Today:
  • Entropy conditions and functions
  • Lax-Wendroff theorem

Wednesday  February 23:
  • Nonlinear systems

Reading: Chapter 13
Entropy-violating numerical solutions

Riemann problem for Burgers’ equation at \( t = 1 \)

with \( u_\ell = -1 \) and \( u_r = 2 \):
Vanishing viscosity solution

We want $q(x, t)$ to be the limit as $\epsilon \to 0$ of solution to

$$qt + f(q)x = \epsilon q_{xx}.$$ 

This selects a unique weak solution:

- Shock if $f'(q_l) > f'(q_r)$,
- Rarefaction if $f'(q_l) < f'(q_r)$.

Lax Entropy Condition:

A discontinuity propagating with speed $s$ in the solution of a convex scalar conservation law is admissible only if $f'(q_{\ell}) > s > f'(q_r)$, where $s = \frac{f(q_r) - f(q_{\ell})}{q_r - q_{\ell}}$. 

Note: This means characteristics must approach shock from both sides as $t$ advances, not move away from shock!
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A discontinuity propagating with speed \( s \) in the solution of a convex scalar conservation law is admissible only if

\[
f'(q_l) > s > f'(q_r), \text{ where } s = (f(q_r) - f(q_l))/(q_r - q_l).
\]

Note: This means characteristics must approach shock from both sides as \( t \) advances, not move away from shock!
Approximate Riemann solvers

For nonlinear problems, computing the exact solution to each Riemann problem may not be possible, or too expensive.

Often the nonlinear problem \( q_t + f(q)_x = 0 \) is approximated by

\[
q_t + A_{i-1/2}q_x = 0, \quad q_\ell = Q_{i-1}, \quad q_r = Q_i
\]

for some choice of \( A_{i-1/2} \approx f'(q) \) based on data \( Q_{i-1}, Q_i \).
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Solve linear system for \( \alpha_{i-1/2} \):

\[
Q_i - Q_{i-1} = \sum_p \alpha_{i-1/2}^p r_{i-1/2}^p.
\]

Waves \( \mathcal{W}_{i-1/2}^p = \alpha_{i-1/2}^p r_{i-1/2}^p \) propagate with speeds \( s_{i-1/2}^p \),

\( r_{i-1/2}^p \) are eigenvectors of \( A_{i-1/2} \),

\( s_{i-1/2}^p \) are eigenvalues of \( A_{i-1/2} \).
Approximate Riemann solvers

\[ q_t + \hat{A}_{i-1/2}q_x = 0, \quad q_\ell = Q_{i-1}, \quad q_r = Q_i \]

Often \( \hat{A}_{i-1/2} = f'(Q_{i-1/2}) \) for some choice of \( Q_{i-1/2} \).

In general \( \hat{A}_{i-1/2} = \hat{A}(q_\ell, q_r) \).
Approximate Riemann solvers

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In general \( \hat{A}_{i-1/2} = \hat{A}(q_\ell, q_r) \).

**Roe conditions** for consistency and conservation:

- \( \hat{A}(q_\ell, q_r) \to f'(q^*) \) as \( q_\ell, q_r \to q^* \),
- \( \hat{A} \) diagonalizable with real eigenvalues,
- For conservation in wave-propagation form,

\[ \hat{A}_{i-1/2}(Q_i - Q_{i-1}) = f(Q_i) - f(Q_{i-1}). \]
Approximate Riemann solvers

For a scalar problem, we can easily satisfy the Roe condition

\[ \hat{A}_{i-1/2}(Q_i - Q_{i-1}) = f(Q_i) - f(Q_{i-1}). \]

by choosing

\[ \hat{A}_{i-1/2} = \frac{f(Q_i) - f(Q_{i-1})}{Q_i - Q_{i-1}}. \]
Approximate Riemann solvers

For a scalar problem, we can easily satisfy the Roe condition

\[ \hat{A}_{i-1/2}(Q_i - Q_{i-1}) = f(Q_i) - f(Q_{i-1}). \]

by choosing

\[ \hat{A}_{i-1/2} = \frac{f(Q_i) - f(Q_{i-1})}{Q_i - Q_{i-1}}. \]

Then \( r_{i-1/2}^1 = 1 \) and \( s_{i-1/2}^1 = \hat{A}_{i-1/2} \) (scalar!).

