right).$$

We say that such a scheme is accurate of order (p, q).

Order of Accuracy and Consistency

In a sense the definition of the order of accuracy is an extension of consistency.

Consistency requires that $P_{k,h}\Phi - P\Phi \to 0$, as $(k, h) \to 0$. The order of accuracy is a measure of how fast this convergence is.

The Lax-Wendroff (slide 9) and Crank-Nicolson (slide 11) schemes are accurate of order $(2, 2)$.

Note that the Lax-Wendroff scheme must be written in the *consistent form*

$$\begin{aligned}\frac{v_m^{n+1} - v_m^n}{k} &= -\frac{a}{2h}\left(v_{m+1}^n - v_{m-1}^n\right) + \frac{a^2 k}{2h^2}\left(v_{m+1}^n - 2v_m^n + v_{m-1}^n\right) \\ &+\frac{1}{2}\left(f_m^{n+1} + f_m^n\right) - \frac{a\lambda}{4}\left(f_{m+1}^n - f_{m-1}^n\right) + \mathcal{O}\left(h^2 + k^2\right),\end{aligned}$$

in order for the order of accuracy to be apparent.

Another Definition

The given definition of order of accuracy breaks for the Lax-Friedrichs scheme, in which the Taylor expansion contains the term $\frac{h^2}{k}\Phi_{xx}$.

A more general definition of order of accuracy is needed. Assuming that $k = \Lambda(h)$, where $\Lambda(h)$ is smooth, and $\Lambda(0) = 0$, we define:

Definition (Order of Accuracy)

A scheme $P_{k,h}v = R_{k,h}f$ with $k = \Lambda(h)$ that is consistent with the differential equation $Pu = f$ is accurate of order ρ if for any smooth function $\Phi(t, x)$,

$$P_{k,h}\Phi - R_{k,h}P\Phi = \mathcal{O}\left(h^{\rho}\right).$$

With $\Lambda(h) = \lambda \cdot h$, the Lax-Friedrichs scheme is consistent with the one-way way equation; and 1st-order accurate $(\rho = 1)$.

Symbols of Difference Schemes

Another way of checking the accuracy of a scheme is to compare the **symbols** of the scheme and differential operator. This is usually more convenient than using the previous definition directly.

Definition (Symbol of the Difference Operator $P_{k,h}$)

The symbol $p_{k,h}(s,\xi)$ of a difference operator $P_{k,h}$ is defined by

$$P_{k,h}\left(e^{skn}e^{imh\xi}\right) = p_{k,h}(s,\xi)\, e^{skn}e^{imh\xi}.$$

That is, the symbol is the quantity multiplying the grid function $e^{skn}e^{imh\xi}$ after operating on this function with the difference operator.

Example: The Symbol of the Lax-Wendroff Scheme

We write the scheme as $P_{k,h} v_m^n = R_{k,h} f_m^n$:

$$\frac{v_m^{n+1} - v_m^n}{k} + \frac{a}{2h}\left(v_{m+1}^n - v_{m-1}^n\right) - \frac{a^2 k}{2h^2}\left(v_{m+1}^n - 2v_m^n + v_{m-1}^n\right)$$
$$= \frac{1}{2}\left(f_m^{n+1} + f_m^n\right) - \frac{a\lambda}{4}\left(f_{m+1}^n - f_{m-1}^n\right)$$

and can identify the symbols

$$p_{k,h} = \frac{e^{sk} - 1}{k} + \frac{ia}{h}\sin(h\xi) + 2\frac{a^2 k}{h^2}\sin^2\left(\frac{h\xi}{2}\right)$$
$$r_{k,h} = \frac{e^{sk} + 1}{2} - \frac{iak}{2h}\sin(h\xi)$$

$$1 - \cos\theta = 2\sin^2\left(\frac{\theta}{2}\right), \quad \sin\theta = 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right).$$

Symbols of Differential Operators

We need something the compare our finite difference scheme against:

Definition (Symbol of the Differential Operator P)

The symbol $p(s, \xi)$ of the differential operator P is defined by

$$P\left(e^{st}e^{i\xi x}\right) = p(s,\xi)e^{st}e^{i\xi x}.$$

That is, the symbol is the quantity multiplying the function $e^{st}e^{i\xi x}$ after operating on this function with the differential operator.

