Stability of finite difference schemes for hyperbolic initial boundary value problems I

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Plan of the first course

We consider the **one-dimensional** Cauchy problem for a first order system :

$$\begin{cases} \partial_t u + A\,\partial_x u = 0\,, & \text{in } [0,T]\times\mathbb{R}\,,\\ u|_{t=0} = f\,, & \text{on } \mathbb{R}\,. \end{cases}$$

Space domain $\mathbb{R}$, $A \in M_N(\mathbb{R})$, $u(t,x) \in \mathbb{R}^N$.

Linear **system** with **constant coefficients** (for simplicity).

Question

Under which condition is the Cauchy problem well-posed ? (Existence, uniqueness and continuous dependence of the solution on the initial condition. Of course, this heavily depends on the functional framework, as usual in the study of partial differential equations.)

Hyperbolicity

Answer by Fourier transform :

$$\begin{cases} \partial_t \widehat{u} + i\,\xi\,A\,\widehat{u} = 0\,, & \text{in } [0,T]\,,\\ \widehat{u}(0,\xi) = \widehat{f}(\xi)\,, & \text{on } \mathbb{R}\,. \end{cases}$$

This gives the formula

$$\widehat{u}(t,\xi) = \exp(-i\,t\,\xi\,A)\,\widehat{f}(\xi)\,.$$

Hyperbolicity

Definition (hyperbolicity)

The operator $\partial_t + A\,\partial_x$ is said to be hyperbolic if

$$\sup_{\eta \in \mathbb{R}} \| \exp(i\,\eta\,A) \| < +\infty\,.$$

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Proposition (easy case of a more general result by Kreiss)

The operator $\partial_t + A\,\partial_x$ is hyperbolic **if and only if** the matrix A is diagonalizable with real eigenvalues.

In this case, the Cauchy problem is well-posed in $L^2(\mathbb{R})$: for all $f \in L^2(\mathbb{R})$, there exists a unique solution $u \in C(\mathbb{R}_t; L^2(\mathbb{R}_x))$, and this solution satisfies the estimate

$$\sup_{t\in\mathbb{R}} \|u(t,\cdot)\|_{L^2(\mathbb{R})} \leq C_0\,\|f\|_{L^2(\mathbb{R})}\,,$$

for a certain numerical constant $C_0 > 0$.

Integration along characteristics

We consider the eigenvalues and eigenvectors of A : λ_j, r_j, $j = 1, \dots, N$.
The solution u is decomposed on the basis $(r_1, \dots, r_N)$:

$$u(t,x) = \sum_{j=1}^{N} \alpha_j(t,x)\, r_j \,,$$

$$f(x) = \sum_{j=1}^{N} \beta_j(x)\, r_j \,.$$

The system of PDEs decouples into

$$\begin{cases} \partial_t \alpha_j + \lambda_j\, \partial_x \alpha_j = 0\,, & \text{in } [0,T] \times \mathbb{R}\,, \\ \alpha_j|_{t=0} = \beta_j\,, & \text{on } \mathbb{R}\,. \end{cases}$$

Integration along characteristics

Each function α_j solves a scalar transport equation, which can be solved by the method of characteristics :

$$\alpha_j(t,x) = \beta_j(x - \lambda_j\, t)\,.$$

This gives the explicit formula

$$u(t,x) = \sum_{j=1}^{N} \beta_j(x - \lambda_j\, t)\, r_j\,.$$

Corollary

If A is diagonalizable with real eigenvalues, then the Cauchy problem is also well-posed in any $L^p(\mathbb{R})$, $1 \leq p < +\infty$.
This property is **specific to one-dimensional problems**.

To remember

• We only consider the case of hyperbolic systems (A diagonalizable) : there is an explicit formula for the solution (in particular, finite speed of propagation.)

• When the initial condition belongs to $L^2(\mathbb{R})$, there holds

$$\widehat{u}(t,\xi) = \exp(-i\,t\,\xi\,A)\,\widehat{f}(\xi)\,.$$

• The L^2 well-posedness theory is the only one that extends to general systems in several space dimensions (Brenner, Rauch...). This is the reason why we do not consider here the well-posedness theory in $BV(\mathbb{R})$. The ultimate goal is to get results in any space dimension.

