Shock profiles in the numerical analysis of hyperbolic systems of conservation laws

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1st order systems of conservation laws

Space-time domain:

$$t \geq 0, \qquad x = (x_1, \ldots, x_d).$$

Vector-valued unknown

$$egin{array}{ccc} (x,t) &\mapsto & u(x,t) \in \mathcal{U} & \left(\subset \mathbb{R}^N
ight), \end{array}$$

having the meaning of physically conserved densities: mass density, energymomentum, charge, electro-magnetic field, ...

Conservation laws:

$$\frac{\partial u}{\partial t} + \sum_{\alpha=1}^{d} \frac{\partial f^{\alpha}(u)}{\partial x_{\alpha}} = 0.$$

Examples

Gas Dynamics: $1 \le d \le 3$ and N = 2 + d. Unknowns $u = (\rho, \rho v, \rho \varepsilon)$. Euler equations:

- Conservation of mass $\partial_t \rho + \operatorname{div}(\rho v) = 0$,
- C. of momentum $\partial_t(\rho v) + \operatorname{div}(\rho v \otimes v) + \nabla p(\rho, e) = 0$,
- C. of energy

$$\partial_t \left(\rho e + \frac{1}{2} \rho |v|^2 \right) + \operatorname{div} \left(\left(\rho e + \frac{1}{2} \rho |v|^2 + p \right) v \right) = 0.$$

Traffic flow (Lighthill, Whitham): scalar unknown $u = \rho$, the density of cars along a road (d = 1).

Conservation of "mass"

$$\partial_t \rho + \partial_x q = 0, \quad q = f(\rho) := \kappa \rho (\rho_{\max} - \rho).$$

Maxwell's equations: d = 3 and N = 6. Unknown u = (B, D). Faraday and Ampère conservation laws

 $\partial_t B + \operatorname{curl} E = 0, \quad \partial_t D - \operatorname{curl} H = 0, \quad \operatorname{div} B = \operatorname{div} D = 0,$

with equations of state

$$E = E(B, D), \qquad H = H(B, D).$$

The Cauchy Problem

For the sake of simplicity: d = 1 (planar waves).

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \qquad (1)$$

where

$$egin{array}{ccc} u &\mapsto & f(u) \ \mathcal{U} & o & \mathbb{R}^N \end{array}$$

is called the *flux*.

Given an initial data $u^0 : \mathbb{R} \to \mathcal{U}$, find the solution such that $u(x, 0) \equiv u^0(x)$.

An example: the Riemann problem

• Hypothesis: u^0 is invariant under $x \mapsto \sigma x$:

$$u^{0}(x) \equiv a$$
 if $x < 0$, $u^{0}(x) \equiv b$ if $x > 0$,

- The PDEs are invariant under $(x, t) \mapsto (\sigma x, \sigma t)$,
- Uniqueness is expected: The solution must be self-similar,

$$u(x,t) = R\left(\frac{x}{t}\right).$$

Solve the *implicit* Differential Equation

$$\frac{d}{d\xi}f(R(\xi)) = \xi \frac{dR}{d\xi}.$$
(2)

If $\xi \mapsto R(\xi)$ is Lipschitz:

$$(\mathrm{d}f(R(\xi)) - \xi)\frac{dR}{d\xi} = 0.$$

Whence either $\xi \mapsto R(\xi)$ is constant (locally), or

- $\frac{dR}{d\xi} = r_k(R(\xi))$ is an eigenvector,
- $\xi = \lambda_k(R(\xi))$ the corresponding eigenvalue.

 \longrightarrow Suggests to assume **hyperbolicity**: df(u) is diagonalisable with real eigenvalues.

Differentiation yields

$$d\lambda_{k}(R(\xi)) \cdot \frac{dR}{d\xi} = 1, \qquad (3)$$

which raises two obstacles:

- 1. (3) is impossible for linear systems ($\lambda_k \equiv \text{cst}$), or more generally if $d\lambda_k(R(\xi)) \cdot r_k = 0.$
- 2. (3) does not allow us to solve the Riemann problem for certain data.

Example: the Burgers equation (d = 1),

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2}u^2\right) = 0.$$

Then $\lambda(u) = f'(u) \equiv u$,

 $u(\xi) = \xi$

yields the NC

 $a \leq b$.

What to do if b < a instead ?

Answer: Accept discontinuous solutions.

Then (2) to be understood in the distributional sense,

$$\frac{d}{d\xi}\left\{f(R(\xi)) - \xi R(\xi)\right\} = -R(\xi).$$

Whence $\xi \mapsto f(R(\xi)) - \xi R(\xi)$ is Lipschitz continuous. Yields a jump relation,

. . .

the Rankine-Hugoniot condition:

$$[f(R)] = \xi[R], \quad (4)$$

with

$$[R] := R(\xi + 0) - R(\xi - 0).$$

Warning. Not all discontinuities are admissible.

Example: in Burgers' equation, discontinuities are restricted by

$$R(\xi+0) < R(\xi-0).$$

Construction: to solve the Riemann problem, glue

- constant states,
- C^1 -solutions (*rarefaction waves*),
- discontinuities (*shock waves*).

Definition. $R = R\left(a, b; \frac{x}{t}\right)$ is the *Riemann solver*.



Conservative difference schemes

Choose $\Delta x > 0$, $\Delta t > 0$.

Rectangular grid: $t_n = n\Delta t$ and $x_j = j\Delta x$.

Aspect ratio:

$$\sigma := \frac{\Delta t}{\Delta x}$$

Dimensional analysis:

$$rac{1}{\sigma}$$
 is a velocity.

Discretized unknown:

$$u_j^n \sim u(x_j, t_n).$$

Driven by a *difference scheme*

$$\frac{u_{j}^{n+1} - u_{j}^{n}}{\Delta t} + \frac{g_{j+\frac{1}{2}}^{n} - g_{j-\frac{1}{2}}^{n}}{\Delta x} = 0,$$

with g the numerical flux.

Initial sampling:

$$u_j^0 := u^0(j\Delta x)$$
 or $u_j^0 := \frac{1}{\Delta x} \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} u^0(x) dx.$

Designing a scheme

Choose a flux map

$$(\ldots, u_j, u_{j+1}, \ldots) \mapsto g_{j+\frac{1}{2}}$$

with shift invariance.

Example: Three-point schemes

$$g_{j+\frac{1}{2}} := F(u_j, u_{j+1}).$$

Yields

$$u_{j}^{n+1} = u_{j}^{n} + \sigma \left(F(u_{j-1}^{n}, u_{j}^{n}) - F(u_{j}^{n}, u_{j+1}^{n}) \right).$$

Reconstruction

 \longrightarrow Approximated solution $u^{app}(x,t)$.

Extra- / inter-polated from the points u_j^n .

- piecewise constant,
- piecewise linear,
- exact solution in strips $n\Delta t \leq t < (n+1)\Delta t$ (uses the Riemann solver),

• ...

There remains to choose F.

