Numerical Schemes for Scalar One-Dimensional Conservation Laws
Finite Volume Discretization

\[ x_j = j \Delta x \]

\[ t^n = n \Delta t \]
We think of $\hat{u}_{j}^{n}$ as representing cell averages.

$$\hat{u}_{j}^{n} \approx \frac{1}{\Delta x} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} u(x, t^{n}) \, dx$$
Conservative Methods

Applying integral form of conservation law to a cell $j$

\[
\frac{d}{dt} \int_{x_j - \frac{1}{2}}^{x_j + \frac{1}{2}} u \, dx = - \left[ f(u(x_j + \frac{1}{2}, t)) - f(u(x_j - \frac{1}{2}, t)) \right]
\]

suggests

\[
\hat{u}_{j}^{n+1} - \hat{u}_j^n \frac{\Delta t}{\Delta x} = - \left( F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}} \right)
\]

\[
\hat{u}_j^{n+1} = \hat{u}_j^n - \frac{\Delta t}{\Delta x} \left( F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}} \right)
\]
Conservative Methods

Numerical Flux function

\[ F_{j+1/2} \equiv F(\hat{u}_{j-l}, \hat{u}_{j-l+1}, \ldots, \hat{u}_j, \ldots, \hat{u}_{j+r}) \]

and \( F \) is a numerical flux function of \( l + r + 1 \) arguments that satisfies the following consistency condition

\[ F(u, u, \ldots, u, u) = f(u) \]
If the solution of a conservative numerical scheme converges as $\Delta x \to 0$ with $\Delta t / \Delta x$ fixed, then it converges to a weak solution of the conservation law.

$\Rightarrow$ shock capturing schemes are possible
Conservative Methods

Lax-Wendroff Theorem

Shock Capturing

In the exact problem:

\[
\frac{d}{dt} \int_{x_0}^{x_J} u \, dx = -(f_0 - f_J)
\]

A conservative numerical scheme satisfies an analogous discrete condition:

\[
\Delta x \sum_{j=0}^{J} (\hat{u}_{j+1}^n - \hat{u}_j^n) = - \sum_{j=0}^{J} \left(F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}\right)
\]

\[
= - \left(F_J+\frac{1}{2} - F_{-\frac{1}{2}}\right)
\]
Conservative Methods

First Order Upwind

Linear Advection Equation...

\[ \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad a \text{ constant } > 0 \]

\[ \hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} - \frac{\Delta t}{\Delta x} \left( F_{j+\frac{1}{2}}^{UP} - F_{j-\frac{1}{2}}^{UP} \right) \]

Let \[ F_{j+\frac{1}{2}}^{UP} \equiv a \hat{u}_{j} \quad \left( F_{j-\frac{1}{2}}^{UP} = a \hat{u}_{j-1} \right) \]

\[ \Rightarrow \quad \hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} - \frac{\Delta t}{\Delta x} a (\hat{u}_{j} - \hat{u}_{j-1}) \]
Conservative Methods

First Order Upwind

...Linear Advection Equation...

What about $a < 0$?

We can write,

$$
\hat{u}_j^{n+1} = \hat{u}_j^n - \frac{a \Delta t}{\Delta x} \begin{cases} 
\hat{u}_j^n - \hat{u}_{j-1}^n & a > 0 \\
\hat{u}_{j+1}^n - \hat{u}_j^n & a < 0 
\end{cases}
$$

or

$$
\hat{u}_j^{n+1} = \hat{u}_j^n - \frac{a \Delta t}{2 \Delta x} (\hat{u}_{j+1}^n - \hat{u}_{j-1}^n) + \frac{|a| \Delta t}{2 \Delta x} (\hat{u}_{j+1}^n - 2\hat{u}_j^n + \hat{u}_{j-1}^n)
$$

MIT © 2011

Hyperbolic Equations 8
In conservative form:

\[
\hat{u}^{n+1}_j = \hat{u}^n_j - \frac{\Delta t}{\Delta x} \left( F^{UPn}_{j+\frac{1}{2}} - F^{UPn}_{j-\frac{1}{2}} \right)
\]

\[
F^{UP}_{j+\frac{1}{2}} = \frac{1}{2}a(\hat{u}_{j+1} + \hat{u}_j) - \frac{1}{2}|a|(\hat{u}_{j+1} - \hat{u}_j)
\]

\[
F^{UP}_{j+\frac{1}{2}} = a\hat{u}_j \quad a > 0
\]