Plan

Discretizing the Cauchy problem

We still consider the Cauchy problem

$$\begin{cases} \partial_t u + A\,\partial_x u = 0\,, & \text{in } [0,+\infty[\,\times\mathbb{R}\,, \\ u|_{t=0} = f\,. \end{cases}$$

Our goal is to construct an approximation the solution $u(t,x)$.

$\Delta t, \Delta x$: time and space steps. The ratio $\lambda = \Delta t/\Delta x$ is kept **fixed**, and Δt is allowed to be small (Δx varies accordingly).

λ is called the Courant-Friedrichs-Lewy number (CFL).

Discretizing the Cauchy problem

In what follows, we let U_j^n denote the approximation of the solution u on the cell $[n\,\Delta t, (n+1)\,\Delta t[\times[j\,\Delta x, (j+1)\,\Delta x[$, with $n \in \mathbb{N}$ and $j \in \mathbb{Z}$.

U_j^n is not necessarily a pointwise approximation of $u(t^n, x_j)$. If U_Δ denotes the corresponding step function, the approximation should be understood in the following sense :

$$\|u - U_\Delta\|_{L^\infty([0,T];L^2(\mathbb{R}))} = o(1)\,.$$

(Observe that U_Δ does not belong to $C(L^2)$ but only to $L^\infty(L^2)$. Continuity is only recovered in the limit $\Delta t \to 0$.)

Numerical scheme for the Cauchy problem

A numerical scheme with one time step reads :

$$\begin{cases} U_j^{n+1} = Q\, U_j^n\,, & j \in \mathbb{Z}\,, \\ U_j^0 = f_j\,, & j \in \mathbb{Z}\,, \end{cases}$$

with a discretized **evolution operator**

$$Q := \sum_{\ell=-r}^{p} A_\ell\, T^\ell\,, \quad (TU)_j := U_{j+1}\,.$$

The scheme involves "r points on the left, and p points on the right". Usually, the matrices A_ℓ are polynomial functions of $\lambda\, A$.

Numerical scheme for the Cauchy problem

• Here we only consider linear schemes : the mapping $U^0 \mapsto U^1$ is linear. The matrices A_ℓ do not depend on j, n nor on the initial condition U^0.

• More elaborate schemes (flux limiters, ENO, WENO...) are **non-linear** ! Their analysis may be much more complicated.

• One possible discretization of the initial condition is

$$f_j := \frac{1}{\Delta x} \int_{j\,\Delta x}^{(j+1)\,\Delta x} f(y)\,\mathrm{d}y \,.$$

Good stability property (use Cauchy-Schwarz) :

$$\sum_{j \in \mathbb{Z}} \Delta x \, |f_j|^2 \le \|f\|_{L^2(\mathbb{R})} \,.$$

Fundamental examples

- The **upwind** scheme : for a scalar transport equation

$$\begin{cases} U_j^{n+1} = U_j^n - \dfrac{\lambda}{2}(a+|a|)\,(U_j^n - U_{j-1}^n) \\ \qquad\qquad -\dfrac{\lambda}{2}(a-|a|)\,(U_{j+1}^n - U_j^n)\,, & j \in \mathbb{Z}\,, \\ U_j^0 = f_j\,, & j \in \mathbb{Z}\,. \end{cases}$$

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For a hyperbolic system :

$$\begin{cases} U_j^{n+1} = U_j^n - \dfrac{\lambda\, A}{2}\,(U_{j+1}^n - U_{j-1}^n) \\ \qquad\qquad +\dfrac{\lambda\,|A|}{2}\,(U_{j+1}^n + U_{j-1}^n - 2\,U_j^n)\,, & j \in \mathbb{Z}\,, \\ U_j^0 = f_j\,, & j \in \mathbb{Z}\,. \end{cases}$$

Fundamental examples

- The **Lax-Friedrichs** scheme

$$\begin{cases} U_j^{n+1} = \dfrac{U_{j-1}^n + U_{j+1}^n}{2} - \dfrac{\lambda\, A}{2}\,(U_{j+1}^n - U_{j-1}^n) & j \in \mathbb{Z}\,, \\ U_j^0 = f_j\,, & j \in \mathbb{Z}\,. \end{cases}$$

Same form as the upwind scheme but with a different "viscous term".