Consistency

- Assume that σ is constant.
- Let $\Delta t \rightarrow 0^+$. Assume that u^{app} converges boundedly almost everywhere.
- **Theorem** (Lax–Wendroff). Then the limit u(x, t) satisfies

$$\partial_t u + \partial_x F(u, u) = 0.$$

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• Want to fit $\partial_t u + \partial_x f(u) = 0$? Require that

$$F(a,a) \equiv f(a), \qquad \forall a \in \mathbb{R}^N.$$

Examples of schemes

Centered scheme (Von Neumann):

$$F_c(a,b) := \frac{1}{2}(f(a) + f(b)).$$

Highly unstable!!!

Lax-Friedrichs scheme:

$$F_{LF}(a,b) := \frac{1}{2}(f(a) + f(b)) + \frac{1}{2\sigma}(a-b).$$

Can be defined through the Riemann problem !

Lax–Wendroff scheme. A second-order variant of Lax–Friedrichs.

$$F_{LW}(a,b) := \frac{1}{2}(f(a) + f(b)) + \frac{\sigma}{2} df_m(f(a) - f(b)),$$

with df_m a "middle point" between df(a) and df(b), *e.g.*

$$df\left(\frac{a+b}{2}\right), \qquad \frac{1}{2}(df(a)+df(b)), \qquad \int_0^1 df(\theta a+(1-\theta)b) d\theta.$$

Godunov scheme:

$$F_G(a,b) = f(c), \qquad c := R(a,b;0),$$

where $(x, t) \mapsto R(a, b; x/t)$ is the Riemann solver.

Nota. Godunov's flux f(R(0)) is well-defined even in the case of a stationary shock, since

$$f(R(0+)) = f(R(0-)).$$

Other schemes: Roe, Osher, Leveque, ...

Linearized stability of schemes

- Still assume σ constant.
- Let $\Delta t \rightarrow 0^+$.
- Write the scheme

$$u_j^{n+1} = G(u_{j-1}^n, u_j^n, u_{j+1}^n),$$

with

$$G(a_{-1}, a_0, a_1) := a_0 + \sigma \left(F(a_{-1}, a_0) - F(a_0, a_1) \right).$$

• Constants are solutions.

• Linearize about a constant state u^* :

$$w_j^{n+1} = \sum_{-1 \le k \le 1} A_k w_{j+k}^n, \qquad A_k := \frac{\partial G}{\partial a_j} (u^*, u^*, u^*).$$

One has

$$\sum_{-1 \le k \le 1} A_k = I_N.$$

• Linearized stability: Given $w(\cdot, 0) \in L^2(\mathbb{R})^N$, the approximate solution $w^{app}(\cdot, t)$, has to remain bounded in L^2 as $\Delta t \to 0^+$:

There should exist C(t) (independent of Δt), such that

$$\sum_{j=-\infty}^{+\infty} \|w_j^n\|^2 \le C(t) \sum_{j=-\infty}^{+\infty} \|w_j^0\|^2,$$

with

$$n = E[t/\Delta t] \to +\infty.$$

• Apply discrete Fourier transform:

$$\widehat{w}(\xi) := \sum_{k=-\infty}^{\infty} e^{ik\xi} w_k.$$

The scheme becomes

$$\widehat{w}^{n+1}(\xi) = M(\xi)\widehat{w}^n(\xi),$$

with

$$M(\xi) := e^{i\xi}A_{-1} + A_0 + e^{-i\xi}A_1.$$

• Induction yields

$$\widehat{w}^n(\xi) = M(\xi)^n \widehat{w}^0(\xi).$$

By Uniform Boundedness Principle, stability requires (Lax–Wendroff)
 sup { ||M(ξ)ⁿ|| ; ξ ∈ ℝ, n ≥ 0 } < ∞.

Depends on both u^* and σ .

• NC, the *Courant–Friedrichs–Lewy condition*:

 $\rho(M(\xi)) \leq 1, \quad \forall \xi \in \mathbb{R}.$

Centered scheme: $\xi \neq 0$ implies $\rho(M(\xi)) > 1$.

Hadamard instability

Warning

Linearized analysis is not appropriate in presence of shock waves

The **Courant–Friedrichs–Lewy condition** (again)

Propagation in the discrete world: u_j^n depends only on $u_{j-n}^0, \ldots, u_{j+n}^0$.

That is, $u^{app}(x,t)$ depends only on the restriction of the initial data to

$$\left[x - \frac{t}{\sigma}, x + \frac{t}{\sigma}\right]$$

Propagation in the PDE world: at a linearized level,

$$\partial_t w + A \partial_x w = 0, \qquad A := df(u^*).$$

Decomposing the data and the solution onto the eigenbasis of $df(u^*)$ yields pure transport:

$$w(x,t) = \sum_{m=1}^{N} a_m (x - \lambda_m t) r_m, \qquad \mathrm{d} f(u^*) r_m = \lambda_m r_m.$$

Whence w(x,t) depends on the restriction of the initial data to

$$[x + \lambda_1 t, x + \lambda_N t].$$

Necessary condition for consistency:

The aspect ratio may not be so large that the waves travel slowlier in the discretized world than in the real world.

In other words, one needs

$$[x + \lambda_1 t, x + \lambda_N t] \subset \left[x - \frac{t}{\sigma}, x + \frac{t}{\sigma}\right].$$

Whence the C.-F.-L. condition:

For every likely u^* ,

$$\sigma
ho(df(u^*)) \le 1.$$
 (5)

Lax–Friedrichs or Godunov schemes: CFL amounts precisely to (5).

The Cauchy problem: the state of the art

Only partial results for the Cauchy problem:

Smooth initial data: Existence and uniqueness of classical solutions, on a strip

$$\mathbb{R}^d \times \left[0, T(u^0)\right).$$

Of little interest for applications.

• No other result for systems ($N \ge 2$) in several space dimensions ($d \ge 2$).

. . .

- Nice theory for the scalar case ($N = 1, d \ge 1$), Volpert, Kruzhkov (1970).
 - Existence and uniqueness for L^{∞} -data.
 - Contraction in the L^1 -distance.
 - Error estimates for approximate solutions (Kutznetsov).
 - Kinetic formulation (Perthame, P.-L. Lions & Tadmor)
- Systems ($N \ge 2$) when d = 1, Glimm (1965), Bressan (1994–ff):
 - Existence for quite general systems and small initial data in $BV(\mathbb{R})$.
 - Uniqueness, L^1 -continuous semi-group.

- Systems with many entropies (mainly N = 2 and d = 1) and some convexity, DiPerna (1983):
 - Existence of solutions for arbitrarily large initial data in L^{∞} ,
 - Uniqueness is not known.

One cause of troubles: shock waves.

A related one is: irreversibility.

Entropies

In physics and mechanics, C^1 -solutions of

 $\partial_t u + \mathsf{Div}_x f(u) = 0$

do satisfy an additional conservation law

$$\partial_t \phi(u) + \operatorname{div}_x \vec{q}(u) = 0,$$

where $D^2 \phi > 0_n$.

Terminology (math^{al}):

• ϕ is an *entropy* (!?!), *q* its *entropy* flux.

Proposition (Godunov, Lax & Friedrichs). A strongly convex entropy ensures the hyperbolicity: df(u) diagonalizable with real eigenvalues.