Note: This is the Rankine-Hugoniot shock speed.

\[ \Rightarrow \] shock waves are correct,

rarefactions replaced by entropy-violating shocks.
Weak solutions to Burgers’ equation

$$u_t + \left( \frac{1}{2} u^2 \right)_x = 0, \quad u_\ell = 1, \quad u_r = 2$$

Characteristic speed: $u$  
Rankine-Hugoniot speed: $\frac{1}{2}(u_\ell + u_r)$.

“Physically correct” rarefaction wave solution:
Weak solutions to Burgers’ equation

\[ u_t + \left( \frac{1}{2} u^2 \right)_x = 0, \quad u_\ell = 1, \quad u_r = 2 \]

Characteristic speed: \( u \)    Rankine-Hugoniot speed: \( \frac{1}{2} (u_\ell + u_r) \).

Entropy violating weak solution:
Weak solutions to Burgers’ equation

\[ u_t + \left( \frac{1}{2} u^2 \right)_x = 0, \quad u_\ell = 1, \quad u_r = 2 \]

Characteristic speed: \( u \)  
Rankine-Hugoniot speed: \( \frac{1}{2} (u_\ell + u_r) \).

Another Entropy violating weak solution:
Transonic rarefactions

**Sonic point:** $u_s = 0$ for Burgers’ since $f'(0) = 0$.

Consider Riemann problem data $u_\ell = -0.5 < 0 < u_r = 1.5$.

In this case wave should spread in both directions:
Transonic rarefactions

Entropy-violating approximate Riemann solution:

\[ s = \frac{1}{2}(u_\ell + u_r) = 0.5. \]

Wave goes **only to right**, no update to cell average on left.
If $u_\ell = -u_r$ then Rankine-Hugoniot speed is 0:

Similar solution will be observed with Godunov’s method if entropy-violating approximate Riemann solver used.
Entropy-violating numerical solutions

Riemann problem for Burgers’ equation at $t = 1$

with $u_\ell = -1$ and $u_r = 2$:
Approximate Riemann solver

\[ Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} \left[ A^{+} \Delta Q_{i-1/2} + A^{-} \Delta Q_{i+1/2} \right] . \]

For scalar advection \( m = 1 \), only one wave.
\[ W_{i-1/2} = \Delta Q_{i-1/2} = Q_{i} - Q_{i-1} \quad \text{and} \quad s_{i-1/2} = u, \]

\[ A^{-} \Delta Q_{i-1/2} = s_{i-1/2}^{-} W_{i-1/2}, \]
\[ A^{+} \Delta Q_{i-1/2} = s_{i-1/2}^{+} W_{i-1/2}. \]

For scalar nonlinear: Use same formulas with
\[ W_{i-1/2} = \Delta Q_{i-1/2} \quad \text{and} \quad s_{i-1/2} = \Delta F_{i-1/2} / \Delta Q_{i-1/2}. \]

Need to modify these by an entropy fix in the trans-sonic rarefaction case.
Entropy fix

\[ Q_{i+1}^n = Q_i^n - \frac{\Delta t}{\Delta x} \left[ A^+ \Delta Q_{i-1/2} + A^- \Delta Q_{i+1/2} \right]. \]

Revert to the formulas

\[ A^- \Delta Q_{i-1/2} = f(q_s) - f(Q_{i-1}) \quad \text{left-going fluctuation} \]
\[ A^+ \Delta Q_{i-1/2} = f(Q_i) - f(q_s) \quad \text{right-going fluctuation} \]

if \( f'(Q_{i-1}) < 0 < f'(Q_i) \).

