Numerical Solutions to PDEs

Lecture Notes #4
— Analysis of Finite Difference Schemes —
Fourier Analysis; Von Neumann Analysis

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Outline

Previously... 1 of 2

Convergence: The desired result; as we refine the grid, the numerical solution of the Finite Difference Scheme (FDS) should better and better represent the exact (continuous) solution of the PDE.

Consistency: Easily checked by **Taylor expansion** — the expansion of the FDS should give the PDE + terms that go to zero as $(h, k) \to 0$.

Stability: An ℓ_2-energy bound on the solution of the FDS in terms of the initial condition (+ further levels of initialization for multi-step schemes). Hard to check using the definitions — we start developing tools today!

Well-Posedness: A property of the PDE for IVPs — An L^2-energy bound on the solution in terms of the initial conditions.

Previously... 2 of 2

The CFL-condition

Courant-Friedrichs-Lewy condition $|a\lambda| \leq 1$ (for explicit one-step schemes applied to $u_t + au_x + bu = f$) is **necessary** (but not sufficient) for stability. It expresses the need for the numerical speed of propagation λ^{-1} to match or exceed the physical speed of propagation a.

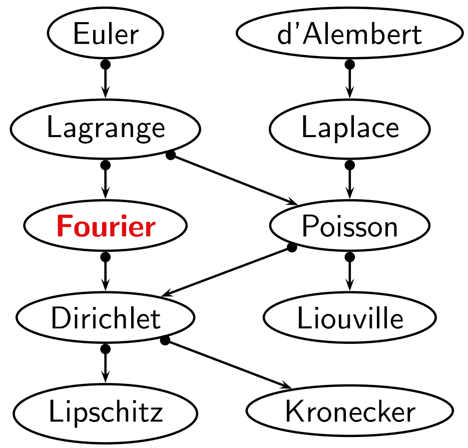
Theorem (The Lax-Richtmyer Equivalence Theorem)

A consistent finite difference scheme for a partial differential equation for which the initial value problem is well-posed is convergent if and only if it is stable.

A Crash Course in Fourier Analysis

Figure: Jean-Baptiste Joseph Fourier (21 March 1768 – 16 May 1830). Advisor: Joseph Louis Lagrange. Student: Gustav Peter Lejeune Dirichlet (+1).

Truncated Genealogy (Advisor $\rightarrow$ Student)



A Crash Course in Fourier Analysis

The **Fourier transform** of a function $u(x)$, $x \in \mathbb{R}$ is defined by

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

The **Fourier inversion formula**

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

recovers the function from its Fourier transform.

Essentially, the Fourier transform representation expresses $u(x)$ as an infinite superposition of (complex) waves $e^{i\omega x} = \cos(\omega x) + i\sin(\omega x)$, with amplitudes $\widehat{u}(\omega)$.

(!) $u(x)$ and $\widehat{u}(\omega)$ must satisfy certain criteria for the integrals (above) to be well-defined. We sweep those details under the rug, and refer to **Math 668: Applied Fourier Analysis**.

Example — With Correction of Typo (Strikwerda p.38)

We consider the function

$$u(x) = \begin{cases} e^{-x} & x \geq 0 \\ 0 & x < 0. \end{cases}$$

The Fourier transform of $u(x)$ is given by

$$\underbrace{\widehat{u}(\omega)}_{\text{correction}} = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} e^{-i\omega x}\, e^{-x}\, dx = \frac{1}{\sqrt{2\pi}}\, \frac{1}{1+i\omega}.$$

The tools needed for evaluation of such integrals can be found in **Math 532 + 631A + 631B: Complex Analysis**.

Tables of Fourier transforms can be found online in various places; ask uncle Google for guidance.

Fourier Transform Tables: A Warning

There are several ways of defining the Fourier transform — the normalization constants for the forward and inverse transforms are chosen from one of the following three set

$$\left\{\frac{1}{\sqrt{2\pi}}, \frac{1}{\sqrt{2\pi}}\right\}, \quad \left\{1, \frac{1}{2\pi}\right\}, \quad \left\{\frac{1}{2\pi}, 1\right\},$$

and the factors in the integrals can be chosen to be

$$\left\{e^{-i\omega x}, e^{i\omega x}\right\}, \quad \left\{e^{i\omega x}, e^{-i\omega x}\right\}.$$

For a total of six "natural" ways to define the transform and its inverse. Of course, mathematicians and engineers have agreed to disagree on the definition of the One True Fourier Transform™. — These choices also affect numerical implementations of the discrete Fourier transform...