Example (gas dynamics):

Define the physical entropy $s = s(\rho, e)$ by

$$\theta ds = de + p(\rho, e) d\frac{1}{\rho}.$$

Then smooth flows satisfy

$$\frac{\partial}{\partial t}(\rho s) + \operatorname{Div}(\rho s \mathbf{v}) = 0.$$

Whence

$$\phi = -\rho s, \qquad \vec{q} = -\rho s \mathbf{v} = \phi \mathbf{v}.$$

Shock waves

Typical solutions of $\partial_t u + \partial_x f(u) = 0$ display discontinuities along curves x = X(t).

Limits $u(X(t) \pm 0, t) =: u^{\pm}(t)$ are expected, together with a *shock speed*

$$s := \frac{dX}{dt}$$

The PDEs translate into jump relations: the Rankine–Hugoniot condition,

$$f(u^+) - f(u^-) = s(u^+ - u^-).$$

Nota: the shock velocity is a $\lambda_k(u^*)$ (Taylor formula).

Irreversibility: the Lax entropy inequality

Relevant to thermodynamics and its 2nd principle.

Translates through a differential inequality.

For *genuinely nonlinear systems*, the R.-H. condition is **not compatible** with the jump relation

$$q(u^{+}) - q(u^{-}) = s\left(\phi(u^{+}) - \phi(u^{-})\right)$$
(6)

associated to the additional conservation law.

So what ?

Example: Burgers equation, N = 1 and $f(u) = \frac{1}{2}u^2$.

• Rankine–Hugoniot:

$$s = \frac{f(u^+) - f(u^-)}{u^+ - u^-} = \frac{u^+ + u^-}{2}.$$

• With
$$\phi(u) := u^2/2$$
 (thus $q(u) = u^3/3$), (6) reads

$$s = \frac{q(u^+) - q(u^-)}{\phi(u^+) - \phi(u^-)} = \frac{2}{3} \times \frac{(u^+)^2 + u^+ u^- + (u^-)^2}{u^+ + u^-}.$$

• Together, these identities give
$$u^- = u^+$$
.

Means that for discontinuous solutions,

$$\partial_t \phi(u) + \partial_x q(u) \neq 0.$$

So what ?

Require only the *Lax entropy inequality* (say $d \ge 1$)

$$\partial_t \phi(u) + \operatorname{div}_x \vec{q}(u) \leq 0,$$

in the sense of distributions.

Translated as

$$q(u^+) - q(u^-) \le s \left(\phi(u^+) - \phi(u^-) \right)$$

across discontinuities.

 \longrightarrow irreversibility.

Entropy consistent schemes

Definition (d = 1). Have a discrete entropy flux Q(a, b) with $Q(a, a) \equiv q(a)$, such that

$$\phi(u_j^{n+1}) \leq \phi(u_j^n) + \sigma\left(Q(u_{j-1}^n, u_j^n) - Q(u_j^n, u_{j+1}^n)\right)$$

for every sequency $(u_j^m)_{j,m}$ generated by the scheme.

Lax & Wendroff: one recovers again

$$\partial_t \phi(u) + \operatorname{div}_x \vec{q}(u) \leq 0$$

in the limit.
Shock profile

Principle: Every admissible solution of $\partial_t u + \partial_x f(u) = 0$, depending only on d' = 0 or 1 variable should have a counterpart at the discrete level.

• Constants \longrightarrow constants !

OK for conservative finite differences:

$$\left(u_{j-1}^n = u_j^n = u_{j+1}^n = a\right) \Longrightarrow \left(u_j^{n+1} = a\right).$$

• Discontinuous travelling waves (shocks)

$$u(x,t) = \begin{cases} u^-, & x < st, \\ u^+, & x > st. \end{cases}$$

 \longrightarrow "discrete" shock profile (DSP).

What is a DSP ?

• Look for a travelling wave in

$$x - ct = j\Delta x - cn\Delta t.$$

Normalized variable

$$y := \frac{x - ct}{\Delta x} = j - \sigma cn.$$

• Look for a travelling discrete wave

$$u_j^n = U(y) = U\left(\frac{x - ct}{\Delta x}\right).$$

...

• Plug into the difference scheme:

$$U(y - \sigma c) = U(y) + \sigma \{ F(U(y - 1), U(y)) - F(U(y), U(y + 1)) \}.$$

Terminology: the Profile Equation.

• Ask for limits

$$U(y) \to u^{\pm}, \qquad x \to \pm \infty.$$

Then

$$u^{\mathsf{app}}(x,t) \xrightarrow{\Delta x \to 0} \begin{cases} u^-, & x < ct, \\ u^+, & x > ct. \end{cases}$$

The velocity of a discrete shock

Integrate the profile equation over $y \in (-\infty, +\infty)$:

$$\int_{-\infty}^{+\infty} (U(y) - U(y - \sigma c)) \, dy = \sigma \int_{-\infty}^{+\infty} \{F(U(y), U(y + 1)) - F(U(y - 1), U(y))\} \, dy.$$

Apply twice the formula

$$\int_{-\infty}^{+\infty} (Z(y) - Z(y - h)) \, dy = h(Z(+\infty) - Z(-\infty)).$$

$$F(u^+, u^+) - F(u^-, u^-) = c(u^+ - u^-).$$

Remember the consistency

$$F(a,a) = f(a).$$

$$\longrightarrow$$
 The Rankine–Hugoniot condition for $(u^-, u^+; c)$!

Proposition: If a DSP exists from a state u^- to a state u^+ , then

1. (u^-, u^+) satisfy the Rankine–Hugoniot condition,

2. the velocity c of the DSP and the shock speed s coincide.

The latter is specific to conservation laws. When discretizing reaction-diffusion equations, say

$$\partial_t v - \Delta v = g(v),$$

then

- the velocity of a discrete front differs from the front speed in the PDE,
- the velocity may not be unique,
- there is a "pinning" phenomenon: as parameters in the PDE vary smoothly, the velocity of the discrete front may vary as in a "devil staircase".

Example: KPP–Fisher equation.

Integration also gives:

Proposition. Assume that the scheme be entropy-consistent. Let U be a DSP with limits u^{\pm} and velocity s.

Then the shock $(u^-, u^+; s)$ satisfies the Lax entropy inequality

$$q(u^+) - q(u^-) \le s \left(\phi(u^+) - \phi(u^-) \right).$$

Thus DSPs are a valuable tool. They represent faithfully shock waves.

Existence of DSPs

Question.

? Given a shock wave $(u^-, u^+; s)$, does there exist a profile $y \mapsto U(y)$, satisfying

- the limits $U(\pm \infty) = u^{\pm}$,
- the profile equation

$$U(y - \sigma s) = U(y) + \sigma \{F(U(y - 1), U(y)) - F(U(y), U(y + 1))\}.$$

Notation: the equation involves a dimensionless parameter, the 'grid velocity'

$$\eta := \sigma s$$

The domain ${\mathcal D}$ of a DSP

$$y \in \mathcal{D} \quad \mapsto \quad U(y).$$

For the PE to make sense, ${\cal D}$ must be invariant under both

$$y \mapsto y \pm 1$$
 and $y \mapsto y - \eta$.

Simplest choice:

$$\mathcal{D} = \mathbb{Z} + \eta \mathbb{Z}.$$

Rational case: If $\eta = \frac{p}{q}$, then $\mathcal{D} = \frac{1}{q}\mathbb{Z}$ is OK.

Irrational case: If $\eta \notin \mathbb{Q}$, then \mathcal{D} is dense in \mathbb{R} . Take

 $\mathcal{D}=\mathbb{R}$

instead.