\[
F^{UP}_{j+\frac{1}{2}} = a\hat{u}_{j+1} \quad a < 0
\]
In the nonlinear case,
\[
\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0
\]
the flux becomes
\[
F_{j+\frac{1}{2}}^{UP} = \frac{1}{2} \left( \hat{f}_{j+1} + \hat{f}_j \right) - \frac{1}{2} |\hat{a}_{j+\frac{1}{2}}| \left( \hat{u}_{j+1} - \hat{u}_j \right)
\]
\[
\hat{a}_{j+\frac{1}{2}} = \begin{cases} 
\frac{\hat{f}_{j+1} - \hat{f}_j}{\hat{u}_{j+1} - \hat{u}_j} & \text{if } \hat{u}_{j+1} \neq \hat{u}_j \\
 f'(\hat{u}_j) & \text{if } \hat{u}_{j+1} = \hat{u}_j
\end{cases}
\]
Conservative Methods

Lax-Wendroff

\[ F_{j+\frac{1}{2}}^{LW} = \frac{1}{2} \left( \hat{f}_{j+1} + \hat{f}_j \right) - \frac{1}{2} \hat{a}^2_{j+\frac{1}{2}} \frac{\Delta t}{\Delta x} (\hat{u}_{j+1} - \hat{u}_j) \]

For the linear equation

\[ \hat{u}_{j}^{n+1} = \hat{u}_j - \frac{C}{2} \left( \hat{u}_{j+1}^{n} - \hat{u}_{j-1}^{n} \right) + \frac{C^2}{2} \left( \hat{u}_{j+1}^{n} - 2\hat{u}_{j}^{n} + \hat{u}_{j-1}^{n} \right) \]

\[ C = a\Delta x/\Delta t \]
Conservative Methods

Do these schemes converge to the entropy satisfying solution?

EXAMPLE:

Consider a non-physical solution to Burgers’ equation:

\[
\begin{align*}
  u(x,t) &= \begin{cases} 
    1 & x \geq 0 \\
    -1 & x < 0 
  \end{cases} \\
\end{align*}
\]

i.e. \( \hat{u}_j^n \) is either 1 or -1 \( \Rightarrow f_j = \frac{1}{2} \ \forall j \)
Conservative Methods

Entropy Solutions

Example

First order upwind:

\[ F_{j+\frac{1}{2}}^{UP} = \frac{1}{2} \left( \hat{f}_{j+1} + \hat{f}_j \right) - \frac{1}{2} \left| \hat{a}_{j+\frac{1}{2}} \right| \left( \hat{u}_{j+1} - \hat{u}_j \right) \]

Since either \( \hat{a}_{j+\frac{1}{2}} \) or \( \hat{u}_{j+1} - \hat{u}_j \) is zero \( \forall j \)

\[ \Rightarrow \quad F_{j+\frac{1}{2}}^{UP} = \frac{1}{2} \quad \forall j \quad \Rightarrow \quad F_{j+\frac{1}{2}}^{UP} - F_{j-\frac{1}{2}}^{UP} = 0 \quad \forall j \]

\[ \Rightarrow \quad \hat{u}_{j+1}^n = \hat{u}_j^n \]

The entropy-violating solution is preserved
If a scheme can be written in the form
\[ \hat{u}^{n+1}_j = H \left( \hat{u}^n_{j-l}, \hat{u}^n_{j-l+1}, \ldots, \hat{u}^n_{j}, \ldots, \hat{u}^n_{j+r} \right) \]
with \( \frac{\partial H}{\partial u_i} \geq 0 \quad i = j - l, \ldots, j, \ldots, j + r, \)
then the scheme is monotone and is

- entropy satisfying
- at most first order accurate
Entropy Satisfying Schemes

Monotone Schemes

Godunov’s Method...

Assume piecewise constant solution over each cell. Compute interface flux by solving interface (Riemann) problem exactly.
Entropy Satisfying Schemes

Monotone Schemes

...Godunov’s Method...

\[ F_{j+\frac{1}{2}}^{Gn} = f\left(u(x_{j+\frac{1}{2}}, t^{n+})\right) \]

\[ = \begin{cases} 
\min_{u \in [u_j, u_{j+1}]} f(u) & u_j < u_{j+1} \\
\max_{u \in [u_j, u_{j+1}]} f(u) & u_j > u_{j+1}
\end{cases} \]

Then,

\[ \hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} - \frac{\Delta t}{\Delta x} \left( F_{j+\frac{1}{2}}^{Gn} - F_{j-\frac{1}{2}}^{Gn} \right) \]
Entropy Satisfying Schemes