Extending the Fourier Transform to Grid Functions, I

For a grid function v_m defined for all integers coordinates m, the Fourier transform is given by

$$\widehat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-im\xi}\, v_m,$$

where $\xi \in [-\pi, \pi]$, and $\widehat{v}(\pi) = \widehat{v}(-\pi)$.

The inversion formula is given by

$$v_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{im\xi}\, \widehat{v}(\xi)\, d\xi.$$

Extending the Fourier Transform to Grid Functions, II

For a grid function v_m defined for all coordinates $x_m = h \cdot m$, the Fourier transform is given by

$$\widehat{v}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-imh\xi}\, v_m$$

where $\xi \in [-\pi/h, \pi/h]$, and $\widehat{v}(\pi/h) = \widehat{v}(-\pi/h)$.

The inversion formula is given by

$$v_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\, \widehat{v}(\xi)\, d\xi.$$

Parseval's Relations: Preservation of L^2 Energy

With the following definition for the L^2 (continuous) energy

$$\|u\|_2 = \sqrt{\int_{-\infty}^{\infty} |u(x)|^2\, dx},$$

the following holds

Parseval's Relations

$$\sqrt{\int_{-\infty}^{\infty} |u(x)|^2\, dx} = \|u\|_2 = \|\widehat{u}\|_2 = \sqrt{\int_{-\infty}^{\infty} |\widehat{u}(\omega)|^2\, d\omega}$$

$$\sqrt{h \sum_{m=-\infty}^{\infty} |v_m|^2} = \|v\|_2 = \|\widehat{v}\|_2 = \sqrt{\int_{-\pi/h}^{\pi/h} |\widehat{v}(\xi)|^2\, d\xi}$$

These relations are key to our stability analysis, and are also a big reason why measuring quantities in the L^2 (and/or ℓ_2) norm is usually a Good Thing™ — many times the norm expresses a natural physical energy, *and* that energy is preserved under the Fourier transform.

The Road to Stability: Using Parseval's Relations

Using Parseval's relations, we can rewrite the inequalities that appeared in the definition of stability (last lecture)

$$h \sum_{m=-\infty}^{\infty} |v_m^n|^2 \leq C_T h \sum_{j=0}^{J} \sum_{m=-\infty}^{\infty} |v_m^j|^2,$$

and

$$\|v^n\|_h \leq \left[C_T \sum_{j=0}^{J} \|v^j\|_h^2 \right]^{1/2} \quad \Leftrightarrow \quad \|v^n\|_h \leq C_T^* \sum_{j=0}^{J} \|v^j\|_h,$$

by the equivalent inequality (applied in the Fourier domain...)

$$\|\widehat{v}^n\|_h \leq C_T^* \sum_{j=0}^{J} \|\widehat{v}^j\|_h.$$

So???

Fourier Analysis and PDEs

Given the Fourier inversion formula

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

we formally compute the derivative with respect to x:

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

This leads us to the stunningly simple, and extremely useful conclusion that

$$\widehat{\left(\frac{\partial u}{\partial \mathbf{x}} \right)} = i\omega\, \widehat{u}(\omega)$$

i.e. **differentiation** on the physical side, corresponds to **multiplication by** $i\omega$ on the Fourier transform side.