Ask that $y \mapsto U(y)$ be continuous.

Existence: the rational case

$$\eta = \frac{p}{q}, \qquad p \wedge q = 1.$$

General method:

• "Integrate" once the profile equation (Benzoni).

Example: if $\eta = \frac{1}{2}$, then

$$U(y) - \sigma\{F(U(y-1/2), U(y+1/2)) + F(U(y), U(y+1))\} \equiv \text{ cst }.$$

Calculation of the constant:

- Take the limit as $y \to -\infty$,
- use $\eta = \sigma s$ and apply consistency.

In the example:

$$U(y) - \sigma \left(F(U(y - \frac{1}{2}), U(y + \frac{1}{2})) + F(U(y), U(y + 1)) \right)$$

= $u_{-} - \frac{1}{s} f(u_{-}).$

- This integrated form encodes the conditions at infinity $U(\pm \infty) = u^{\pm}$.
- More generally, rewrite the profile equation as

$$G\left(V_k, V_{k+1}; u^-, \sigma\right) = 0$$

for the extended state

$$V_k = \left(U\left(\frac{k}{q} - 1\right), U\left(\frac{k+1}{q} - 1\right), \dots, U\left(\frac{k-1}{q} + 1\right) \right)$$

• If possible, apply the IFT, to convert the integrated profile equation into a *discrete dynamical system*

$$V_{k+1} = H\left(V_k; u^-, \sigma\right).$$

- $V^- = (u^-, \dots, u^-)$ is a rest point (obvious).
- $V^+ = (u^+, \dots, u^+)$ is a rest point (Rankine–Hugoniot).
- Look for a heteroclinic orbit between V^- and V^+ .
- Tools: bifurcation theory, center manifold theorem applied to the map

$$(V, u, \sigma) \mapsto \widehat{H}(V, u, \sigma) := (H(V; u), u, \sigma).$$

Results in the rational case

Theorem (Majda & Ralston, 1979). Under the assumptions that

- the scheme is "non-resonant" and "linearly stable",
- the system is "genuinely non-linear",
- $(u^-, u^+; s)$ is an admissible shock,
- $||u^+ u^-|| \ll \frac{1}{q}$,

there exists a one-parameter family of DSPs with limits u^{\pm} .

Sketch of the proof ($\eta = 0$)

For steady shocks (s = 0), one has $\eta = 0$.

1-Geometry of the R.–H. condition. Select an index $1 \le k \le N$. Select a state u^* such that

$$\lambda_k(u^*) = 0, \qquad \mathrm{d}\lambda_k(u^*)r_k(u^*) \neq 0.$$

• Define locally

$$\Sigma := \{ u \in \mathcal{U} ; \lambda_k(u) = 0 \}.$$

 Σ is a hypersurface, transversal to $r_k(u)$.

- $f(\Sigma)$ is a hypersurface too.
- Locally, $f(\Sigma)$ splits \mathbb{R}^N into two open sets \mathcal{O}_0 and \mathcal{O}_2 .

• The graph of $u \mapsto f(u)$ folds over Σ . The equation

 $f(v) = \bar{f}$

has zero, one or two solutions, depending on whether

$$\overline{f} \in \mathcal{O}_0, \quad \in f(\Sigma), \quad \in \mathcal{O}_2.$$

• In a neighbourhood \mathcal{U}^* of $u^*,$

$$f(v) = f(v')$$

defines a smooth involution

$$v\mapsto v',$$

such that

$$(v'=v) \iff (v \in \Sigma).$$

• One has

$$\lambda_k(v)\lambda_k(v') < 0, \qquad \forall v \notin \Sigma.$$

2- The dynamical system.

• Define M(a, v) by I.F.T.:

$$F(a, M(a, v)) = f(v).$$

Works for Lax–Friedrichs, but not for Godunov.

• Write the Profile Equation $F(u_j, u_{j+1}) = f(u^-)$ in the form

 $(u_{j+1}, v_{j+1}) = H(u_j, v_j), \qquad H(a, v) := (M(a, v), v).$ (7) Meaning that $v_j \equiv \text{cst.}$

- Fixed points correspond to f(a) = f(v). Two families:
 - (v, v) for $v \in \mathcal{U}^*$,
 - (v', v) for $v \in \mathcal{U}^*$.

- These N-dimensional manifolds intersect transversally along diag($\Sigma \times \Sigma$).
- **3-** Center manifold theory.
 - Compute

$$\mathsf{D}H(u^*, u^*) = \begin{pmatrix} \mathsf{d}_a M & \mathsf{d}_b M \\ \mathsf{0}_N & I_N \end{pmatrix}.$$

• Differentiating, one has

$$\mathsf{d}_a F + \mathsf{d}_b F \,\mathsf{d}_a M = \mathsf{0}, \qquad \mathsf{d}_b F \,\mathsf{d}_v M = \mathsf{d} f.$$

• Recall that

$$\mathsf{d}_a F + \mathsf{d}_b F = df,$$

along the diagonal.

$$1 \in \mathsf{Sp}\left(\mathsf{d}_a M(u^*, u^*)\right),$$

• and $\mu = 1$ is an eigenvalue of $DH(u^*, u^*)$,

$$\#\{\mu = 1\} \ge N + 1.$$

- Non-resonnance:
 - the multiplicity is exactly N + 1,
 - no other eigenvalue on the unit circle.

• Center Manifold Theorem. There exists locally a smooth manifold \mathcal{M} of dimension N + 1, invariant under the dynamics, containing every trajectory which remains globally in \mathcal{U}^* .

The center manifold is tangent at (u^*, u^*) to

 $\ker \mathsf{D}H(u^*, u^*).$

• Here, ker $DH(u^*, u^*)$ is made of vectors

$$\begin{pmatrix} X\\ X+\alpha r_k(u^*) \end{pmatrix}, \quad \forall X \in \mathbb{R}^N, \, \alpha \in \mathbb{R}.$$

- The center manifold contains
 - fixed points in \mathcal{U}^* (two hypersurfaces),
 - heteroclinic orbits within \mathcal{U}^* .

• Since $v_{j+1} = v_j$, \mathcal{M} is foliated by curves

$$\delta(\bar{v}) := \{(a, v) \in \mathcal{M} ; v = \bar{v}\},\$$

invariant under the dynamics.

• These curves are transversal to the fixed point locuses. Each $\delta(\bar{v})$ contains exactly two fixed points:

$$P := (\overline{v}, \overline{v})$$
 and $Q := (\overline{v}', \overline{v}).$

- The restriction of *H* to $\delta(\bar{v})$ is orientation-preserving: *H* maps the arc *PQ* onto itself *PQ*, monotonically.
- Every point R in PQ yields a heteroclinic orbit such that

$$(u_0, v_0) = R.$$

Other values of η (sketchy)

- 1. Still use the integrated profile equation
- 2. Pretend that u^- and σ are not constant, and write the dynamics as

 $V_{k+1} = H(V_k, z_k, \sigma_k), \qquad z_{k+1} = z_k, \qquad \sigma_{k+1} = \sigma_k, \qquad (!!)$ that is

$$(V_{k+1}, z_{k+1}, \sigma_{k+1}) = \widehat{H}(V_k, z_k, \sigma_k),$$

but with z_k and σ_k constant ...