Stability

Definition (stability)

The numerical scheme is (ℓ^2-) stable if there exists a constant $C_0 > 0$ such that for all $\Delta t \in]0,1]$, for all initial condition $(f_j)_{j\in\mathbb{Z}} \in \ell^2$ and for all $n \in \mathbb{N}$, there holds

$$\sum_{j\in\mathbb{Z}} \Delta x \, |U_j^n|^2 \leq C_0 \sum_{j\in\mathbb{Z}} \Delta x \, |f_j|^2 \, .$$

We wish to determine when a scheme is stable.

Stability

Start from

$$\forall\, x \in \mathbb{R}\,, \quad U^{n+1}(x) = \sum_{\ell=-r}^{p} A_\ell \, U^n(x+\ell\,\Delta x)\,,$$

and apply Fourier transform to obtain :

$$\forall\, \xi \in \mathbb{R}\,, \quad \widehat{U^{n+1}}(\xi) = \mathcal{A}(\mathrm{e}^{i\,\Delta x\,\xi})\,\widehat{U^n}(\xi)\,,$$

with

$$\forall\, \kappa \in \mathbb{C} \setminus \{0\}\,, \quad \mathcal{A}(\kappa) := \sum_{j=-r}^{p} \kappa^\ell \, A_\ell\,.$$

Stability

Proposition (characterization of stability)

The numerical scheme is stable **if and only if** the matrices A_ℓ satisfy, for some numerical constant C_1, the uniform bound :

$$\forall\, n \in \mathbb{N}\,, \quad \forall\, \eta \in \mathbb{R}\,, \quad \left| \mathcal{A}(\mathrm{e}^{i\,\eta})^n \right| \le C_1\,.$$

This property is called **uniform power boundedness**.

The matrix $\mathcal{A}$ is called the amplification matrix or symbol.

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Examples

The upwind and Lax-Friedrichs schemes are stable if and only if $\lambda\,\rho(A) \le 1$.

Multistep schemes

A numerical scheme with several time steps reads :

$$\begin{cases} U_j^{n+1} = \sum_{\sigma=0}^{s} Q_\sigma \, U_j^{n-\sigma} \,, & n \geq s \,, \, j \in \mathbb{Z} \,, \\ U_j^n = f_j^n \,, & n = 0, \dots, s \,, \, j \in \mathbb{Z} \,, \end{cases}$$

with discretized operators

$$Q_\sigma := \sum_{\ell=-r}^{p} A_{\ell,\sigma} \, T^\ell \,.$$

Fundamental example

- The **leap-frog** scheme

$$\begin{cases} U_j^{n+1} = U_j^{n-1} - \lambda\, A\,(U_{j+1}^n - U_{j-1}^n) & j \in \mathbb{Z}\,, \\ U_j^0 = f_j^0\,, & j \in \mathbb{Z}\,, \\ U_j^1 = f_j^1\,, & j \in \mathbb{Z}\,. \end{cases}$$

Stability

Definition (stability)

The numerical scheme is (ℓ^2-) stable if there exists a constant $C_2 > 0$ such that for all $\Delta t \in]0,1]$, for all initial conditions $(f_j^0)_{j \in \mathbb{Z}}, \dots, (f_j^s)_{j \in \mathbb{Z}} \in \ell^2$ and for all $n \in \mathbb{N}$, there holds

$$\sum_{j \in \mathbb{Z}} \Delta x \, |U_j^n|^2 \leq C_2 \sum_{n=0}^{s} \sum_{j \in \mathbb{Z}} \Delta x \, |f_j^n|^2 \, .$$

Stability

Proposition (characterization of stability)

The scheme is stable **if and only if** the amplification matrix

$$\mathcal{A}(\kappa) := \begin{pmatrix} \widehat{Q_0}(\kappa) & \dots & \dots & \widehat{Q_s}(\kappa) \\ I & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ 0 & 0 & I & 0 \end{pmatrix} , \quad \widehat{Q_\sigma}(\kappa) := \sum_{\ell=-r}^{p} \kappa^\ell A_{\ell,\sigma} ,$$

is uniformly power bounded for $\kappa = \mathrm{e}^{i\,\eta} \in \mathbb{S}^1$.