Higher Derivatives — L^2 — Parseval

It now follows that the squared L^2-norm of the r-th derivative is given by

$$\int_{-\infty}^{\infty} \left| \frac{\partial^r u(x)}{\partial x^r} \right|^2 dx = \int_{-\infty}^{\infty} |\omega|^{2r}\, |\widehat{u}(\omega)|^2\, d\omega,$$

These quantities exist (*i.e.* u has L^2 integrable derivatives of order through r, if and only if

$$\int_{-\infty}^{\infty} (1 + |\omega|^2)^r\, |\widehat{u}(\omega)|^2\, d\omega < \infty.$$

From this we can define the **function space** (**Sobolev space**, also denoted $W_2^r(\mathbb{R})$, or $W^{r,2}(\mathbb{R})$) $H^r(\mathbb{R})$ ($r > 0$) as the set of functions $u \in L^2(\mathbb{R})$, for which (note $H^0(\mathbb{R}) \equiv L^2(\mathbb{R})$)

$$\|u\|_{H^r} = \sqrt{\int_{-\infty}^{\infty} (1 + |\omega|^2)^r\, |\widehat{u}(\omega)|^2\, d\omega} < \infty.$$

Notations for Norms of Derivatives

We introduce the notation

$$\|D^r u\|^2 = \int_{-\infty}^{\infty} \left| \frac{\partial^r}{\partial x^r} u(x) \right|^2 dx = \int_{-\infty}^{\infty} |\omega|^{2r}\, |\widehat{u}(\omega)|^2\, d\omega,$$

and note (for future reference), that the integral over x is only defined when r is an integer, but the integral over ω can be used for "fractional derivatives."

OK, lets return to the one-way wave equation...

Fourier Analysis and the One-Way Wave Equation, I

Consider, with $u(0,x) = u_0(x)$ specified,

$$u_t + au_x = 0, \quad \Leftrightarrow \quad u_t = -au_x.$$

Fourier transforming in the x-coordinate, we get

$$\widehat{u}_t = -ia\omega\widehat{u}, \quad \widehat{u}_0(\omega) \text{ given}.$$

This is an Ordinary Differential Equation (ODE) in t, and the solution is given by

$$\widehat{u}(t,\omega) = e^{-ia\omega t}\,\widehat{u}_0(\omega).$$

With the help of the tools we have developed, we can show that this Initial Value Problem is well-posed.

Fourier Analysis and the One-Way Wave Equation, II

We have, using Parseval's equality

$$\int_{-\infty}^{\infty} |u(t,x)|^2\,dx = \int_{-\infty}^{\infty} |\widehat{u}(t,\omega)|^2\,d\omega = \int_{-\infty}^{\infty} |e^{-ia\omega t}\,\widehat{u}_0|^2\,d\omega =$$
$$\int_{-\infty}^{\infty} \underbrace{|e^{-ia\omega t}|^2}_{1} |\widehat{u}_0|^2\,d\omega = \int_{-\infty}^{\infty} |\widehat{u}_0|^2\,d\omega = \int_{-\infty}^{\infty} |u_0|^2\,dx = \|u_0\|_2^2.$$

Hence, not only do we have a bound on the energy — we have an exact value, which does not change in time. $\Rightarrow$ **The IVP is well-posed**.

Von Neumann Analysis

The application of Fourier analysis which presently is of interest to us is the application to the stability analysis of finite difference schemes; known as **von Neumann analysis**.

Starting from the forward-time-backward-space scheme (suitable only when $a > 0$, think about the characteristic) applied to the one-way wave equation ($u_t + au_x = 0$):

$$\frac{v_m^{n+1} - v_m^n}{k} + a\,\frac{v_m^n - v_{m-1}^n}{h} = 0.$$

We rewrite this in the form ($\lambda = k/h$)

$$v_m^{n+1} = (1 - a\lambda)v_m^n + a\lambda v_{m-1}^n.$$

Next we, use the Fourier inversion formula to represent the quantities on the right-hand side....

Von Neumann Analysis... Moving Along

With

$$v_m^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\,\widehat{v}^n(\xi)\,d\xi,$$

we get

$$v_m^{n+1} = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi} \left[(1 - a\lambda) + a\lambda \underbrace{e^{-ih\xi}}_{\text{from } v_{m-1}^n} \right] \widehat{v}^n(\xi)\,d\xi.$$

From the inversion formula we also have

$$v_m^{n+1} = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\,\widehat{v}^{n+1}(\xi)\,d\xi.$$

We have two representations of the same quantity...