3. Given $u^- \in \mathcal{U}$ and $1 \leq j \leq N$, the state (V^-, u^-, σ^-) is a fixed point, where

$$V^- := (u^-, \dots, u^-), \qquad \sigma^- \in \mathbb{R}$$

is arbitrary

- 4. Nearby fixed points are of the form (V^+, u^+, σ^+) with $V^+ := (u^+, \dots, u^+)$ and $(u^-, u^+; \eta/\sigma^+)$ satisfying R–H.
- 5. The dynamics stands in a space of dimension (2q + 1)N + 1... but The Center Manifold Theorem reduces the dynamics to an (N + 2)dimensional manifold \mathcal{M} .
- 6. There are N + 1 constants of the dynamics: (u, σ) . Thus \mathcal{M} is foliated by curves invariant under the dynamics.

7. ...

QED

• In other words, there exists a *continuous* "D"SP

$$U: \mathbb{R} \to \mathbb{R}^N \qquad !$$

• For every $h \in \mathbb{R}$, the following defines a travelling wave

$$u_j^n = U\left(h+j-\frac{pn}{q}\right).$$

• **Re-parametrization**: If U is a continuous DSP, then so is $U \circ \psi$ for every one-to-one mapping $\psi : \mathbb{R} \to \mathbb{R}$ with (circle homeomorphism)

$$\psi\left(y+\frac{1}{q}\right)=\psi(y)+\frac{1}{q}.$$

• The theorem applies mainly to Lax "compressive" shocks.

Non-resonance vs Lax–Friedrichs

Lax–Friedrichs scheme:

$$u_j^{n+1} = \frac{1}{2} \left(u_{j-1}^n + u_{j+1}^n \right) + \frac{1}{2\sigma} \left(f(u_{j-1}^n) - f(u_{j+1}^n) \right).$$

The odd / even subgrids ignore each other:

$$j+n \in 2\mathbb{Z}, \qquad / \qquad j+n+1 \in 2\mathbb{Z}.$$

 \longrightarrow L.–F. is resonant.

To apply Majda–Ralston Theorem: iterate the scheme

$$u_{j}^{n+2} = \frac{1}{4} \left(u_{j-2}^{n} + 2u_{j}^{n} + u_{j+2}^{n} \right) + \cdots$$

Doubling the scales Δt and Δx yields

$$v_k^m := u_{2k}^{2m},$$

which obeys a conservative difference scheme with numerical flux

$$F_{LF2}(a,b) := \frac{1}{4\sigma}(a-b) + \frac{1}{4}(f(a) + f(b)) + \frac{1}{2}f\left(\frac{a+b}{2} + \frac{\sigma}{2}(f(a) - f(b))\right)$$

This scheme is non-resonant.

The irrational case

Warning: $\mathbb{Z} + \eta \mathbb{Z}$ is dense in \mathbb{R} .

 $\longrightarrow \qquad \text{Search for a$ *continuous* $DSP} \\ U : \mathbb{R} \to \mathbb{R}^N.$

First attempt: Pass to the limit as rationals tend to irrationals.

Failure, because of the restriction

$$\|u^+ - u^-\| \ll \frac{1}{q}$$

in Majda–Ralston Theorem.

In the limit, $q \rightarrow +\infty$. There remains the useless situation

$$u^+ = u^-.$$

A complete theory: the scalar case (N = 1)

Scalar conservation laws satisfy a comparison principle (Kruzkhov): If u and v solve the Cauchy problem, then

$$(u^0 \le v^0, a.e.) \Longrightarrow (u \le v, \forall t > 0).$$

Suggests to employ monotone schemes

$$u_j^{n+1} = G\left(u_{j-1}^n, u_j^n, u_{j+1}^n\right),$$

with

$$(a,b,c) \mapsto G(a,b,c)$$

(componentwise) monotonous non-decreasing.

Often related to the CFL condition.

Examples:

• Lax–Friedrichs and Godunov schemes are monotone under $\sigma |f'| \leq 1$,

$$G_{LF}(a,b,c) = \frac{1}{2}(a+\sigma f(a)) + \frac{1}{2}(c-\sigma f(c)).$$
$$G_G(a,b,c) = b + \sigma \left(f_G(a,b) - f_G(b,c)\right)$$

with

$$f_G(a,b) := \begin{cases} \inf\{f(u) ; u \in [a,b]\},\\\\ \sup\{f(u) ; u \in [b,a]\}. \end{cases}$$

- Lax–Wendroff is never monotone (2nd order).
- Monotone schemes are only first-order.

Theorem (G. Jennings).

For scalar equations and monotone schemes, continuous DSPs

- 1. exist for every admissible shock with $\eta \in \mathbb{Q}$,
- 2. are strictly monotone,
- 3. are essentially unique,
- 4. are Lipschitz:

$$|U(x+h) - U(x)| \le |h(u^+ - u^-)|, \qquad \forall x, h \in \mathbb{R}.$$

 \bigcirc

"Admissible shocks": those satisfying the Oleinik condition.

The latter justifies the passage to the limit:

Theorem (H. Fan , D. S.).

The same existence / uniqueness / monotonicity result holds true regardless the (ir)rationality of η , for every (weakly) monotone scheme.

 \Diamond

Sketch of proof:

- Apply Ascoli–Arzela
- Pass to the limit in the "integrated form" of the profile equation.
- From 1- monotonicity of the profile U, 2- the integrated profile equation,
 3- the Oleinik inequality, prove that U(±∞) = u[±].

The shift function

Back to systems. Let $U : \mathbb{R} \to \mathcal{U}$ be a DSP, with bounded variations.

Given $h \in \mathbb{R}$, define

$$Y(h) := \sum_{j \in \mathbb{Z}} (U(j+h) - U(j)) \qquad \left(Y(h) \in \mathbb{R}^N \right).$$

Properties:

• Because
$$U(\pm \infty) = u^{\pm}$$
,

$$Y(h+1) - Y(h) = u^{+} - u^{-}.$$

• Because of the profile equation (+ Rankine–Hugoniot and $\sigma s = \eta$):

$$Y(h + \eta) - Y(h) = \eta(u^+ - u^-).$$

$Y(h) = h(u^+ - u^-), \qquad \forall h \in \mathbb{Z} + \eta \mathbb{Z}.$ (8)

Application:

 \Longrightarrow

The scalar case with a monotone scheme. The monotonicity of U together with (8) imply

$$|U(y+h) - U(y)| \le |h(u^+ - u^-)|$$

(see above).

Irrational case. By continuity and density of $\mathbb{Z} + \eta \mathbb{Z}$, (8) yields

$$Y(h) = h(u^+ - u^-), \quad \forall h \in \mathbb{R}.$$
 (9)

But $\mathbb{R} \setminus \mathbb{Q}$ is dense …

Thus (9) is expected to hold even when $\eta \in \mathbb{Q}$.

In particular for

$$h \not\in \frac{1}{q}\mathbb{Z},$$

... well, if the life is smooth.

Something must go wrong !