The symbol of $P = \frac{\partial}{\partial t} + a\frac{\partial}{\partial x}$ (the one-way wave-equation differential operator), with the right-hand-side $R = f$ are given by:

$$p(s,\xi) = s + ia\xi, \quad r(s,\xi) = 1.$$

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Using the Symbols $p_{k,h}$, $r_{k,h}$, $p(s,\xi)$ and $r(s,\xi)$

Consistency requires

$$\lim_{k,h\to 0} p_{k,h} = p(s,\xi), \quad \lim_{k,h\to 0} r_{k,h} = r(s,\xi),$$

the following theorem gives the order of accuracy:

Theorem (Order of Accuracy)

A scheme $P_{k,h}v = R_{k,h}f$ that is consistent with $Pu = f$ is accurate of order (p,q) if and only if for each value of s and ξ,

$$p_{k,h}(s,\xi) - r_{k,h}(s,\xi)p(s,\xi) = \mathcal{O}\left(k^p + h^q\right), \qquad \textbf{(*)}$$

or equivalently

$$\frac{p_{k,h}(s,\xi)}{r_{k,h}} - p(s,\xi) = \mathcal{O}\left(k^p + h^q\right).$$

Using the Symbols $p_{k,h}$, $r_{k,h}$, $p(s,\xi)$ and $r(s,\xi)$

Usually, the form **(*)** from the theorem is the most convenient form for showing the order of accuracy. For the Lax-Wendroff scheme applied to the one-way wave equation, we get

$$\begin{aligned} & p_{k,h}(s,\xi) - r_{k,h}(s,\xi)p(s,\xi) = \\ & \frac{e^{sk}-1}{k} + \frac{ia}{h}\sin(h\xi) + 2\frac{a^2 k}{h^2}\sin^2\left(\frac{h\xi}{2}\right) \\ & -\left[\frac{e^{sk}+1}{2} - \frac{iak}{2h}\sin(h\xi)\right]\cdot[s+ia\xi]. \end{aligned}$$

This looks like a hopeless mess... We get the Taylor expansion using Maple™, and find

$$p_{k,h}(s,\xi) - r_{k,h}(s,\xi)p(s,\xi) \sim -\left[\frac{s^3}{12} + \frac{is^2 a\xi}{4}\right]k^2 - \left[\frac{ia\xi^3}{6}\right]h^2 + \ldots$$

hence, the Lax-Wendroff scheme is $\mathcal{O}\left(k^2+h^2\right)$, *i.e.* order (2,2).

How to use Matlab / Maple™ for Taylor Expansions

Maple:

```
S := ( exp(s*k) - 1 ) / k + I*a/h * sin(h*xi) +
2*a^2*k/h^2 * sin(h*xi/2)^2 - ( (exp(s*k) + 1 )/2 -
I*a*k / 2 / h * sin(h*xi) ) * (s + I*a*xi);
```

```
collect(simplify(mtaylor(S, [k,h], 4)),k);
```

Matlab:

```
syms s k h xi a
```

S = $(exp(s*k)-1)/k+i*a/h*sin(h*xi)+2*a^2*k/h^2*sin(h*xi/2)^2-((exp(s*k)+1)/2-i*a*k/2/h*sin(h*xi))*(s+i*a*xi)$

```
taylor(S,[k,h],'ExpansionPoint',[0,0],'Order',3)
```

ans = $(-(s^2*(s+a*xi*i))/4+s^3/6)*k^2+a*h^2*xi^3*(-i/6)$

Corollary to the Theorem

Corollary (Order of Accuracy)

A scheme $P_{k,h}v = R_{k,h}f$ with $k = \Lambda(h)$ that is consistent with $Pu = f$ is accurate of order ρ if and only if for each value of s and ξ,

$$\frac{p_{k,h}(s,\xi)}{r_{k,h}} - p(s,\xi) = \mathcal{O}\left(h^{\rho}\right).$$

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Order of Accuracy for Homogeneous Equations

Often, we are interested in the IVP with the homogeneous equation $Pu = 0$, rather than $Pu = f$. As stated, our theorem breaks, since we have no meaningful definition of $R_{k,h}$.

