

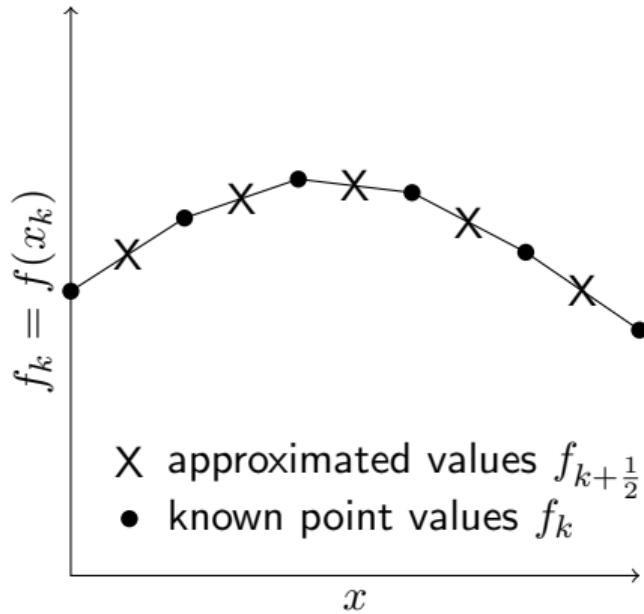
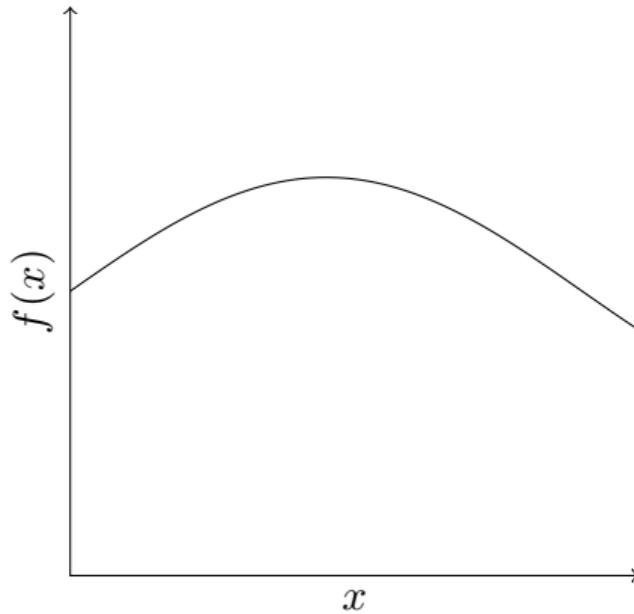
Essentially Non-Oscillatory Methods

Nick Derr

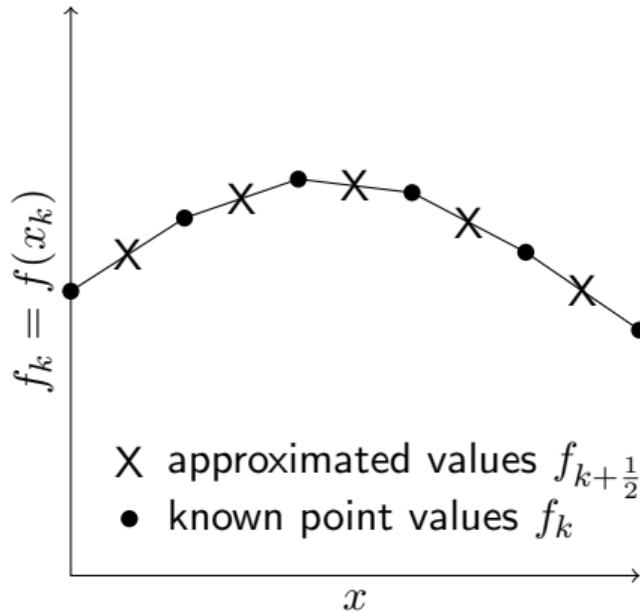
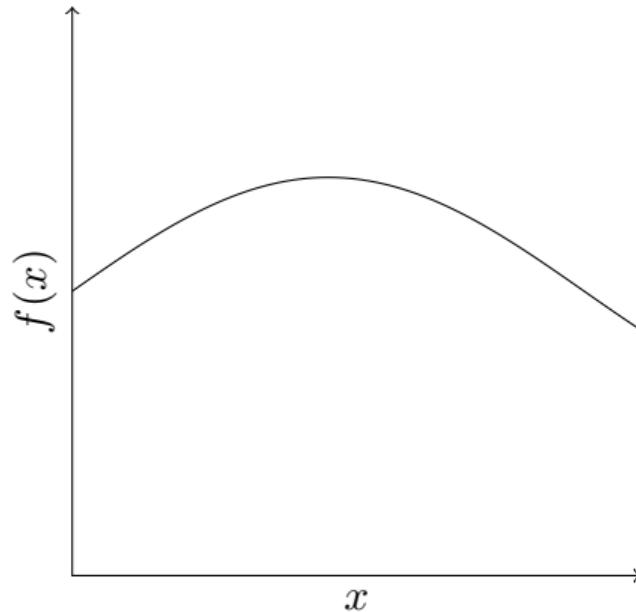
Applied Math 205
Harvard University

October 20, 2020

Approximating derivatives by finite differences is at the heart of many numerical methods.

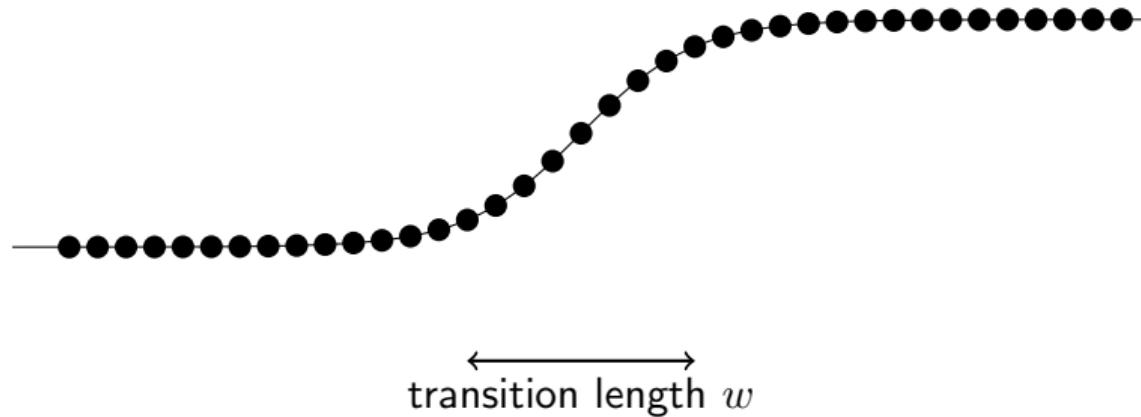


Approximating derivatives by finite differences is at the heart of many numerical methods.