In the rational case, the shift function compares two profiles

$$\mathbf{u} = (u_y)_{y \in \frac{1}{q}\mathbb{Z}}$$
 and $\mathbf{v} = (v_y)_{y \in \frac{1}{q}\mathbb{Z}}$,
 $U(j) = u_j, \qquad U(j+h) = v_j.$

- If $h \in \frac{1}{q}\mathbb{Z}$, u and v are identical, up to a shift ; (9) is OK because it is (8).
- But if $h \notin \frac{1}{q}\mathbb{Z}$, u and v are distinct.

If $N \ge 2$, there is no reason why Y(h) should be parallel to $u^+ - u^-$.

Counter-example

Here is a construction with

$$Y(h) \not\parallel u^+ - u^-.$$

- $\eta = 0$: the shock (u^-, u^+) is stationnary,
- The scheme is Godunov's (Lax–Wendroff scheme works too).
- The "integrated" profile equation for steady shocks:

$$f(R(u_j, u_{j+1}; 0)) = f(u^-) = f(u^+).$$

• \longrightarrow Typically:

$$R(u_j, u_{j+1}; 0) \in \{u^-, u^+\}, \quad \forall j \in \mathbb{Z}.$$
Lemma. If $(u^-, u^+; 0)$ is an admissible shock, it is not possible that

$$R(u_{j-1}, u_j; 0) = u^+$$
 and $R(u_j, u_{j+1}; 0) = u^-$

Proof: 1- Since $R(u_j, u_{j+1}; 0) = u^-$, the Riemann problem from u_j to u^- consists only in backward waves.

2- One passes from u^- to u^+ by a steady admissible shock.

3- Since $R(u_{j-1}, u_j; 0) = u^+$, the Riemann problem from u^+ to u_j consists only in forward waves.

Gluing these pieces, the Riemann problem from u_j to u_j admits a non-constant solution. This contradicts the Lax entropy inequality.

Consequence: up to a shift,

$$R(u_j, u_{j+1}; 0) = \begin{cases} u^-, & j < 0, \\ u^+, & j \ge 0. \end{cases}$$

Same idea as in the proof above: if j < 0, the solution of the Riemann problem from u^- to itself passes through u_j . Likewise, if j > 0, ... Whence

$$u_j = \begin{cases} u^-, & j < 0, \\ u^+, & j > 0. \end{cases}$$

There remains

$$R(u^-, u_0; 0) = u^-, \qquad R(u_0, u^+; 0) = u^+.$$

These conditions define an arc $\gamma \subset \mathcal{U}$ with ends u^- and u^+ .

[For specialists only: if $(u^-, u^+; 0)$ is an *N*-shock, then γ is the portion of the shock curve $S_N(u^-)$ between u^- and u^+ .]

The continuous DSP:

Arbitrary parametrization of γ

 $y \in [0,1] \mapsto U(y), \quad U(0) = u^{-}, \quad U(1) = u^{+}.$

Extend it by

$$U(y) \equiv \left\{ egin{array}{cc} u^-, & y < 0, \\ u^+, & y > 1. \end{array}
ight.$$

To every point $a = U(h) \in \gamma$, there corresponds a DSP

$$u_j = U(h+j) = \begin{cases} u^-, & j < 0, \\ a, & j = 0, \\ u^+, & j > 0. \end{cases}$$

The shift function Y measures the difference between two DSPs. If a is as above, then

$$Y(h) = \sum_{j \in \mathbb{Z}} (u_j - v_j) = a - u^-.$$

Not parallel to $u^+ - u^-$, unless $\gamma = [u^-, u^+]$.

QED

Thus (9) does not pass to the limit from irrationals to rationals.

The alternative

- 1. Either DSPs do not exist for irrationals too close to rationals (non-Diophantine numbers),
- 2. or their have an infinite total variation,
- 3. or they do not depend smoothly on the data $(u^-, u^+; s, \sigma)$.

Causes:

- Small divisors problem,
- Resonnance between the shock front and the grid.

Why the scalar case is not that bad

For a monotone scheme:

- DSPs do exist,
- they have a finite total variation $|u^+ u^-|$,
- they depend smoothly on the data.

So what ?

Two vectors in \mathbb{R} are always parallel ! $\longrightarrow Y(h) \parallel u^+ - u^-.$

Monotonicity forbids infinite total variation.

(back to systems) The Diophantine case

Definition. A real number η is *Diophantine* if there exists $C = C(\eta) < \infty$ and $\nu = \nu(\eta) > 0$ such that

$$\left|\eta - \frac{r}{\ell}\right| \ge \frac{C}{\ell^{\nu}}, \quad \forall \frac{r}{\ell} \in \mathbb{Q}, \quad r \land \ell = 1.$$

- Lebesgue-almost every number is Diophantine of degree $\nu = 2$.
- $\pi = 3.14159...$ is Diophantine of degree $\nu \leq 8.0161...$
- $\zeta(3)$ is Diophantine of degree $\nu \leq 5.513891...$
- But

$$\sum_{m=1}^{\infty} 10^{-m!}$$
 is not (Liouville).

The small divisor problem

• Look at the integrated profile equation

$$\int_{x-\eta}^{x} U(y) \, dy - \sigma \int_{x}^{x+1} F(U(y-1), U(y)) \, dy = \eta u^{-} - \sigma f(u^{-}).$$

• Linearize the r.-h.-s.:

$$Lv(x) = \int_{x-\eta}^{x} v(y) \, dy - \sigma \left(A \int_{x-1}^{x} v(y) \, dy + B \int_{x}^{x+1} v(y) \, dy \right).$$

• The operator *L* diagonalizes *via* Fourier transform:

$$e^{-i\xi x}L\left[e^{i\xi x}X\right] = M(\xi)X,$$

with

$$M(\xi) := \frac{1}{i\xi} \left((1 - e^{-i\xi\eta})I_N - \sigma((1 - e^{-i\xi})A - \sigma(e^{i\xi} - 1)B) \right).$$

• The operator *L* is not Fredholm:

$$M(2\pi\ell) = \frac{1}{2i\pi\ell} \left(1 - e^{-2i\pi\ell\eta} \right) I_N.$$

The right-hand side is

$$O\left(\frac{1}{\ell^2}\right)$$
 for infinity many ℓ 's.

• If η is not Diophantine: $\forall \nu > 2, \exists \frac{r}{\ell} \in \mathbb{Q}$ with

$$\left|\eta - \frac{r}{\ell}\right| \le \frac{1}{\ell^{\nu}}.$$

Then

$$\|M(2\pi\ell)\|\leq rac{1}{\ell^{
u}}.$$

• Very fast decay !!

Even Nash–Moser technique does not apply in this case.

• Diophantine case:

 $\exists \nu \geq 2$ such that

$$\|M(2\pi\ell)\| = \mathcal{O}\left(\frac{1}{\ell^{\nu}}\right).$$

 \longrightarrow Tame estimates for the Green function of the linearized scheme.

Theorem (T.-P. Liu & S.-H. Yu).

Assume that the scheme is dissipative and non-resonant.

Assume that η is Diophantine and that $(u^-, u^+; s)$ is a small enough $(|u^+ - u^-| \ll 1)$ admissible shock.

Then there exists a continuous DSP.

Smallness is measured in terms of $C(\eta)$ and $\nu(\eta)$.

These DSPs are orbitally stable for the numerical scheme.