Plan

Some facts on matrices

We study when a matrix (a family of matrices) is (uniformly) power bounded.

Lemma

Let $M \in M_d(\mathbb{C})$ be power bounded. Then $\rho(M) \leq 1$.

Corollary (von Neumann condition)

If the numerical scheme is stable, then $\rho(\mathcal{A}(e^{i\,\eta})) \leq 1$ for all $\eta \in \mathbb{R}$.

Some facts on matrices

We would like to know when the von Neumann condition is also **sufficient** for stability.

Lemma (easy case)

Let us consider a one step scheme for which the matrices $A_{-r}, \dots, A_p$ can be simultaneously diagonalized (for instance when they are all polynomial functions of λA).

Then the scheme is stable if and only if the von Neumann condition holds.

Some facts on matrices

Is there a more accurate description of power bounded matrices ?

Lemma

A matrix $M \in M_d(\mathbb{C})$ is power bounded if and only if $\rho(M) \leq 1$ and furthermore the eigenvalues of M whose modulus equals 1 are semi-simple (that is, their geometric multiplicity equals their algebraic multiplicity).

This Lemma is unfortunately inapplicable for an infinite family of matrices (main reason : the Jordan reduction is highly ill-conditionned).

The only general characterization of uniformly power bounded matrices is due to Kreiss.

Geometrically regular operators

Definition (geometrically regular operators)

The finite difference operator Q, resp. the operators Q_σ, is said to be geometrically regular if the amplification matrix $\mathcal{A}$ satisfies the following property : if $\underline{\kappa} \in \mathbb{S}^1$ and $\underline{z} \in \mathbb{S}^1 \cap \mathrm{sp}(\mathcal{A}(\underline{\kappa}))$ has algebraic multiplicity $\underline{\alpha}$, then there exist some functions $\beta_1(\kappa), \dots, \beta_{\underline{\alpha}}(\kappa)$ that are **holomorphic** in a neighborhood $\mathcal{W}$ of $\underline{\kappa}$ in $\mathbb{C}$ and that satisfy

$$\beta_1(\underline{\kappa}) = \cdots = \beta_{\underline{\alpha}}(\underline{\kappa}) = \underline{z}\,, \quad \det\left(z\,I - \mathcal{A}(\kappa)\right) = \vartheta(\kappa, z) \prod_{j=1}^{\underline{\alpha}} \left(z - \beta_j(\kappa)\right),$$

with ϑ a holomorphic function of (κ, z) in some neighborhood of $(\underline{\kappa}, \underline{z})$ such that $\vartheta(\underline{\kappa}, \underline{z}) \neq 0$,

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with ϑ a holomorphic function of (κ, z) in some neighborhood of $(\underline{\kappa}, \underline{z})$ such that $\vartheta(\underline{\kappa}, \underline{z}) \neq 0$,and if furthermore, there exist some vectors $e_1(\kappa), \dots, e_{\underline{\alpha}}(\kappa) \in \mathbb{C}^N$, resp. $\mathbb{C}^{N(s+1)}$, that depend **holomorphically** on $\kappa \in \mathcal{W}$, that are linearly independent for all $\kappa \in \mathcal{W}$, and that satisfy

$$\forall\, \kappa \in \mathcal{W}\,, \quad \forall\, j = 1, \dots, \underline{\alpha}\,, \quad \mathcal{A}(\kappa)\, e_j(\kappa) = \beta_j(\kappa)\, e_j(\kappa)\,.$$

Geometrically regular operators

In other words, for geometrically regular operators, when $\underline{z} \in \mathbb{S}^1 \cap \mathrm{sp}(\mathcal{A}(\underline{\kappa}))$, the eigenvalues and eigenvectors close to $\underline{\kappa}$ can be chosen holomorphically with respect to κ.

A necessary condition is that $\underline{z}$ is a semi-simple eigenvalue.

If the eigenvalue is simple, geometric regularity holds. For multiple eigenvalues, this is the simplest behavior for crossing.