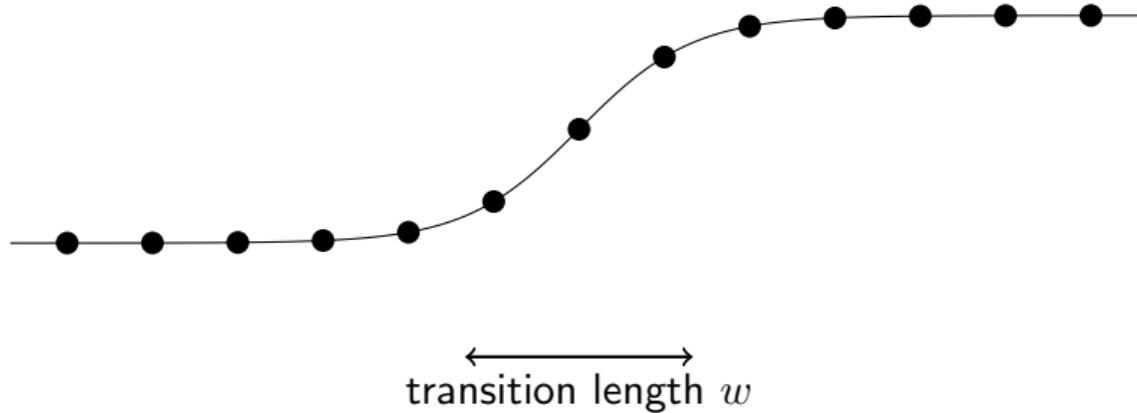


We can approximate any derivative value by evaluating that of an interpolant through a set of nearby points.

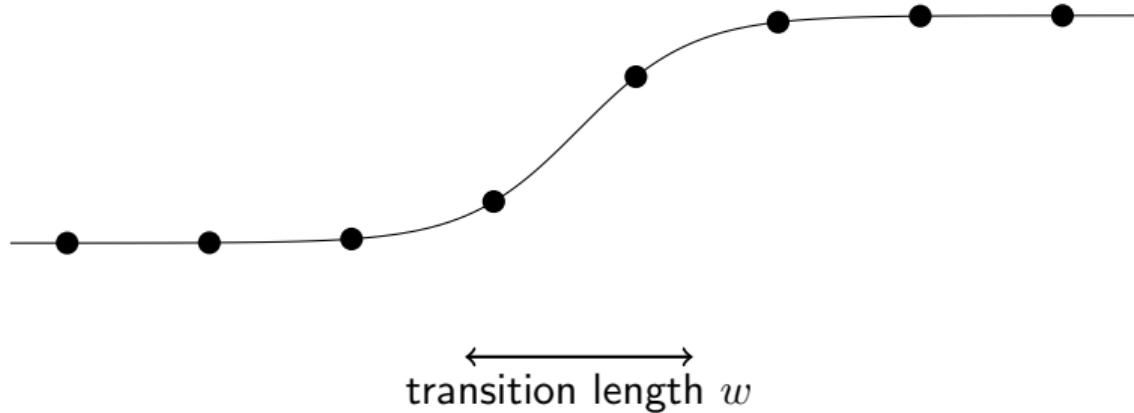
If grid points are spaced too far apart, fine features in the solution may not be captured.



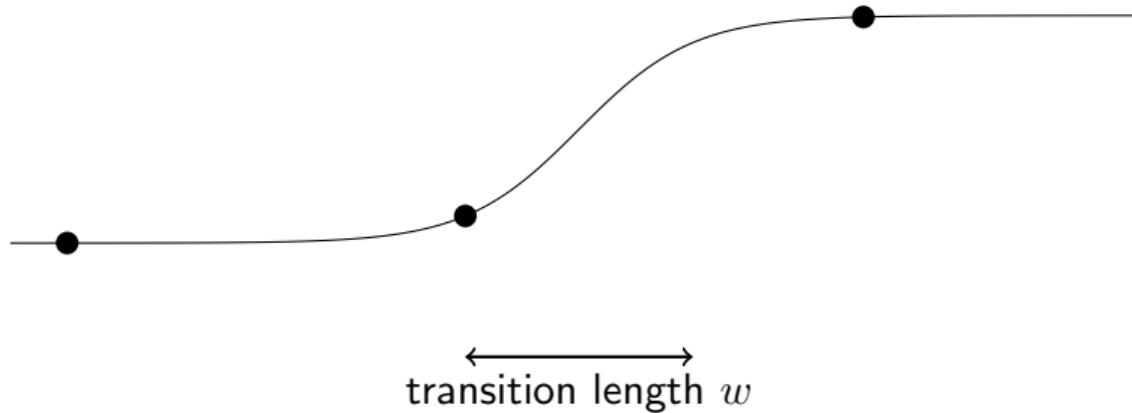
If grid points are spaced too far apart, fine features in the solution may not be captured.



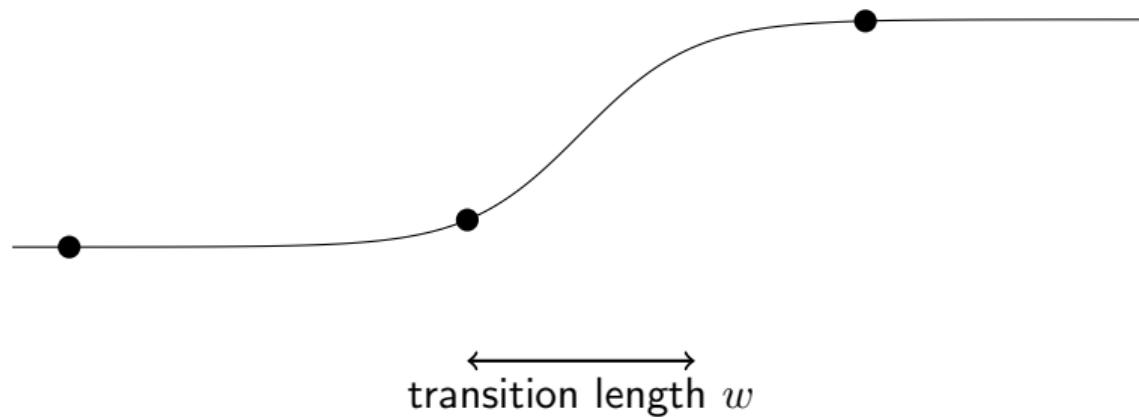
If grid points are spaced too far apart, fine features in the solution may not be captured.