Large total variation problem

(Baiti, Bressan & Jenssen) consider semi-decoupled systems

$$\partial_t v + \partial_x f(v) = 0, \qquad (10)$$

$$\partial_t w + \partial_x (\lambda w + g(v)) = 0. \qquad (11)$$

- Either apply Jennings Theorem to (10), a scalar equation.
 Or compute explicit DSPs (Lax) for certain fluxes *f*.
- Evaluate Green function for the linear part (11)

$$(\partial_t + \lambda \partial_x)w = r.h.s.$$

Resonance may occur, depending on $\lambda\sigma$.

Lax–Friedrichs scheme. Here $\sigma_m \rightarrow \sigma \in \mathbb{Q}$.

The DSP U_m converges uniformly but its total variation increases unboundedly.

The variations concentrate on an interval

$$\left[-a(\sigma_m-\sigma)^{-2},-b(\sigma_m-\sigma)^{-2}\right],$$

far away the shock front.

Godunov scheme. More or less the same result.

By-products

- The schemes (L.-F. or G.) produce sequences (a_{ν}, u_{ν}^{app}) with
 - initial data a_{ν} whose total variation remains bounded as $\nu \to \infty$.
 - approximate solution u_{ν}^{app} whose total variation over $\mathbb{R} \times \{T\}$ does not remain bounded as $\nu \to \infty$.
- Considering a_{ν} and $a_{\nu}(\cdot h)$, the approximations are unstable in the L^1 norm, with respect to the initial data:

$$\sup_{\nu,h} \frac{1}{h} \|a_{\nu}(\cdot - h) - a_{\nu}\|_{L^{1}(\mathbb{R})} < \infty,$$
$$\lim_{\nu \to \infty} \left(\sup_{0 < h < 1} \frac{1}{h} \|u_{\nu}^{\mathsf{app}}(\cdot - h, T) - u_{\nu}^{\mathsf{app}}(\cdot, T)\|_{L^{1}(\mathbb{R})} \right) = \infty.$$

• However, compensated-compactness method yields convergence $u^{app} \rightarrow u$ towards an admissible solution of the Cauchy problem.

This convergence cannot be very strong; at least, it is not uniform.

- The convergence of finite difference schemes cannot be proven by *a priori* BV bounds.
- For small initial data, *BV*-bounds do hold (Glimm, Bressan & coll.). Thus the counter-example build by Baiti & coll. are not that small.

The mathematics of the stability / convergence of conservative difference schemes must be very hard !

Comparison with Viscous Shock Profiles

Shortcoming: VSP

Approximate (1) by some amount of viscosity:

$$\partial_t u + \partial_x f(u) = \epsilon \partial_x (B(u) \partial_x u).$$

Examples:

- Euler vs Navier-Stokes in gas dynamics,
- Viscoelasticity,
- second-order model of traffic flow,

Normalized travelling wave

$$u^{\epsilon}(x,t) = U\left(\frac{x-st}{\epsilon}\right).$$

with

$$(B(U)U')' = f(U)' - sU', \qquad U(\pm \infty) = u^{\pm}.$$
 (12)

Integrate once:

$$B(U)' = f(U) - sU - f(u^{-}) + su^{-}.$$
 (13)

(13) includes:

- Conditions at infinity,
- Rankine–Hugoniot.

Existence theory for VSPs

- A VSP is a heteroclinic orbit of a continuous dynamical system.
- VSPs form the intersection of W^u(u⁻) and W^s(u⁺), unstable / stable invariant manifolds of u[±] for (13).

• If

$$\dim \mathcal{W}^u(u^-) + \dim \mathcal{W}^s(u^+) \ge N+1,$$

then generically,

$$\dim \left(\mathcal{W}^u(u^-) \cap \mathcal{W}^s(u^+) \right) = \dim \mathcal{W}^u(u^-) + \dim \mathcal{W}^s(u^+) - N.$$

Tools: again, bifurcation analysis, Center Manifold Theorem.

The case of a Lax shock

Notation: The k-th characteristic field

$$df(u)r_k(u) = \lambda_k(u)r_k(u).$$

Definition: A discontinuity $(u^-, u^+; s)$ is a Lax shock if $\exists k$ such that

$$\lambda_{k-1}(u^-) < s < \lambda_k(u^-), \qquad \lambda_k(u^+) < s < \lambda_{k+1}(u^+).$$

Interpretation: Among the 2N characteristic curves

$$\dot{x} = \lambda_j(u(x,t))$$

(N curves at right of the shock and N at left), N + 1 enter the shock.

Lemma (Lax).

1. Small discontinuities are approximately parallel to one of the eigenvectors r_k :

$$u^+ - u^- \sim \rho r_k(u^-)$$

for some $1 \leq k \leq N$.

2. Assume that the *k*-th characteristic field is *genuinely nonlinear*.

$$\mathrm{d}\lambda_k(u)\cdot r_k(u)\neq 0.$$

Then small k-discontinuities are Lax shocks, up to a switch $u^- \leftrightarrow u^+$.

 \bigcirc

For a Lax shock,

 $\dim \mathcal{W}^u(u^-) = N - k + 1, \qquad \dim \mathcal{W}^s(u^+) = k.$

 \rightarrow Generically (always true for small shocks)

$$\dim \left(\mathcal{W}^u(u^-) \cap \mathcal{W}^s(u^+) \right) = 1.$$

Whence the existence and uniqueness of a VSP, up to a shift.

This is a one-parameter family of VSPs.

Parameter = shift.

Qualitatively similar to DSPs.

Question. Does this similarity occur for non-Lax shocks ?

Non-Lax shocks: VSPs

• Undercompressive shocks

$$\lambda_k(u^-) < s < \lambda_{k+1}(u^-), \qquad \lambda_k(u^+) < s < \lambda_{k+1}(u^+).$$

Only N characteristics enter the shock:

$$\dim \mathcal{W}^u(u^-) + \dim \mathcal{W}^s(u^+) = N.$$

• Overcompressive shocks

$$\lambda_{k-2}(u^-) < s < \lambda_{k-1}(u^-), \qquad \lambda_k(u^+) < s < \lambda_{k+1}(u^+).$$

N + 2 characteristics enter the shock.

$$\dim \mathcal{W}^u(u^-) + \dim \mathcal{W}^s(u^+) = N + 2.$$

Undercompressive shocks: VSPs

Generically,

$$\dim \left(\mathcal{W}^u(u^-) \cap \mathcal{W}^s(u^+) \right) \le N - N = 0$$

But $\mathcal{W}^{u}(u^{-}) \cap \mathcal{W}^{s}(u^{+})$ is made of integral curves of the field $u \mapsto B(u)^{-1} \left(f(u) - su - f(u^{-}) + su^{-} \right).$

Therefore

$$\mathcal{W}^u(u^-) \cap \mathcal{W}^s(u^+) = \emptyset$$

Principle. Most undercompressive shocks do not admit a VSP. The existence of a shock profile is a codimension-1 property.

Undercompressive shocks: DSPs

Assume $\eta \in \mathbb{Q}$. Example: $\eta = 0$.

Recall:

Integrated profile equation:

$$F(u_j, u_{j+1}) = f(u^-) \stackrel{(\mathsf{R}.-\mathsf{H}.)}{=} f(u^+).$$

When IFT applies, rewrite

$$u_{j+1} = H(u_j).$$
 (14)

Then

DSP
$$\longleftrightarrow$$
 heteroclinic orbit from u^- to u^+

Again, DSPs correspond to an intersection

 $\mathcal{W}^u(u^-) \cap \mathcal{W}^s(u^+),$

unstable / stable manifolds for H, a *diffeormorphism*.