Geometrically regular operators

Proposition (characterization of stability for geometrically regular operators)

Let the finite difference operator Q, resp. the operators Q_σ, be geometrically regular. Then the one step, resp. multistep, numerical scheme is stable **if and only if** the von Neumann condition holds.

Geometrically regular operators

Proposition (characterization of stability for geometrically regular operators)

Let the finite difference operator Q, resp. the operators Q_σ, be geometrically regular. Then the one step, resp. multistep, numerical scheme is stable **if and only if** the von Neumann condition holds.

Examples : • the upwind and Lax-Friedrichs schemes for $\lambda\,\rho(A) \leq 1$,
• the leap-frog scheme for $\lambda\,\rho(A) < 1$.

Plan

Consistency analysis

Recall the formula

$$\widehat{u}(\Delta t, \xi) = \exp(-i\,\Delta t\,\xi\,A)\,\widehat{f}(\xi) \simeq (I - i\,\Delta t\,\xi\,A)\,\widehat{f}(\xi)\,.$$

For a one-step scheme, we also have

$$\forall\, \xi \in \mathbb{R}\,, \quad \widehat{U^1}(\xi) = \mathcal{A}(\mathrm{e}^{i\,\Delta x\,\xi})\,\widehat{U^0}(\xi)\,.$$

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Performing a finite expansion with respect to Δt, we find the following **necessary conditions** for consistency :

$$\mathcal{A}(1) = \sum_{\ell=-r}^{p} A_\ell = I\,, \quad \mathcal{A}'(1) = \sum_{\ell=-r}^{p} \ell\,A_\ell = -\lambda\,A\,.$$

Plan

- Stability is **characterized** by uniform power boundedness of the amplification matrix.

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- In the framework of **geometrically regular** operators, stability is **characterized** by the von Neumann condition.
- This notion seems to apply to all "classical" numerical schemes. However, the behavior of eigenvalues of the amplification matrix can be very complex.

The **eigenvalues** of the amplification matrix $\mathcal{A}(e^{i\,\eta})$ should remain within the **closed unit disk**. How can they behave ?

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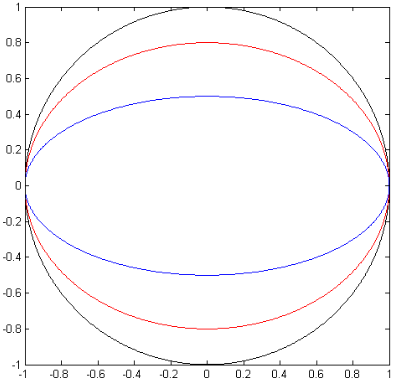
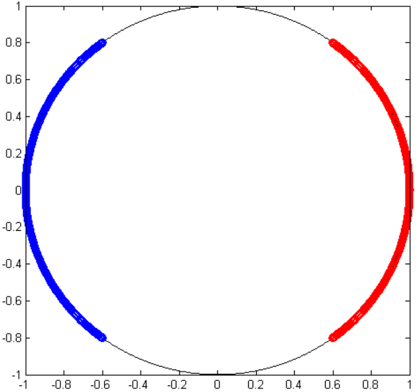
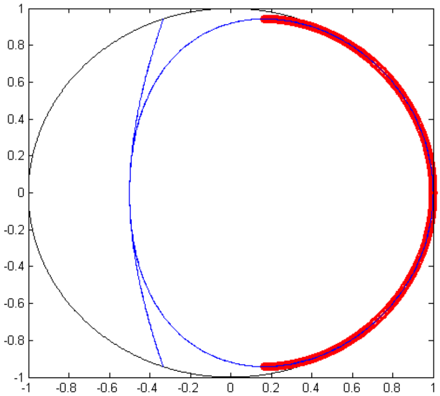
Two regular contact points with the unit circle (Lax-Friedrichs) :



Two singular contact points with the unit circle of even order (leap-frog) : in this case, the eigenvalues always belong to the unit circle.



Two singular contact points with the unit circle of even order ($s = 0$, Runge-Kutta scheme) :



One singular contact point with the unit circle of odd order ($s = 1$, therefore two eigenvalues, based on Adams integration rule) :