If grid points are spaced too far apart, fine features in the solution may not be captured.



If grid points are spaced too far apart, fine features in the solution may not be captured.



Need $\Delta x < w$ — but what happens as $w \rightarrow 0$? Does this happen in “real life” ?

Often, features that appear discontinuous are actually transition regions of some width w , but the cost to simulate with $\Delta x < w$ would be enormous!



Often, features that appear discontinuous are actually transition regions of some width w , but the cost to simulate with $\Delta x < w$ would be enormous!



Often, features that appear discontinuous are actually transition regions of some width w , but the cost to simulate with $\Delta x < w$ would be enormous!



Need methods for simulating discontinuous solutions!

Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

If we assume a wavelike solution, i.e.
 $f(x, t) = f(x - ct)$, we get

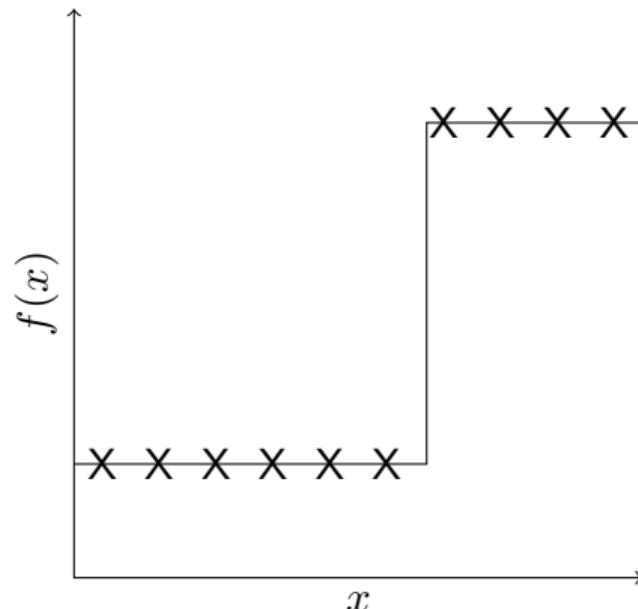
$$\boxed{\dot{f} = -cf, \quad f' = f,}$$

so even with discontinuities the solution sees the function **move to the right**

Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

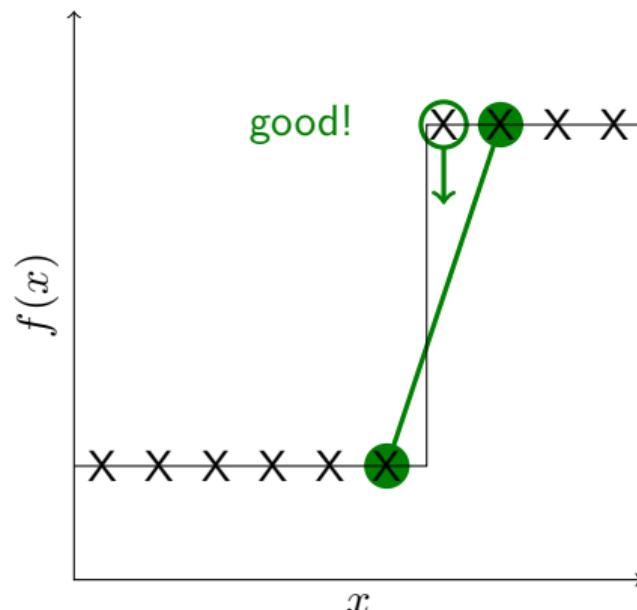
- ▶ solution moves to right



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

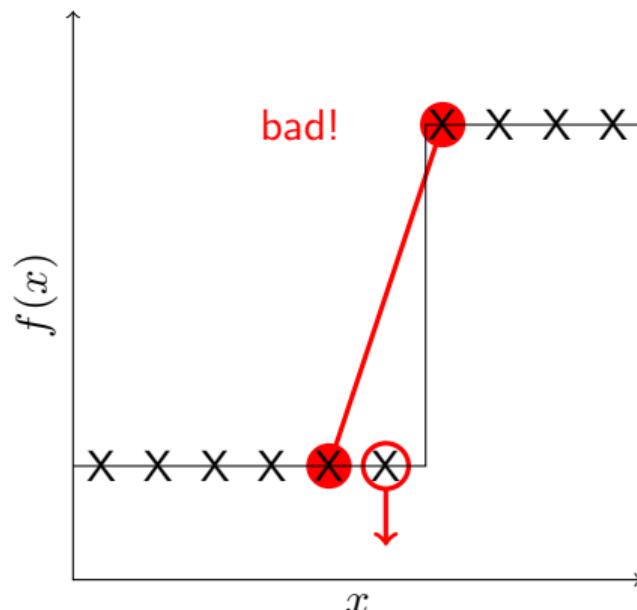
- ▶ solution moves to right
- ▶ some points move in expected direction



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

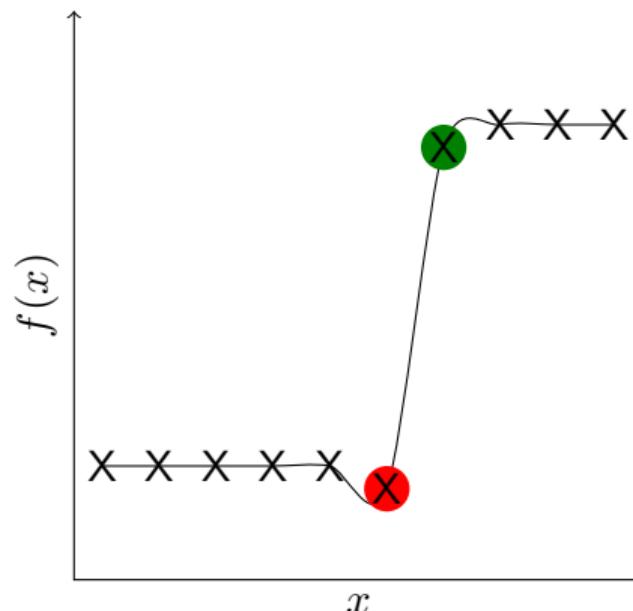
- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