We extend our toolbox:

Definition (Symbol)

A symbol $a(s, \xi)$ is an infinitely differentiable function defined for complex values of s, with $\mathrm{Re}(s) \geq c$ for some constant c and for all real values of ξ.

This definition of a symbol includes the previously defined symbols for finite difference operators (polynomials in e^{ks} with coefficients that are polynomials or rational functions in $e^{ih\xi}$), and differential operators (polynomials in s and ξ), along with many other symbols...

Order of Accuracy for Homogeneous Equations

Definition (Symbol Congruence to Zero)

A symbol $a(s,\xi)$ is congruent to zero modulo a symbol $p(s,\xi)$, written

$$a(s,\xi) \equiv 0 \bmod p(s,\xi),$$

if there is a symbol $b(s,\xi)$ such that

$$a(s,\xi) = b(s,\xi) \cdot p(s,\xi).$$

We also write

$$a(s,\xi) \equiv c(s,\xi) \bmod p(s,\xi),$$

if

$$a(s,\xi) - c(s,\xi) \equiv 0 \bmod p(s,\xi),$$

i.e.

$$a(s,\xi) = b(s,\xi) \cdot p(s,\xi) + c(s,\xi).$$

Order of Accuracy for Homogeneous Equations

With this extended toolbox, we have:

Theorem (Accuracy for Homogeneous Equations)

A scheme $P_{k,h}v = 0$, with $k = \Lambda(h)$, that is consistent with $Pu = 0$ is accurate of order ρ if

$$p_{k,h}(s,\xi) \equiv \mathcal{O}\left(h^{\rho}\right) \bmod p(s,\xi).$$

Consider

$$p_{k,h}^{\mathrm{LW}}(s,\xi) = \frac{e^{sk} - 1}{k} + \frac{ia}{h}\sin\left(h\xi\right) + 2\frac{a^2 k}{h^2}\sin^2\left(\frac{h\xi}{2}\right),$$

and

$$p(s,\xi) = s + ia\xi.$$

Order of Accuracy for Homogeneous Equations

The Taylor expansion of $p_{k,h}^{\text{LW}}(s,\xi)$ is

$$p_{k,h}^{\text{LW}}(s,\xi) \sim \underbrace{[s+ia\xi]}_{p(s,\xi)} + \frac{1}{2}\underbrace{\left(s^2+a^2\xi^2\right)}_{p(s,\xi)\cdot\overline{p(s,\xi)}} k + \left[\frac{1}{6}s^3\right]k^2 - \left[\frac{1}{6}ia\xi^3\right]h^2 + \ldots$$

Hence

$$p_{k,h} \equiv \mathcal{O}\left(k^2+h^2\right) \bmod p(s,\xi),$$

since

$$p_{k,h} = p(s,\xi)\cdot\left(1+\frac{1}{2}\overline{p(s,\xi)}\right) + \mathcal{O}\left(k^2+h^2\right).$$

Explicit One-Step Schemes

Theorem (Accuracy for Explicit One-Step Schemes)

An explicit one-step scheme for hyperbolic equations that has the form

$$v_m^{n+1} = \sum_{\ell=-\infty}^{\infty} \alpha_\ell v_{m+\ell}^n$$

for homogeneous problems can be at most first-order accurate if all the coefficients α_l *are non-negative, except for trivial schemes for the one-way wave-equation with* $a\lambda = \ell$*, where* ℓ *is an integer, given by*

$$v_m^{n+1} = v_{m-\ell}^n.$$

The proof (Strikwerda pp.71–72) uses our new "symbols toolbox" extensively. The Lax-Wendroff scheme is the explicit one-step second-order accurate scheme that uses the fewest number of grid-points.

Order of Accuracy of the Solution

In the last third of the semester we will show that:

The order of accuracy of the solution computed using (multiple time-steps of) the finite difference scheme is **equal** to that of the order of accuracy of the scheme, provided that the initial data is smooth.

Next time:
We examine the stability of the newly introduced schemes — Lax-Wendroff, and Crank-Nicolson; discuss some notation; talk about boundary conditions for finite difference schemes; and discuss how to efficiently propagate the solution using the Crank-Nicolson scheme.

Truncated Genealogy (Advisor → Student)