**High-resolution method:** still define wave \( \mathcal{W} \) and speed \( s \) by

\[ \mathcal{W}_{i-1/2} = Q_i - Q_{i-1}, \]
\[ s_{i-1/2} = \begin{cases} 
\frac{(f(Q_i) - f(Q_{i-1}))(Q_i - Q_{i-1})}{f'(Q_i)} & \text{if } Q_{i-1} \neq Q_i \\
\frac{f'(Q_i)}{f'(Q_i)} & \text{if } Q_{i-1} = Q_i.
\end{cases} \]
The Godunov flux function for the case \( f''(q) > 0 \) is

\[
F^n_{i-1/2} = \begin{cases} 
  f(Q_{i-1}) & \text{if } Q_{i-1} > q_s \text{ and } s > 0 \\
  f(Q_i) & \text{if } Q_i < q_s \text{ and } s < 0 \\
  f(q_s) & \text{if } Q_{i-1} < q_s < Q_i.
\end{cases}
\]

\[
= \begin{cases} 
  \min_{Q_{i-1} \leq q \leq Q_i} f(q) & \text{if } Q_{i-1} \leq Q_i \\
  \max_{Q_i \leq q \leq Q_{i-1}} f(q) & \text{if } Q_i \leq Q_{i-1},
\end{cases}
\]

Here \( s = \frac{f(Q_i) - f(Q_{i-1})}{Q_i - Q_{i-1}} \) is the Rankine-Hugoniot shock speed.
Entropy-violating numerical solutions

Riemann problem for Burgers’ equation with \( q_l = -1 \) and \( q_r = 2 \):
We generally require additional conditions on a weak solution to a conservation law, to pick out the unique solution that is physically relevant.

**In gas dynamics:** entropy is constant along particle paths for smooth solutions, entropy can only increase as a particle goes through a shock.
We generally require additional conditions on a weak solution to a conservation law, to pick out the unique solution that is physically relevant.

In gas dynamics: entropy is constant along particle paths for smooth solutions, entropy can only increase as a particle goes through a shock.

Entropy functions: Function of $q$ that “behaves like” physical entropy for the conservation law being studied.
We generally require **additional conditions** on a weak solution to a conservation law, to pick out the unique solution that is physically relevant.

**In gas dynamics:** entropy is constant along particle paths for smooth solutions, **entropy can only increase** as a particle goes through a shock.

**Entropy functions:** Function of $q$ that “behaves like” physical entropy for the conservation law being studied.

**NOTE:** Mathematical entropy functions generally chosen to **decrease** for admissible solutions, **increase** for entropy-violating solutions.
A scalar-valued function $\eta : \mathbb{IR}^m \rightarrow \mathbb{IR}$ is a convex function of $q$ if the Hessian matrix $\eta''(q)$ with $(i, j)$ element

$$\eta_{ij}''(q) = \frac{\partial^2 \eta}{\partial q^i \partial q^j}$$

is positive definite for all $q$, i.e., satisfies

$$v^T \eta''(q)v > 0 \quad \text{for all } q, v \in \mathbb{IR}^m.$$

Scalar case: reduces to $\eta''(q) > 0$. 

R.J. LeVeque, University of Washington
AMath 574, February 14, 2011 [FVMHP Sec. 11.4]
Entropy functions

Entropy function: \( \eta : \mathbb{R}^m \rightarrow \mathbb{R} \)  
Entropy flux: \( \psi : \mathbb{R}^m \rightarrow \mathbb{R} \)

chosen so that \( \eta(q) \) is convex and:

- \( \eta(q) \) is conserved wherever the solution is smooth,
  \[ \eta(q)_t + \psi(q)_x = 0. \]

- Entropy decreases across an admissible shock wave.
Entropy functions

Entropy function: $\eta: \mathbb{R}^m \to \mathbb{R}$  
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• $\eta(q)$ is conserved wherever the solution is smooth,

$$\eta(q)_t + \psi(q)_x = 0.$$ 

• Entropy decreases across an admissible shock wave.