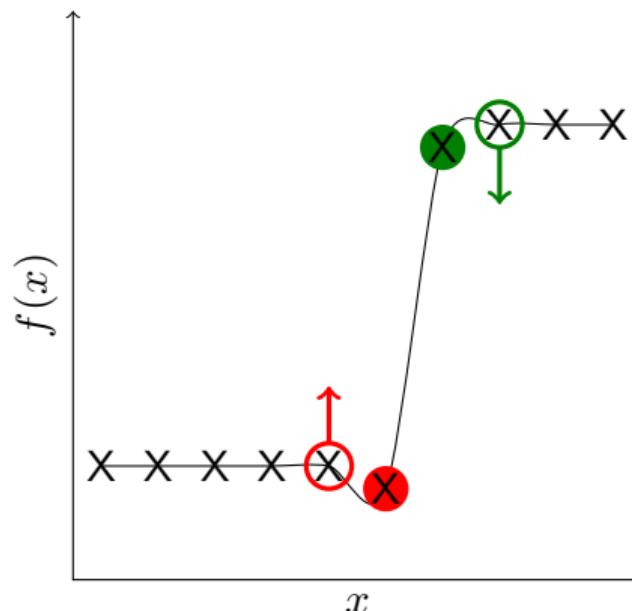
- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!
- ▶ each time step moves points left of shock incorrectly



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

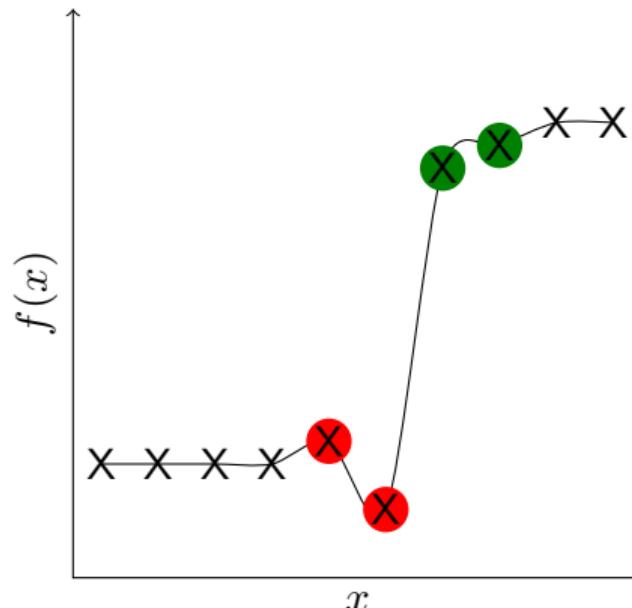
- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!
- ▶ each time step moves points left of shock incorrectly



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

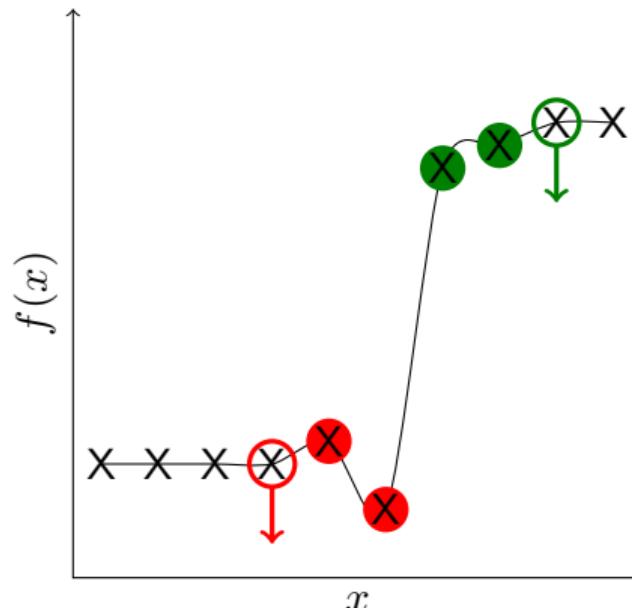
- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!
- ▶ each time step moves points left of shock incorrectly
- ▶ → unstable growth of spurious oscillations



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

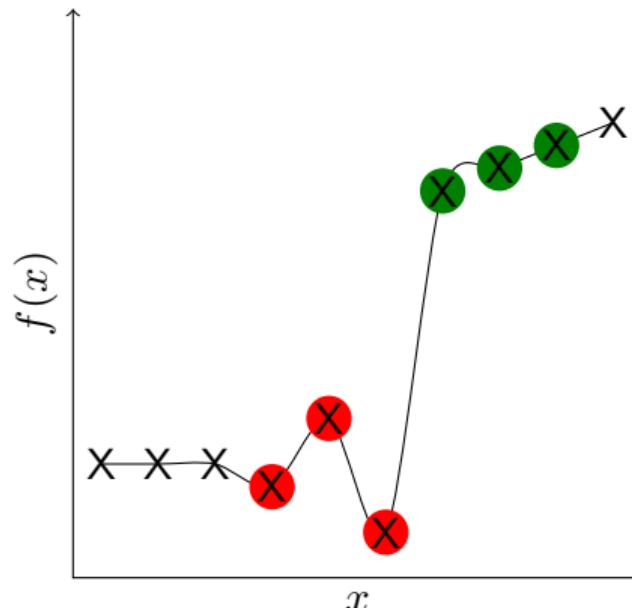
- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!
- ▶ each time step moves points left of shock incorrectly
- ▶ → unstable growth of spurious oscillations



Discontinuities in solutions, or shocks, violate the assumptions on Taylor series truncation error and cause problems for “vanilla” methods.

Example: $\partial_t f = -c \partial_x f \implies \dot{f}_k = -c \left(\frac{f_{k+1} - f_{k-1}}{2\Delta x} \right)$ (centered difference)

- ▶ solution moves to right
- ▶ some points move in expected direction, but others don't!
- ▶ each time step moves points left of shock incorrectly
- ▶ → unstable growth of spurious oscillations



Let's re-write the problem in conservative form:

For some velocity $v = v(x, f)$,

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} (vf) .$$

Let's re-write the problem in conservative form:

For some velocity $v = v(x, f)$,

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} (vf) .$$

Let $q = vf$ equal the **generalized flux**. Then

$$\frac{\partial f_k}{\partial t} = -\frac{q_{k+\frac{1}{2}} - q_{k-\frac{1}{2}}}{\Delta x}$$

f_0	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	----------

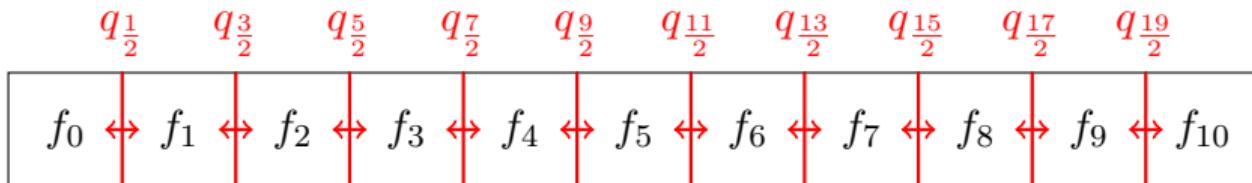
Let's re-write the problem in conservative form:

For some velocity $v = v(x, f)$,

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} (vf).$$

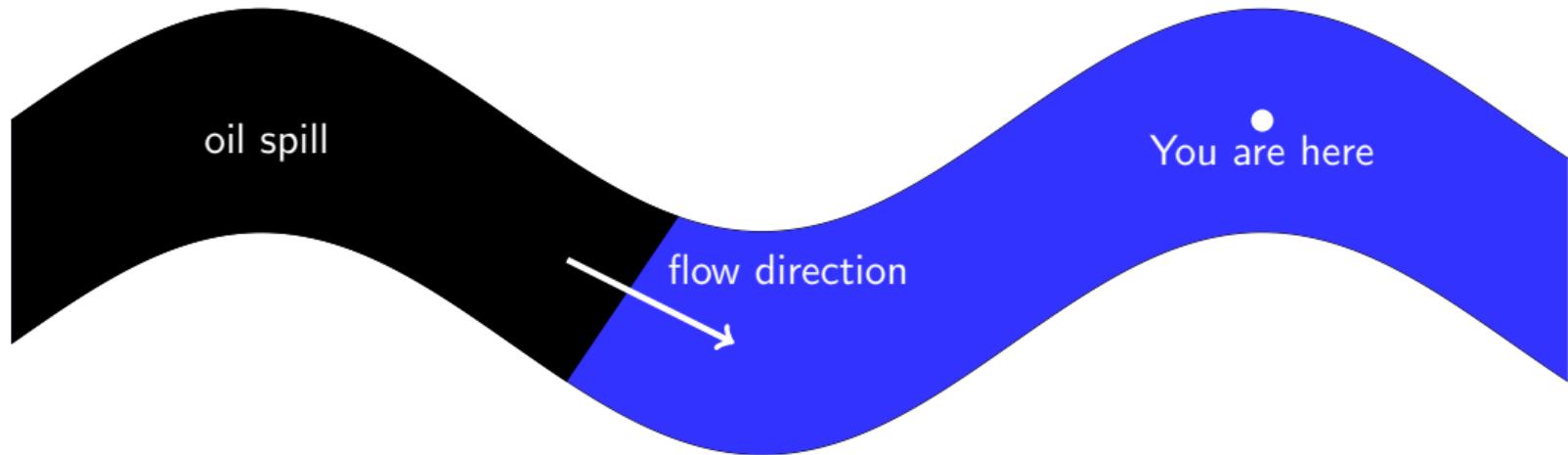
Let $q = vf$ equal the **generalized flux**. Then

$$\frac{\partial f_k}{\partial t} = -\frac{q_{k+\frac{1}{2}} - q_{k-\frac{1}{2}}}{\Delta x}$$

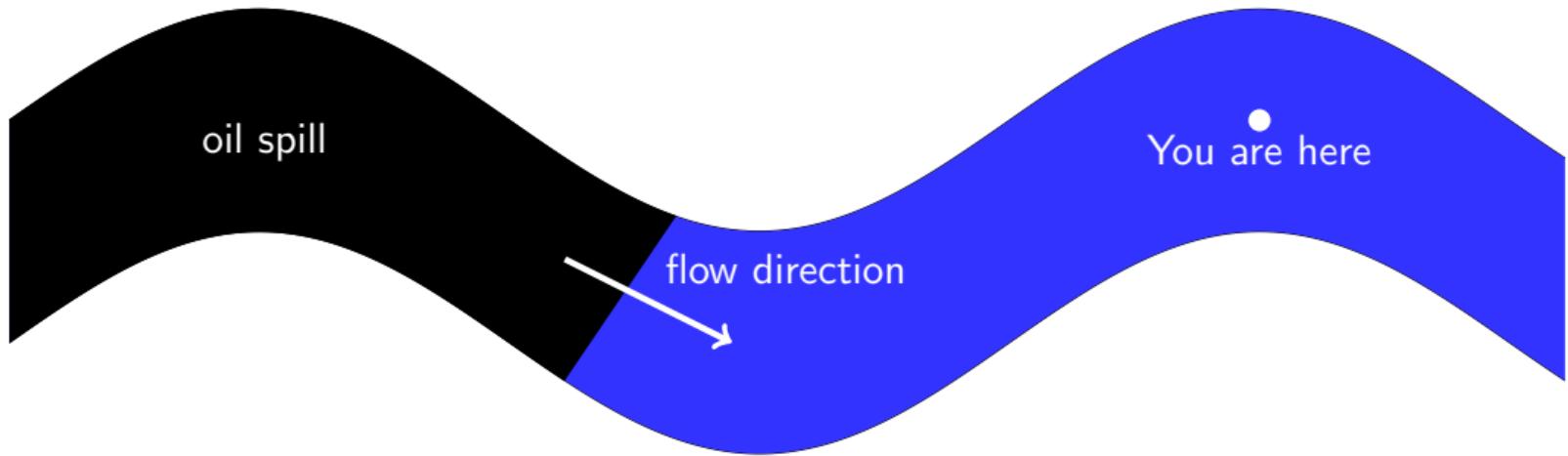


Example: centered difference on previous slide used $q_{k+\frac{1}{2}} = cf_{k+\frac{1}{2}} = \frac{c}{2}(f_k + f_{k+1})$.
Can we understand failure of the previous example in terms of the stencil $\{\frac{1}{2}, \frac{1}{2}\}$?

Big Idea 1: The sign of the velocity v tells us the direction of information flow. Look upstream! (Downstream? Garbage in, garbage out.)