Monotone Schemes

...Godunov’s Method

Applied to Burgers’ equation

\[
F_{j+\frac{1}{2}}^G = \left\{ \begin{array}{ll}
\frac{1}{2} \hat{u}_{j+1}^2 & \hat{u}_j, \hat{u}_{j+1} < 0 \\
\frac{1}{2} \hat{u}_j^2 & \hat{u}_j, \hat{u}_{j+1} > 0 \\
0 & \hat{u}_j < 0 < \hat{u}_{j+1} \quad \text{(expansion)} \\
\frac{1}{2} \hat{u}_{j+1}^2 & \hat{u}_j > 0 > \hat{u}_{j+1} \\
\frac{1}{2} \hat{u}_j^2 & \hat{u}_j > 0 > \hat{u}_{j+1} \\
\end{array} \right.
\]

MIT © 2011 Hyperbolic Equations 17
If the numerical flux $F_{j+\frac{1}{2}}$ satisfies

$$\text{sign}(\hat{u}^n_{j+1} - \hat{u}^n_j)(F^n_{j+\frac{1}{2}} - f(u)) \leq 0 \quad \forall u \in [\hat{u}_j, \hat{u}_{j+1}]$$

An E-scheme is

- entropy satisfying
- at most first order accurate
Entropy Satisfying Schemes

Summary

first order

entropy satisfying

MIT © 2011
First order schemes give poor resolution but can be made to produce entropy satisfying and non-oscillatory solutions.

Higher order schemes (at least the ones we have seen so far) produce non-entropy satisfying and oscillatory solutions.

Good criterion to design “high order” oscillation free schemes is based on the Total Variation of the solution.
TVD Methods

First Order Upwind

\[ J = 100, \ \Delta x = 1/100, \ C = 0.5, \ N = 200 \]
Lax-Wendroff

\[ J = 100, \quad \Delta x = 1/100, \quad C = 0.5, \quad N = 200 \]
Total Variation of the discrete solution

$$TV(\hat{u}^n) = \sum_j |\hat{u}_{j+1}^n - \hat{u}_j^n|$$

If new extrema are generated $TV(\hat{u})$ will increase.

$$TV(\hat{u}^{n+1}) \leq TV(\hat{u}^n)$$

Total Variation Diminishing Schemes
TVD Methods

Some Properties

- All E-Schemes are TVD
- Conservative TVD Schemes \( \Rightarrow Converge \) to weak solutions
TVD Methods

Conditions for TVD schemes

If a scheme is written in the form

\[
\hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} + D_{j+\frac{1}{2}} \Delta \hat{u}_{j+\frac{1}{2}}^{n} - C_{j-\frac{1}{2}} \Delta \hat{u}_{j-\frac{1}{2}}^{n}
\]

it is TVD iff

\[
\Delta \hat{u}_{j+\frac{1}{2}} = \hat{u}_{j+1} - \hat{u}_{j}
\]

\[
\begin{align*}
C_{j+\frac{1}{2}} & \geq 0 \\
D_{j+\frac{1}{2}} & \geq 0 \\
C_{j+\frac{1}{2}} + D_{j+\frac{1}{2}} & \leq 1
\end{align*}
\]
Conditions for TVD schemes

Example: Upwind

Upwind scheme for linear equation, $a > 0$:

$$u_{j}^{n+1} = u_{j}^{n} - \frac{a \Delta t}{\Delta x} \left( u_{j}^{n} - u_{j-1}^{n} \right)$$

$$C_{j-\frac{1}{2}} = \frac{a \Delta t}{\Delta x}; \quad D_{j+\frac{1}{2}} = 0$$

$$C_{j-\frac{1}{2}} = \frac{a \Delta t}{\Delta x} \leq 1$$

Stability-like condition!
No second or higher order accurate constant coefficient \((\text{linear})\) scheme can be TVD.

\[ \Rightarrow \] Higher order TVD schemes must be nonlinear
Consider the linear equation
\[
\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad \text{for} \quad a > 0
\]

First order upwind (Godunov) scheme is
\[
\hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} - C \left( \hat{u}_{j}^{n} - \hat{u}_{j-1}^{n} \right)
\]
where
\[
C = \frac{a \Delta t}{\Delta x}
\]

Oscillation free but smeared solutions.
TVD Methods

High Resolution Schemes

Lax-Wendroff

\[ \hat{u}_{j}^{n+1} = \hat{u}_{j}^{n} - \frac{C}{2} \left( \hat{u}_{j+1}^{n} - \hat{u}_{j-1}^{n} \right) + \frac{C^2}{2} \left( \hat{u}_{j+1}^{n} - 2\hat{u}_{j}^{n} + \hat{u}_{j-1}^{n} \right) \]