Von Neumann Analysis... Moving Along 2 of 2

The integrands must be the same, hence

$$\widehat{v}^{n+1}(\xi) = \underbrace{\left[(1-a\lambda) + a\lambda\, e^{-ih\xi}\right]}_{g(h\xi)} \widehat{v}^{n}(\xi).$$

$g(h\xi)$ is known as the **amplification factor**, and we note that

$$\widehat{v}^{n}(\xi) = g(h\xi)^n\, \widehat{v}^{0}(\xi).$$

If $|g(h\xi)| > 1$, then the energy grows exponentially; hence **for stability we must require** $|g(h\xi)| \leq 1$.

Von Neumann Analysis... Closing Out

We let $\theta = h\xi$, and use $e^{-i\theta} = \cos\theta - i\sin\theta$, and consider $|g(\theta)|^2$:

$$\begin{aligned}
|g(\theta)|^2 &= (1 - a\lambda + a\lambda\cos\theta)^2 + a^2\lambda^2\sin^2\theta \\
&= \left(1 - 2a\lambda\sin^2\left(\frac{\theta}{2}\right)\right)^2 + 4a^2\lambda^2\sin^2\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right) \\
&= 1 - 4a\lambda\sin^2\left(\frac{\theta}{2}\right) + 4a^2\lambda^2\sin^4\left(\frac{\theta}{2}\right) + 4a^2\lambda^2\sin^2\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right) \\
&= 1 - 4a\lambda(1 - a\lambda)\sin^2\left(\frac{\theta}{2}\right).
\end{aligned}$$

Since $\sin^2\left(\frac{\theta}{2}\right) \geq 0$, we must require $a\lambda \geq 0$ and $a\lambda \leq 1$ in order for $|g(\theta)|^2 \leq 1$. Hence, the scheme is stable for $\mathbf{0 \leq a\lambda \leq 1}$.

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

Von Neumann Analysis: Images of $g(\theta)$

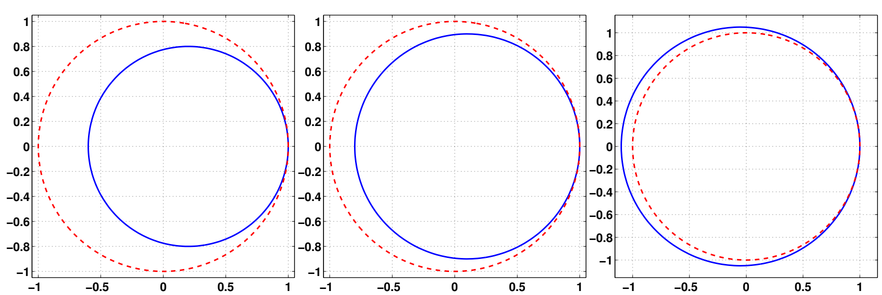


Figure: Images of $g(\theta)$ in the complex plane. For $a\lambda = 0.8$ and $a\lambda = 0.9$, the image (**blue**, solid) is contained in the unit circle (**red**, dashed), but for $a\lambda = 1.05$ we can clearly see that $|g(\theta)| > 1$, except for $g(0) = 1$.

With this example in mind, we are ready for the formal criterion for stability.

Von Neumann Analysis: The Stability Condition

Theorem (Von Neumann Stability)

A one-step finite difference scheme (with constant coefficients) is stable in a stability region Λ if and only if there is a constant K (independent of θ, k, and h) such that

$$|g(\theta, k, h)| \leq 1 + Kk$$

with $(k, h) \in \Lambda$. If $g(\theta, k, h)$ is independent of h and k, the stability condition can be replaced with the restricted stability condition

$$|g(\theta)| \leq 1.$$

Determining stability this way is quite straightforward — only symbolic manipulations of the expression for $|g(\theta, k, h)|^2$ are needed.

Example: Forward-Time-Central-Space

The procedure can be stream-lined quite a bit, consider

$$\frac{v_m^{n+1} - v_m^n}{k} + a\,\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0.$$

Replace v_m^n by $g^n\, e^{im\theta}$, and get

$$\frac{g^{n+1} e^{im\theta} - g^n e^{im\theta}}{k} + a\,\frac{g^n e^{i(m+1)\theta} - g^n e^{i(m-1)\theta}}{2h}$$

$$= g^n e^{im\theta}\left[\frac{g-1}{k} + a\,\frac{e^{i\theta} - e^{-i\theta}}{2h}\right] = 0.$$

The expression in the square bracket must be zero, and $e^{i\theta} - e^{-i\theta} = 2i\sin\theta$, so the amplification factor is given by

$$g(\theta) = 1 - ia\lambda\sin\theta, \quad |g(\theta)|^2 = 1 + (a\lambda)^2\sin^2\theta \geq 1.$$

Hence, this scheme is **unstable**.