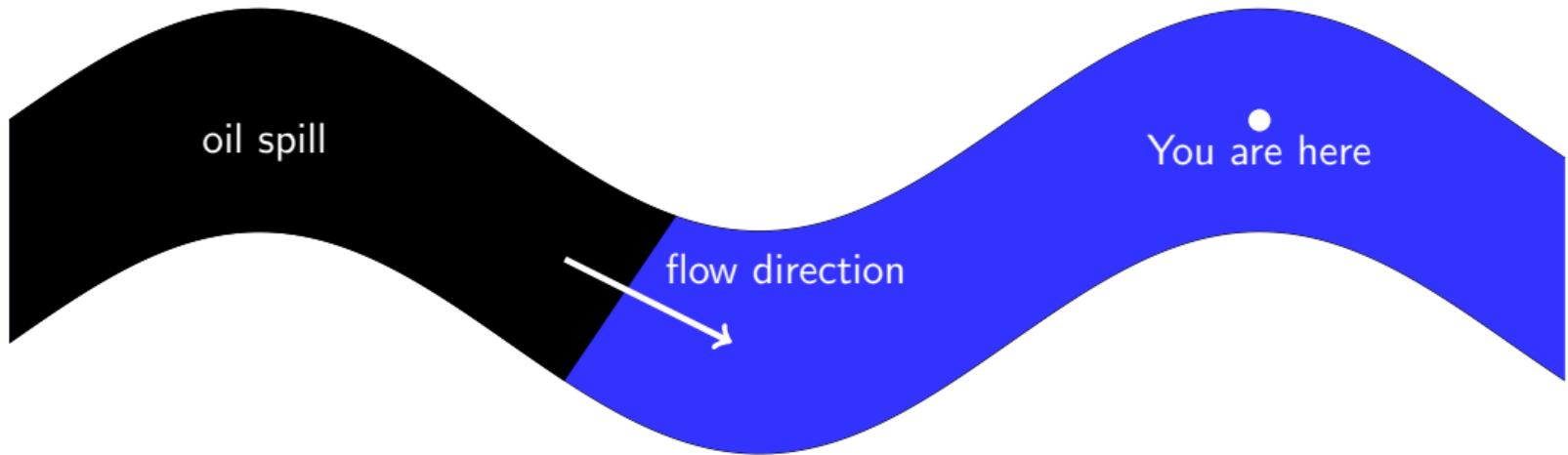


Big Idea 1: The sign of the velocity v tells us the direction of information flow. Look upstream! (Downstream? Garbage in, garbage out.)



Which way are you going to look in order to understand how the local concentration of oil is going to change near you? \Rightarrow Make sure stencils include upstream portion.

Big Idea 1: The sign of the velocity v tells us the direction of information flow. Look upstream! (Downstream? Garbage in, garbage out.)

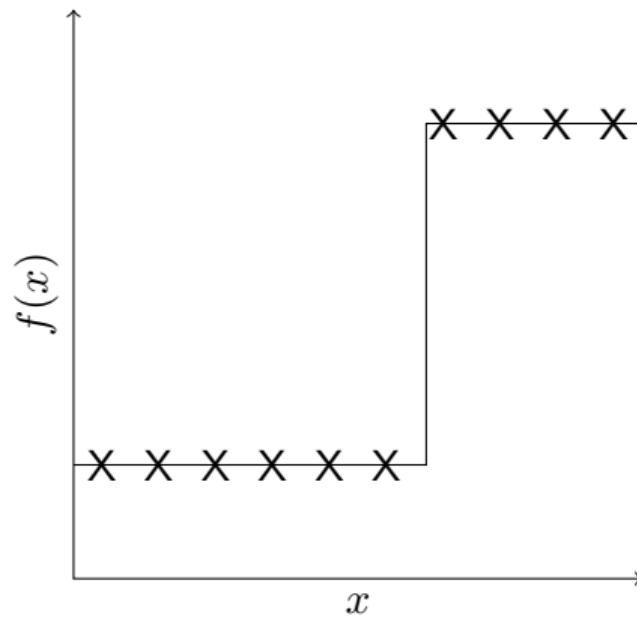


Which way are you going to look in order to understand how the local concentration of oil is going to change near you? \Rightarrow Make sure stencils include upstream portion.

“Upwinding” is essential for shock capture

Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

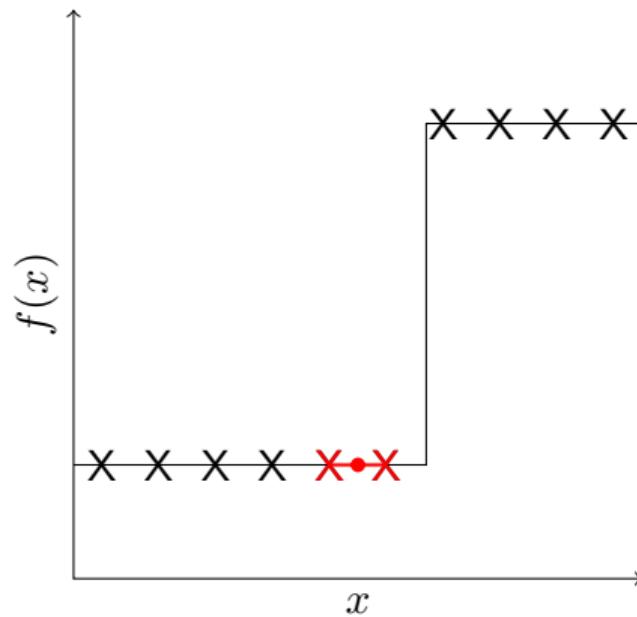
How do various interpolation rules influence the behavior of the problematic point?



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

Original centered difference:

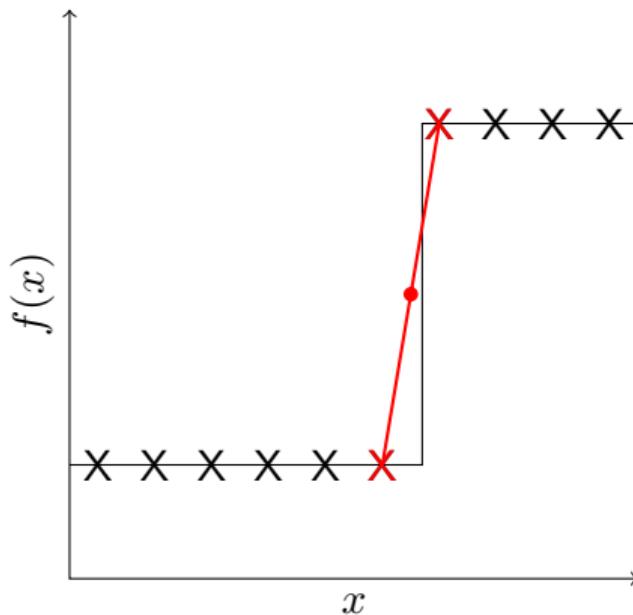
- ▶ point 1 is reasonable



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

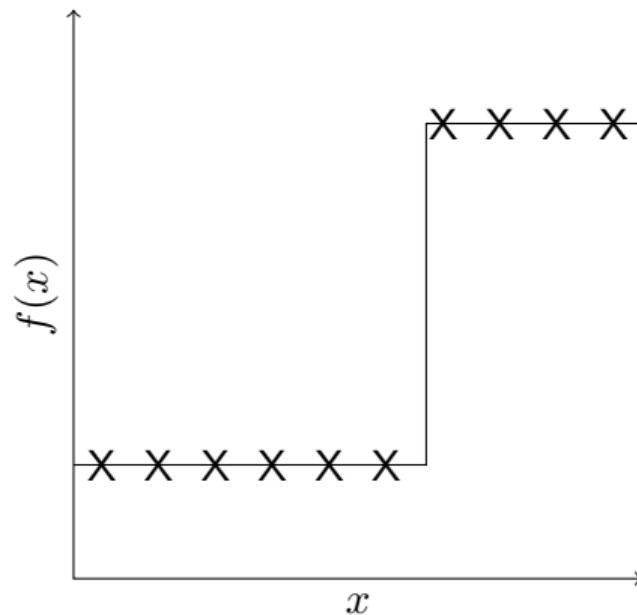
Original centered difference:

- ▶ point 1 is reasonable
- ▶ point 2 creates our unwanted oscillation because it's **interpolating points on either side of a discontinuity**



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

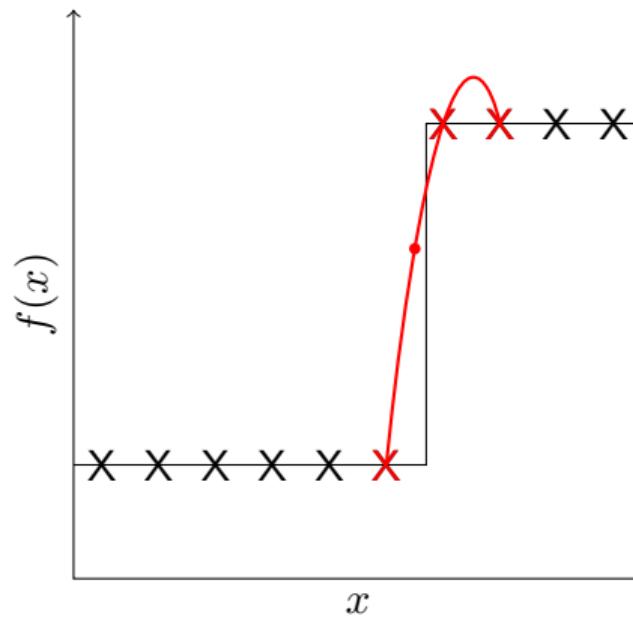
What if we ditch the centered stencil? Use a 3-point stencil to preserve 2nd order. We have three choices that upwind: let's look at them applied to second point.



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

What if we ditch the centered stencil? Use a 3-point stencil to preserve 2nd order. We have three choices that upwind: let's look at them applied to second point.

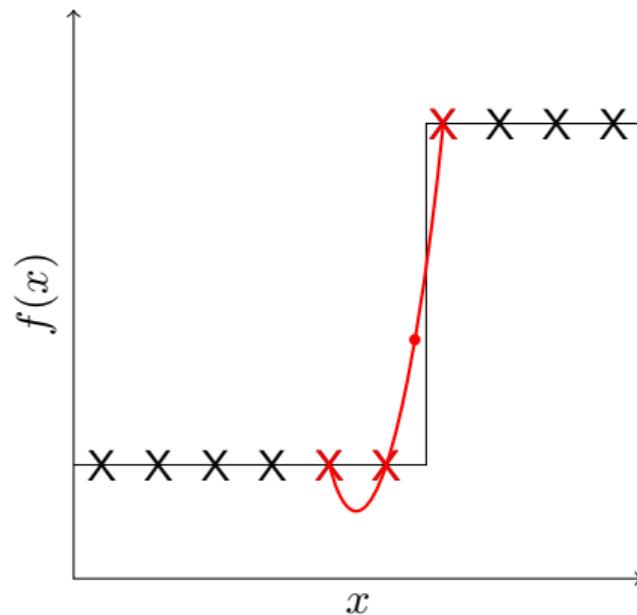
- ▶ between first two: no good



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

What if we ditch the centered stencil? Use a 3-point stencil to preserve 2nd order. We have three choices that upwind: let's look at them applied to second point.

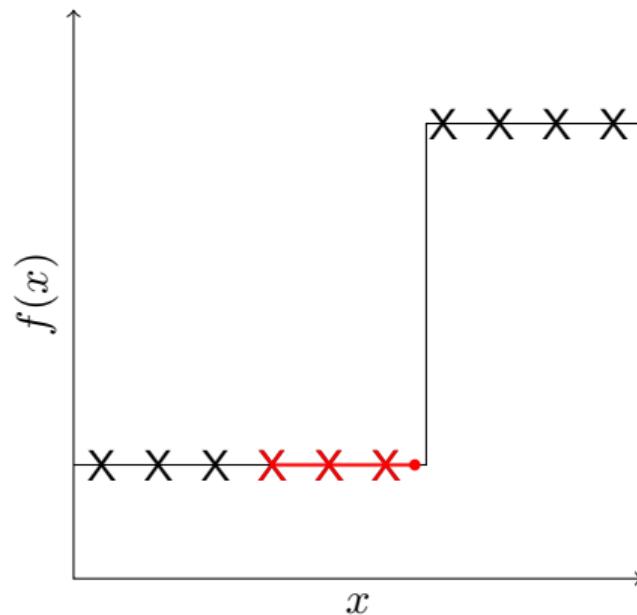
- ▶ between first two: no good
- ▶ between last two: same prob



Big Idea 2: Interpolation error only converges to zero with grid size if it's with respect to a smooth function

What if we ditch the centered stencil? Use a 3-point stencil to preserve 2nd order. We have three choices that upwind: let's look at them applied to second point.

- ▶ between first two: no good
- ▶ between last two: same prob
- ▶ after last: Bingo!