Weak form:

$$\int_{x_1}^{x_2} \eta(q(x, t_2)) \, dx \leq \int_{x_1}^{x_2} \eta(q(x, t_1)) \, dx$$

$$+ \int_{t_1}^{t_2} \psi(q(x_1, t)) \, dt - \int_{t_1}^{t_2} \psi(q(x_2, t)) \, dt$$

with equality where solution is smooth.
Entropy functions

How to find $\eta$ and $\psi$ satisfying this?

$$\eta(q)_t + \psi(q)_x = 0$$

For smooth solutions gives

$$\eta'(q)q_t + \psi'(q)q_x = 0.$$
Entropy functions

How to find $\eta$ and $\psi$ satisfying this?

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For smooth solutions gives

$$\eta'(q)q_t + \psi'(q)q_x = 0.$$ 

Since $q_t = -f'(q)q_x$ this is satisfied provided

$$\psi'(q) = \eta'(q)f'(q)$$
Entropy functions

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For smooth solutions gives

$$\eta'(q)q_t + \psi'(q)q_x = 0.$$  

Since $q_t = -f'(q)q_x$ this is satisfied provided

$$\psi'(q) = \eta'(q)f'(q).$$

Scalar: Can choose any convex $\eta(q)$ and integrate.

Example: Burgers’ equation, $f'(u) = u$ and take $\eta(u) = u^2$.

Then $\psi'(u) = 2u^2 \implies$ Entropy function: $\psi(u) = \frac{2}{3}u^3$. 
The conservation laws

\[ u_t + \left( \frac{1}{2} u^2 \right)_x = 0 \quad \text{and} \quad (u^2)_t + \left( \frac{2}{3} u^3 \right)_x = 0 \]

both have the same quasilinear form

\[ u_t + u u_x = 0 \]

but have different weak solutions, different shock speeds!
Weak solutions and entropy functions

The conservation laws

\[ u_t + \left( \frac{1}{2} u^2 \right)_x = 0 \quad \text{and} \quad (u^2)_t + \left( \frac{2}{3} u^3 \right)_x = 0 \]

both have the same quasilinear form

\[ u_t + uu_x = 0 \]

but have different weak solutions, different shock speeds!

Entropy function: \( \eta(u) = u^2 \).

A correct Burgers’ shock at speed \( s = \frac{1}{2} (u_\ell + u_r) \) will have total mass of \( \eta(u) \) decreasing.
Entropy functions

\[
\int_{x_1}^{x_2} \eta(q(x, t_2)) \, dx \leq \int_{x_1}^{x_2} \eta(q(x, t_1)) \, dx \\
+ \int_{t_1}^{t_2} \psi(q(x_1, t)) \, dt - \int_{t_1}^{t_2} \psi(q(x_2, t)) \, dt
\]

comes from considering the vanishing viscosity solution:

\[
q_t^\epsilon + f(q^\epsilon) x = \epsilon q_{xx}^\epsilon
\]
Entropy functions

\[ \int_{x_1}^{x_2} \eta(q(x, t_2)) \, dx \leq \int_{x_1}^{x_2} \eta(q(x, t_1)) \, dx \]

\[ + \int_{t_1}^{t_2} \psi(q(x_1, t)) \, dt - \int_{t_1}^{t_2} \psi(q(x_2, t)) \, dt \]

comes from considering the vanishing viscosity solution:

\[ q^\varepsilon_t + f(q^\varepsilon)_x = \varepsilon q^\varepsilon_{xx} \]

Multiply by \( \eta'(q^\varepsilon) \) to obtain:

\[ \eta(q^\varepsilon)_t + \psi(q^\varepsilon)_x = \varepsilon \eta'(q^\varepsilon) q^\varepsilon_{xx} \]
Entropy functions

\[\int_{x_1}^{x_2} \eta(q(x,t_2)) \, dx \leq \int_{x_1}^{x_2} \eta(q(x,t_1)) \, dx \]

\[+ \int_{t_1}^{t_2} \psi(q(x_1,t)) \, dt - \int_{t_1}^{t_2} \psi(q(x_2,t)) \, dt\]

comes from considering the vanishing viscosity solution:

\[q_t^\varepsilon + f(q^\varepsilon)_x = \varepsilon q_{xx}^\varepsilon\]

