

Numerical Solutions to PDEs

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

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Outline

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Recap

Previously...

Fourier Analysis — A Crash Course:

We introduced the Fourier transform, and its inverse

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

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

Parseval's equalities → Well-posedness, and stability:

The energy conservation $\|u(x)\|_2 = \|\hat{u}(\omega)\|_2$ 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.



Recap

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].



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 $(h, k) \rightarrow 0$, 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, $(\frac{1}{2}h^*, \frac{1}{2}k^*)$.

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.



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

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

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

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

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

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



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

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

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

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

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



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

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

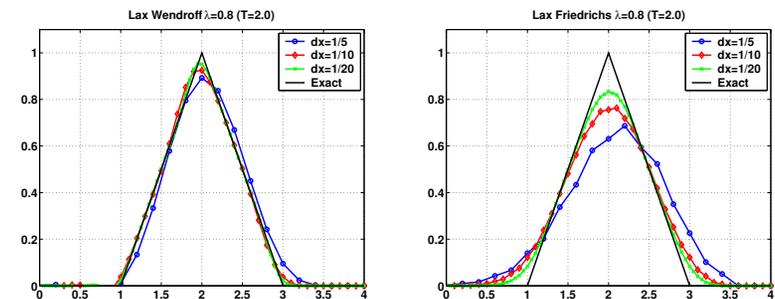
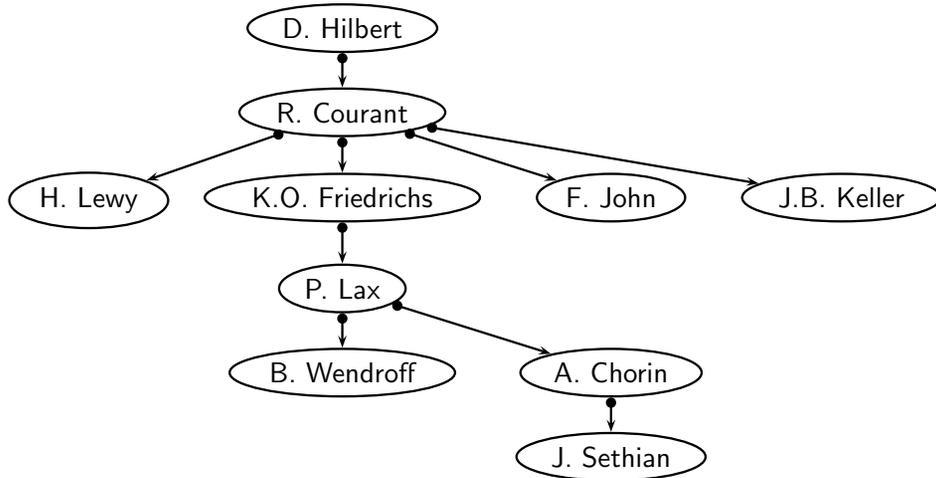


Figure: Comparison of the Lax-Wendroff (left) and Lax-Friedrichs schemes. Clearly, the solutions produced by the L-W scheme is of better quality (for the same grid spacing).



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The Crank-Nicolson Scheme

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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:

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

Then we use

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

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

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



The Crank-Nicolson Scheme

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

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

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

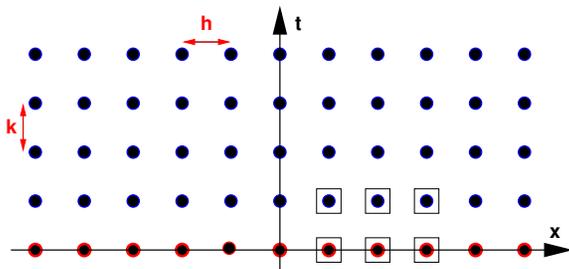


Figure: Illustration of the stencil for the Crank-Nicolson finite difference schemes; it contains three points on the previous (known) time-level, and three points on the new (to-be-determined) time-level.



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 $\Phi(t, x)$,

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

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

The Lax-Wendroff (slide 8) and Crank-Nicolson (slide 10) schemes are accurate of order $(2, 2)$.

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

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

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 $\Phi(t, x)$,

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

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

Additional Tools

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

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

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 $P_{k,h}v_m^n = R_{k,h}f_m^n$:

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

and can identify the symbols

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

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



Symbols of Differential Operators

We need something to 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

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

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:

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



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

Consistency requires

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

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 ,

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

or equivalently

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



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

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

hence, the Lax-Wendroff scheme is $\mathcal{O}(k^2 + h^2)$, 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 ,

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



Order of Accuracy for Homogeneous Equations

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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 $\text{Re}(s) \geq c$ 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

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Definition (Symbol Congruence to Zero)

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

$$a(s, \xi) \equiv 0 \pmod{p(s, \xi)},$$

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

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

We also write

$$a(s, \xi) \equiv c(s, \xi) \pmod{p(s, \xi)},$$

if

$$a(s, \xi) - c(s, \xi) \equiv 0 \pmod{p(s, \xi)},$$

i.e.

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



Order of Accuracy for Homogeneous Equations

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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

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

Consider

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

and

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



Order of Accuracy for Homogeneous Equations

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

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

Hence

$$p_{k,h} \equiv \mathcal{O}(k^2 + h^2) \text{ mod } p(s, \xi),$$

since

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



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.



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