Suffers from oscillations.
Re-write the Lax-Wendroff scheme:

\[
\hat{u}_j^{n+1} = \hat{u}_j^n - C \left( \hat{u}_j^n - \hat{u}_{j-1}^n \right) - \frac{1}{2} C (1 - C) \left( \hat{u}_{j+1}^n - 2\hat{u}_j^n + \hat{u}_{j-1}^n \right)
\]

\(\text{first order upwind}\)

\[F_{j+\frac{1}{2}}^{LW} = a\hat{u}_j + \frac{a}{2} (1 - C) (\hat{u}_{j+1} - \hat{u}_j)\]

\(\text{anti-diffusive flux}\)

Introduce \(\text{flux limiter } \phi_{j+\frac{1}{2}}:\)

\[
F_{j+\frac{1}{2}}^{TVD} = a\hat{u}_j + \frac{a}{2} (1 - C) \phi_{j+\frac{1}{2}} (\hat{u}_{j+1} - \hat{u}_j)
\]
\[
\hat{u}^{n+1}_j = \hat{u}^n_j - C \left( \hat{u}^n_j - \hat{u}^n_{j-1} \right)
\]

\[
- \frac{1}{2}C(1 - C) \left[ \phi_{j+\frac{1}{2}} \left( \hat{u}^n_{j+1} - \hat{u}^n_j \right) - \phi_{j-\frac{1}{2}} \left( \hat{u}^n_j - \hat{u}^n_{j-1} \right) \right]
\]

If \( \phi_j = \phi_{j-1} = 1 \) \( \Rightarrow \) Lax-Wendroff (not TVD)

If \( \phi_j = \phi_{j-1} = 0 \) \( \Rightarrow \) Upwind (TVD)

Choose the limiter as close as possible to 1 but enforcing TVD conditions
Re-write

\[
\hat{u}^{n+1}_j = \hat{u}^n_j - C \Delta \hat{u}_{j-\frac{1}{2}} - \frac{1}{2} C (1 - C) (\phi_{j+\frac{1}{2}} \Delta \hat{u}_{j+\frac{1}{2}} - \phi_{j-\frac{1}{2}} \Delta \hat{u}_{j-\frac{1}{2}})
\]

\[
= u^n_j - C \left\{ 1 + \frac{1}{2} (1 - C) \left[ \phi_{j+\frac{1}{2}} \frac{1}{r_{j+\frac{1}{2}}} - \phi_{j-\frac{1}{2}} \right] \right\} \Delta \hat{u}_{j-\frac{1}{2}}
\]

Recall the TVD test:

\[
\hat{u}^{n+1}_j = \hat{u}^n_j + D_{j+\frac{1}{2}} \Delta \hat{u}^n_{j+\frac{1}{2}} - C_{j-\frac{1}{2}} \Delta \hat{u}^n_{j-\frac{1}{2}}
\]
TVD Methods

High Resolution Schemes

...Flux Limiters

Take

\[ C_{j+\frac{1}{2}} = C \left\{ 1 + \frac{1}{2} (1 - C) \left[ \frac{\phi_{j+\frac{1}{2}}}{r_{j+\frac{1}{2}}} - \phi_{j-\frac{1}{2}} \right] \right\} \]

\[ D_{j+\frac{1}{2}} = 0 \]

TVD criterion \( \Rightarrow \quad 0 \leq C_{j+\frac{1}{2}} \leq 1 \)
Choose $\phi_{j+\frac{1}{2}}$ to be function of $r_{j+\frac{1}{2}}$.
It can be seen that the above TVD conditions are satisfied if

\[
\begin{align*}
\phi(r) &= 0 \quad r \leq 0 \\
0 &\leq \frac{\phi(r)}{r} \leq 2 \\
0 &\leq \phi(r) \leq 2
\end{align*}
\]
TVD Methods

High Resolution Schemes

2nd Order TVD Region

\[ \Phi(r) \]

2nd Order TVD Region

MIT©2011

Hyperbolic Equations 36
Minmod $\phi(r) = \max(0, \min(1, r))$

Superbee $\phi(r) = \max(0, \min(2r, 1), \min(r, 2))$

Van Leer $\phi(r) = \frac{r + |r|}{1 + |r|}$

All produce **second order** schemes when the solution is smooth, and reduce to **upwind** at **discontinuities**.
TVD Methods

High Resolution Schemes

Examples...

BEAM-WARMING

BEAM-WARMING
TVD Methods

High Resolution Schemes

...Examples...
TVD Methods

High Resolution Schemes

...Examples...

TVD - MINMOD

TVD - MINMOD
TVD Methods

High Resolution Schemes

...Examples...