Multiply by \(\eta'(q^\varepsilon)\) to obtain:

\[\eta(q^\varepsilon)_t + \psi(q^\varepsilon)_x = \varepsilon \eta'(q^\varepsilon)q_{xx}^\varepsilon.\]

Manipulate further to get

\[\eta(q^\varepsilon)_t + \psi(q^\varepsilon)_x = \varepsilon \left(\eta'(q^\varepsilon)q_{xx}^\varepsilon\right)_x - \varepsilon \eta''(q^\varepsilon) (q_x^\varepsilon)^2.\]
Entropy functions

Smooth solution to viscous equation satisfies

\[ \eta(q^\epsilon)_t + \psi(q^\epsilon)_x = \epsilon(\eta'(q^\epsilon)q^\epsilon_x)_x - \epsilon\eta''(q^\epsilon)(q^\epsilon_x)^2. \]

Integrating over rectangle \([x_1, x_2] \times [t_1, t_2]\) gives

\[
\int_{x_1}^{x_2} \eta(q^\epsilon(x, t_2)) \, dx = \int_{x_1}^{x_2} \eta(q^\epsilon(x, t_1)) \, dx
\]

\[
- \left( \int_{t_1}^{t_2} \psi(q^\epsilon(x_2, t)) \, dt - \int_{t_1}^{t_2} \psi(q^\epsilon(x_1, t)) \, dt \right)
\]

\[
+ \epsilon \int_{t_1}^{t_2} \left[ \eta'(q^\epsilon(x_2, t)) q^\epsilon_x(x_2, t) - \eta'(q^\epsilon(x_1, t)) q^\epsilon_x(x_1, t) \right] \, dt
\]

\[
- \epsilon \int_{t_1}^{t_2} \int_{x_1}^{x_2} \eta''(q^\epsilon)(q^\epsilon_x)^2 \, dx \, dt.
\]

Let \( \epsilon \rightarrow 0 \) to get result:

Term on third line goes to 0,
Term of fourth line is always \( \leq 0 \).
Weak form of entropy condition:

\[
\int_0^\infty \int_{-\infty}^\infty \left[ \phi_t \eta(q) + \phi_x \psi(q) \right] \, dx \, dt + \int_{-\infty}^\infty \phi(x, 0) \eta(q(x, 0)) \, dx \geq 0
\]

for all \( \phi \in C^1_0(\mathbb{R} \times \mathbb{R}) \) with \( \phi(x, t) \geq 0 \) for all \( x, t \).
Weak form of entropy condition:

\[ \int_0^\infty \int_{-\infty}^\infty \left[ \phi_t \eta(q) + \phi_x \psi(q) \right] \, dx \, dt + \int_{-\infty}^\infty \phi(x, 0) \eta(q(x, 0)) \, dx \geq 0 \]

for all \( \phi \in C^1_0(\mathbb{R} \times \mathbb{R}) \) with \( \phi(x, t) \geq 0 \) for all \( x, t \).

Informally we may write

\[ \eta(q)_t + \psi(q)_x \leq 0. \]
Lax-Wendroff Theorem

Suppose the method is conservative and consistent with

\[ q_t + f(q)_x = 0, \]

\[ F_{i-1/2} = \mathcal{F}(Q_{i-1}, Q_i) \quad \text{with} \quad \mathcal{F}(\bar{q}, \bar{q}) = f(\bar{q}) \]

and Lipschitz continuity of \( \mathcal{F} \).

If a sequence of discrete approximations converge to a function \( q(x, t) \) as the grid is refined, then this function is a weak solution of the conservation law.

**Note:**

Does not guarantee a sequence converges \( \text{(need stability)} \).

Two sequences might converge to different weak solutions.