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Example: Lax-Friedrichs Scheme

The Lax-Friedrichs Scheme is quite similar to FT-CS:

$$\frac{v_m^{n+1} - \frac{1}{2}\left[\mathbf{v_{m+1}^n} + \mathbf{v_{m-1}^n}\right]}{k} + a\,\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0$$

Replace v_m^n by $g^n\, e^{im\theta}$, and get

$$\frac{g^{n+1} e^{im\theta} - g^n \frac{1}{2}\left[\mathbf{e^{i(m+1)\theta}} + \mathbf{e^{i(m-1)\theta}}\right]}{k} + a\,\frac{g^n e^{i(m+1)\theta} - g^n e^{i(m-1)\theta}}{2h}$$

$$= g^n e^{im\theta}\left[\frac{g - \frac{1}{2}\left[\mathbf{e^{i\theta}} + \mathbf{e^{-i\theta}}\right]}{k} + a\,\frac{e^{i\theta} - e^{-i\theta}}{2h}\right] = 0$$

Now, $e^{i\theta} - e^{-i\theta} = 2i\sin\theta$, and $e^{i\theta} + e^{-i\theta} = 2\cos\theta$, so

$$g(\theta) = \cos\theta - ia\lambda\sin\theta, \quad |g(\theta)|^2 = \cos^2\theta + (a\lambda)^2\sin^2\theta$$

Hence, this scheme is **stable**, as long as $|a\lambda| \leq 1$.

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Example: Lax-Friedrichs Scheme... Again

The Lax-Friedrichs scheme applied to the equation

$$u_t + au_x - \mathbf{u} = 0,$$

i.e.

$$\frac{v_m^{n+1} - \frac{1}{2}\left[v_{m+1}^n + v_{m-1}^n\right]}{k} + a\,\frac{v_{m+1}^n - v_{m-1}^n}{2h} - \mathbf{v_m^n} = 0,$$

gives rise to the amplification factor

$$g(\theta, k, h) = \cos\theta - ia\lambda\sin\theta + \mathbf{k},$$

with

$$|g(\theta, k, h)|^2 = (\cos\theta + \mathbf{k})^2 + (a\lambda)^2\sin^2\theta.$$

For which $|g(\theta, k, h)|^2 \leq (1+k)^2 = 1 + 2k + \mathcal{O}(k^2)$ if $|a\lambda| \leq 1$. This scheme is **stable** according to the first inequality in the theorem.

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Modified Schemes and Stability

Corollary (Stability for Modified Schemes)

If a scheme as in the **von Neumann stability theorem** *is modified so that the modifications result only in the addition to the amplification factor of terms that are $\mathcal{O}(k)$ uniformly in ξ, then the modified scheme is stable if and only if the original scheme is stable.*

Proof: If g is the amplification factor for the scheme and satisfies $|g| \leq 1 + Kk$, then the amplification factor of the modified scheme, g', satisfies

$$|g'| = |g + \mathcal{O}(k)| \leq 1 + Kk + Ck = 1 + K'k.$$

Hence the modified scheme is stable if and only if the original scheme is stable, and vice versa. □

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Stability For the One-Way Wave Equation with a Lower-Order Term

Theorem

A consistent one-step scheme for the equation

$$u_t + au_x + bu = 0$$

is stable if and only if it is stable for this equation when $b = 0$*. Moreover, when* $k = \lambda h$*, and* λ *is a constant, the stability condition on* $g(h\xi, k, h)$ *is*

$$|g(\theta, 0, 0)| \leq 1.$$

Because of this theorem, it is usually sufficient to consider $g(h\xi, k, h) \rightsquigarrow g(\theta)$, and ignore the dependence on h, and k.

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Informal Homework — Not Due

Study the examples in chapter 2, and the proofs of the theorems.

Read § 2.3 — **Comments on Instability and Stability**.

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