TVD - VAN LEER

TVD - VAN LEER
TVD Methods

High Resolution Schemes

...Examples

TVD - SUPERBEE

TVD - SUPERBEE
For a nonlinear conservation law the formulation of flux limiters is extended to allow both positive and negative wave speeds.

1. Reconstruct a higher-order polynomial representation within a cell from averages of neighboring cell values

2. Evaluate fluxes at cell interfaces through (approximate) solution of Riemann problems

3. Evolve cell averages in time
Reconstruction

\[ \tilde{u}_j(x) = \tilde{u}_j(x)(\hat{u}_{j-l}, \hat{u}_{j-l+1}, \ldots, \hat{u}_{j+l-1}, \hat{u}_{j+l}) \]
\[ \tilde{u}_j(x) = \hat{u}_j + (x - x_j)\sigma_j \]

- Can be generalized to:
  - varying cell sizes
  - multiple dimensions
  - higher order
Options for $\sigma_j$: 

\[ \sigma_{j}^C \equiv \frac{\hat{u}_{j+1} - \hat{u}_{j-1}}{2\Delta x} \]  

\[ \sigma_{j}^L \equiv \frac{\hat{u}_{j} - \hat{u}_{j-1}}{\Delta x} \]  

\[ \sigma_{j}^R \equiv \frac{\hat{u}_{j+1} - \hat{u}_{j}}{\Delta x} \]
Van Leer suggested the following quadratic $\kappa$-scheme:

$$\tilde{u}_j(x) = \hat{u}_j + (x - x_j)\sigma^C_j + \frac{3\kappa}{2} \left[ (x - x_j)^2 - \frac{\Delta x^2}{12} \right] \frac{\sigma^R_j - \sigma^L_j}{\Delta x}$$

- $\kappa = 1/3$ is the correct second order Taylor series
- $\kappa = 0$ reduces to linear reconstruction with $\sigma_j = \sigma^C_j$ (Fromm’s scheme)
\[ \Delta x \frac{d\hat{u}_j}{dt} = - \left[ F_{j+\frac{1}{2}}^{MUSCL} - F_{j-\frac{1}{2}}^{MUSCL} \right] \]

\[ F_{j+\frac{1}{2}}^{MUSCL} = F \left( \tilde{u}_j(x_{j+\frac{1}{2}}), \tilde{u}_{j+1}(x_{j+\frac{1}{2}}) \right) \]
For linear reconstruction,

\[ \tilde{u}_j(x_{j+\frac{1}{2}}) = \hat{u}_j + \frac{1}{2} \Delta x \sigma_j \]  
(4)

\[ \tilde{u}_j(x_{j-\frac{1}{2}}) = \hat{u}_j - \frac{1}{2} \Delta x \sigma_j \]  
(5)
For $\kappa$ quadratic reconstruction,

$$\tilde{u}_j(x_{j+\frac{1}{2}}) = \hat{u}_j + \frac{1}{4}\Delta x \left( (1 - \kappa)\sigma^L_j + (1 + \kappa)\sigma^R_j \right)$$  (6)

$$\tilde{u}_j(x_{j-\frac{1}{2}}) = \hat{u}_j - \frac{1}{4}\Delta x \left( (1 + \kappa)\sigma^L_j + (1 - \kappa)\sigma^R_j \right)$$  (7)

Note: $\kappa = -1$ gives reconstructions based on data from one-side of interface. When combined with an upwind flux function, the result is a fully-upwinded second-order accurate spatial discretization.
Monotonic reconstructions enforced by requiring $\tilde{u}_j(x)$ to be bounded by averages in cell $j - 1$, $j$, and $j + 1$ (Van Leer 1979).

Reconstruction violates monotonicity condition at circled locations.
For linear reconstructions, this monotonicity condition can be enforced using the gradient \((\sigma_j)_{\text{mono}}\) given by the following formulation:

\[
(\sigma_j)_{\text{mono}} \equiv \frac{1}{2} \left[ \text{sign}(\sigma_j^L) + \text{sign}(\sigma_j^R) \right] \min \left[ 2 |\sigma_j^L| , 2 |\sigma_j^R| , |\sigma_j| \right]
\]

where \(\sigma_j\) is an arbitrary gradient approximation that then defines the scheme.
The flux limiters we have seen previously can be related to specific choices of $\sigma_j$. For example:

- Minmod: $|\sigma_j| = \min(|\sigma_j^L|, |\sigma_j^R|)$
- Superbee: $|\sigma_j| = \max(|\sigma_j^L|, |\sigma_j^R|)$

As an exercise, determine $|\sigma_j|$ for the Van Leer limiter.