Also need to satisfy an **entropy condition**.
Sketch of proof of Lax-Wendroff Theorem

Multiply the conservative numerical method

\[ Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n) \]

by \( \Phi_i^n \) to obtain

\[ \Phi_i^n Q_i^{n+1} = \Phi_i^n Q_i^n - \frac{\Delta t}{\Delta x} \Phi_i^n (F_{i+1/2}^n - F_{i-1/2}^n). \]
Sketch of proof of Lax-Wendroff Theorem

Multiply the conservative numerical method

\[ Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} (F_{i+1/2}^{n} - F_{i-1/2}^{n}) \]

by \( \Phi_{i}^{n} \) to obtain

\[ \Phi_{i}^{n} Q_{i}^{n+1} = \Phi_{i}^{n} Q_{i}^{n} - \frac{\Delta t}{\Delta x} \Phi_{i}^{n} (F_{i+1/2}^{n} - F_{i-1/2}^{n}) \].

This is true for all values of \( i \) and \( n \) on each grid. Now sum over all \( i \) and \( n \geq 0 \) to obtain

\[ \sum_{n=0}^{\infty} \sum_{i=-\infty}^{\infty} \Phi_{i}^{n} (Q_{i}^{n+1} - Q_{i}^{n}) = - \frac{\Delta t}{\Delta x} \sum_{n=0}^{\infty} \sum_{i=-\infty}^{\infty} \Phi_{i}^{n} (F_{i+1/2}^{n} - F_{i-1/2}^{n}) \].

Use summation by parts to transfer differences to \( \Phi \) terms.
Sketch of proof of Lax-Wendroff Theorem

Obtain analog of weak form of conservation law:

\[
\Delta x \Delta t \left[ \sum_{n=1}^{\infty} \sum_{i=-\infty}^{\infty} \left( \frac{\Phi_i^n - \Phi_i^{n-1}}{\Delta t} \right) Q_i^n 
+ \sum_{n=0}^{\infty} \sum_{i=-\infty}^{\infty} \left( \frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta x} \right) F_{i-1/2}^n \right] = -\Delta x \sum_{i=-\infty}^{\infty} \Phi_i^0 Q_i^0.
\]

Consider on a sequence of grids with \( \Delta x, \Delta t \to 0 \).

Show that any limiting function must satisfy weak form of conservation law.
Show that the numerical flux function $F$ leads to a numerical entropy flux $\Psi$

such that the following discrete entropy inequality holds:

$$\eta(Q_i^{n+1}) \leq \eta(Q_i^n) - \frac{\Delta t}{\Delta x} \left[ \Psi_{i+1/2}^n - \Psi_{i-1/2}^n \right].$$
Analog of Lax-Wendroff proof for entropy

Show that the numerical flux function $F$ leads to a numerical entropy flux $\Psi$

such that the following discrete entropy inequality holds:

$$\eta(Q_{i}^{n+1}) \leq \eta(Q_{i}^{n}) - \frac{\Delta t}{\Delta x} \left[ \Psi_{i+1/2}^{n} - \Psi_{i-1/2}^{n} \right].$$

Then multiply by test function $\Phi_{i}^{n}$, sum and use summation by parts to get discrete form of integral form of entropy condition.

$\implies$ If numerical approximations converge to some function, then the limiting function satisfies the entropy condition.
Entropy consistency of Godunov’s method

For Godunov’s method, $F(Q_{i-1}, Q_i) = f(Q_{i-1/2}^\downarrow)$

where $Q_{i-1/2}^\downarrow$ is the constant value along $x_{i-1/2}$ in the Riemann solution.

Let $\Psi_{i-1/2}^n = \psi(Q_{i-1/2}^\downarrow)$

Discrete entropy inequality follows from Jensen’s inequality:

The value of $\eta$ evaluated at the average value of $\tilde{q}^n$ is less than or equal to the average value of $\eta(\tilde{q}^n)$, i.e.,

$$\eta \left( \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \tilde{q}^n(x, t_{n+1}) \, dx \right) \leq \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} \eta(\tilde{q}^n(x, t_{n+1})) \, dx.$$