Undercompressive shock:

$$\dim \mathcal{W}^u(u^-) + \dim \mathcal{W}^s(u^+) = N,$$

whence (generically)

$$\dim\left(\mathcal{W}^{u}(u^{-})\cap\mathcal{W}^{s}(u^{+})\right)\leq N+N-2N=0$$

Special: in discrete dynamics, an invariant subset under *H* may be discrete !

Thus the intersection may have dim = N - N = 0.

Principle. Undercompressive shocks may admit a DSP.

The existence of a shock profile is a generic property (stable under small disturbances of the data).

A DSP is now isolated, instead of a one-parameter family.

Undercompressive shocks: DSPs vs VSPs

Discrete SP. Generic property.

Discrete set, with a \mathbb{Z} -action.

An even number of orbits. Often 2 orbits.

Viscous SP. Codimension-one property.

One-parameter set if any, with an \mathbb{R} -action.

Moral: in the theory of profiles for undercompressive shocks

$$0\cdot\infty=2$$
 or $\mathbb{R}^{-1} imes\mathbb{R}=\mathbb{Z}/2\mathbb{Z}.$

Why two DSPs ?

Say $N = 2, \eta = 0$. Then

$$\dim \mathcal{W}^s(u^+) = \dim \mathcal{W}^u(u^-) = 1.$$

 u^{\pm} are saddle points of (14)





Principle.

- *H* is orientation preserving.
- Let *τ^s(u)* be the tangent to *W^s(u⁺)* at *u*, oriented towards *u⁺*.
 Likewise, let *τ^u(u)* ...

• (Generic) At an intersection point,

$$\mathcal{B}(u) = \{\tau^s(u), \tau^u(u)\}$$

is a basis.

• Define the "sign" of the intersection:

$$\sigma(u) := \begin{cases} +1, & \text{direct basis,} \\ -1, & \text{reverse basis.} \end{cases}$$

- The sign of the intersection is constant along an orbit.
- Two consecutive intersection points u and \bar{u} have opposite intersection signs

Thus u and \bar{u} correspond to distinct orbits,

 \longrightarrow distinct DSPs.

An example taken from reaction-diffusion

Consider the KPP equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \phi'(u), \qquad \phi(u) := \frac{1}{4} \left(u^2 - 1 \right)^2.$$

Steady states are

Constants:

$$u \equiv \pm 1.$$

Fronts:

$$\frac{d^2u}{dx^2} = \phi'(u),$$

whence

$$\frac{1}{2}\left(\frac{du}{dx}\right)^2 = \phi(u), \qquad u(\pm\infty) = \pm 1.$$

Lemma. Fronts minimize the functional

$$J[v] := \int_{\mathbb{R}} \left(\frac{1}{2} \left(\frac{du}{dx} \right)^2 + \phi(u) \right) \, dx,$$

under the constraint

$$u(\pm\infty)=\pm 1.$$

The front is unique up to a shift.

It is odd:

$$u(-x) = -u(x).$$

Actually, -u is another front, from +1 to -1.

Discretization of KPP

$$\frac{u_j^{m+1} - u_j^m}{\Delta t} = \frac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{(\Delta x)^2} - \phi'(u_j^m).$$

Standing discrete waves:

$$\frac{u_{j+1}^m - 2u_j^m + u_{j-1}^m}{(\Delta x)^2} = \phi'(u_j^m).$$
(15)

Interpretation in the phase space

Define

$$v_j := \frac{u_{j+1} - u_j}{\Delta x}.$$

Then

$$\begin{pmatrix} u_j \\ v_j \end{pmatrix} = \begin{pmatrix} u_{j-1} + \Delta x \, v_{j-1} \\ v_{j-1} + \Delta x \, \phi' \left(u_{j-1} + \Delta x \, v_{j-1} \right) \end{pmatrix} =: H \begin{pmatrix} u_{j-1} \\ v_{j-1} \end{pmatrix}.$$

Two fixed points:

$$H\begin{pmatrix}\pm 1\\0\end{pmatrix} = \begin{pmatrix}\pm 1\\0\end{pmatrix}$$

•

These are saddle points.

Discrete fronts from -1 to +1 correspond to heteroclinic orbits of *H*. They are parametrized by

$$\mathcal{W}^u\begin{pmatrix}-1\\0\end{pmatrix}\cap\mathcal{W}^s\begin{pmatrix}+1\\0\end{pmatrix}.$$

Existence of discrete fronts

Lemma. Discrete fronts minimize the functional

$$J_{\Delta}[v] := \frac{1}{2\Delta x} \sum_{j \in \mathbb{Z}} (u_j - u_{j-1})^2 + \Delta x \sum_{j \in \mathbb{Z}} \phi(u_j),$$

under the constraint

$$u_{\pm\infty} = \pm 1.$$

Whence the *idea*:

Minimize J_{Δ} over the set of odd sequences.

Still, minimizers are fronts.

There are two fronts

Two ways to express the oddness:

• Either u is odd with respect to 0,

$$u_{-j} = -u_j.$$

• Or u is odd with respect to $\frac{1}{2}$,

$$u_{1-j} = -u_j.$$

This yields two disjoint sets of odd sequences, whence two distinct minimizers.

Theorem. The KPP equation admits at least two distinct discrete fronts from -1 to +1.

They are monotonous.
There are many fronts !

• We proved that
$$\mathcal{W}^u \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$
 intersect transversally $\mathcal{W}^s \begin{pmatrix} +1 \\ 0 \end{pmatrix}$.

• By symmetry,
$$\mathcal{W}^u \begin{pmatrix} +1 \\ 0 \end{pmatrix}$$
 intersect transversally $\mathcal{W}^s \begin{pmatrix} -1 \\ 0 \end{pmatrix}$.

• $\mathcal{W}^u \begin{pmatrix} -1 \\ 0 \end{pmatrix}$ folds infinitely many times and approaches $\mathcal{W}^u \begin{pmatrix} +1 \\ 0 \end{pmatrix}$, being squeezed.

• Ultimately,
$$\mathcal{W}^u \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$
 intersect transversally $\mathcal{W}^s \begin{pmatrix} -1 \\ 0 \end{pmatrix}$.



• Whence a *Smale horse-shoe* configuration.

Theorem. There are countably many discrete fronts from -1 to +1. Most of them are non-monotone.

 \diamond

Theorem. There are as well countably many discrete fronts homoclinic to -1 (or to +1).

There are also chaotic trajectories, approaching ± 1 infinitely many times on intervals of arbitrary lengths.

The case of a non-even potential ϕ

On the one hand, the Smale horse-shoe configuration is *structurally stable*: it persists under small disturbance of the dynamical systems.

On the other hand, the saddle-saddle connection of

$$\frac{d^2u}{dx^2} = \phi'(u)$$

does not persist, if the wells of ϕ are not equal.

Application: choose ϕ , close enough to an even, double-well potential ϕ_0 .

- Then countably many heteroclinic discrete fronts.
- However, there is no viscous front, when unequal wells.