Takeaway: interpolation $x_{k+\frac{1}{2}}$ from one of several possible stencils at each point

ENO Method:

Given a collection of five points $S = \{f_{k-2}, f_{k-1}, f_k, f_{k+1}, f_{k+2}\}$, we calculate the interpolant $f_{k+\frac{1}{2}}$ as follows. Following the procedure of the last slide, we introduce three stencils $S_j \in S$,

$$\begin{array}{ccccc} & & f_{k+\frac{1}{2}} & & \\ X & X & X & \circ & X & X \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \\ \hline & & S_0 & & \end{array}$$

ENO Method:

Given a collection of five points $S = \{f_{k-2}, f_{k-1}, f_k, f_{k+1}, f_{k+2}\}$, we calculate the interpolant $f_{k+\frac{1}{2}}$ as follows. Following the procedure of the last slide, we introduce three stencils $S_j \in S$,

$$\begin{array}{ccccc} & & f_{k+\frac{1}{2}} & & \\ X & X & X & \circ & X & X \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \\ & & \underbrace{}_{S_1} & & \end{array}$$

ENO Method:

Given a collection of five points $S = \{f_{k-2}, f_{k-1}, f_k, f_{k+1}, f_{k+2}\}$, we calculate the interpolant $f_{k+\frac{1}{2}}$ as follows. Following the procedure of the last slide, we introduce three stencils $S_j \in S$,

$$\begin{array}{ccccc} & & f_{k+\frac{1}{2}} & & \\ X & X & X & X & X \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \\ & & \underbrace{}_{S_2} & & \end{array}$$

ENO Method:

Given a collection of five points $S = \{f_{k-2}, f_{k-1}, f_k, f_{k+1}, f_{k+2}\}$, we calculate the interpolant $f_{k+\frac{1}{2}}$ as follows. Following the procedure of the last slide, we introduce three stencils $S_j \in S$,

$$\begin{array}{ccccc} & & f_{k+\frac{1}{2}} & & \\ X & X & X & \circ & X & X \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \end{array}$$

Let $f_{k+\frac{1}{2}}^{(j)}$ be the interpolant constructed with the points in stencil S_j :

$$f_{k+\frac{1}{2}}^{(0)} = \frac{1}{8} (3f_{k-2} - 10f_{k-1} + 15f_k), \quad X \ X \ X\star$$

$$f_{k+\frac{1}{2}}^{(1)} = \frac{1}{8} (-f_{k-1} + 6f_k + 3f_{k+1}), \quad X \ X \star X$$

$$f_{k+\frac{1}{2}}^{(2)} = \frac{1}{8} (3f_k + 6f_{k+1} - f_{k+2}), \quad X \star X \ X$$

ENO Method:

Given a collection of five points $S = \{f_{k-2}, f_{k-1}, f_k, f_{k+1}, f_{k+2}\}$, we calculate the interpolant $f_{k+\frac{1}{2}}$ as follows. Following the procedure of the last slide, we introduce three stencils $S_j \in S$,

$$\begin{array}{ccccc} & & f_{k+\frac{1}{2}} & & \\ X & X & \circ & X & X \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \end{array}$$

Let $f_{k+\frac{1}{2}}^{(j)}$ be the interpolant constructed with the points in stencil S_j :

$$f_{k+\frac{1}{2}}^{(0)} = \frac{1}{8} (3f_{k-2} - 10f_{k-1} + 15f_k), \quad X \ X \ X\star$$

$$f_{k+\frac{1}{2}}^{(1)} = \frac{1}{8} (-f_{k-1} + 6f_k + 3f_{k+1}), \quad X \ X \star X$$

$$f_{k+\frac{1}{2}}^{(2)} = \frac{1}{8} (3f_k + 6f_{k+1} - f_{k+2}), \quad X \star X \ X$$

How do we choose one?

ENO Method:

If the underlying f is smooth over the region covered by S_j , then

$$\left| f_{k+\frac{1}{2}}^{(j)} - f \left(x_{k+\frac{1}{2}} \right) \right| = \mathcal{O} (\Delta x^3),$$

so the answer is pick an S_j over which f is smooth. But how do we know that?

ENO Method:

If the underlying f is smooth over the region covered by S_j , then

$$\left| f_{k+\frac{1}{2}}^{(j)} - f \left(x_{k+\frac{1}{2}} \right) \right| = \mathcal{O} (\Delta x^3),$$

so the answer is pick an S_j over which f is smooth. But how do we know that?

In the literature, β_j is often used as a measure of the “sharpness” over the stencil S_j . Multiple approaches exist. Simplest: let $\beta_j \propto |f''|$ as calculated with the points in S_j ,

$$\beta_j = |f_{k-2+j} - 2f_{k-1+j} + f_{k+j}|.$$

ENO Method:

If the underlying f is smooth over the region covered by S_j , then

$$\left| f_{k+\frac{1}{2}}^{(j)} - f\left(x_{k+\frac{1}{2}}\right) \right| = \mathcal{O}(\Delta x^3),$$

so the answer is pick an S_j over which f is smooth. But how do we know that?

In the literature, β_j is often used as a measure of the “sharpness” over the stencil S_j . Multiple approaches exist. Simplest: let $\beta_j \propto |f''|$ as calculated with the points in S_j ,

$$\beta_j = |f_{k-2+j} - 2f_{k-1+j} + f_{k+j}|.$$

$$f_{k+\frac{1}{2}} = f_{k+\frac{1}{2}}^{(j_\star)}, \text{ with } j_\star = \operatorname{argmin}_{j \in [0,2]} \{\beta_j\}.$$

ENO Method:

If the underlying f is smooth over the region covered by S_j , then

$$\left| f_{k+\frac{1}{2}}^{(j)} - f\left(x_{k+\frac{1}{2}}\right) \right| = \mathcal{O}(\Delta x^3),$$

so the answer is pick an S_j over which f is smooth. But how do we know that?

In the literature, β_j is often used as a measure of the “sharpness” over the stencil S_j . Multiple approaches exist. Simplest: let $\beta_j \propto |f''|$ as calculated with the points in S_j ,

$$\beta_j = |f_{k-2+j} - 2f_{k-1+j} + f_{k+j}|.$$

$$f_{k+\frac{1}{2}} = f_{k+\frac{1}{2}}^{(j_\star)}, \text{ with } j_\star = \operatorname{argmin}_{j \in [0,2]} \{\beta_j\}.$$

Let's see it in action!

How can we maximize our use of information?

We can use all the points in the stencil S to construct a fourth-order interpolant!

$$\begin{array}{ccccc} \text{X} & \text{X} & \text{X} & \text{X} & \text{X} \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \\ \hline & & S & & \end{array}$$

$f_{k+\frac{1}{2}}$

How can we maximize our use of information?

We can use all the points in the stencil S to construct a fourth-order interpolant!

$$\begin{array}{ccccc} \text{X} & \text{X} & \text{X} & \circ & \text{X} \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \end{array}$$

$f_{k+\frac{1}{2}}$

There is one fifth-order interpolant of these five points, which we'll denote $f_{k+\frac{1}{2}}^{(S)}$. We can write it as a weighted sum of our third-order interpolants,

$$f_{k+\frac{1}{2}}^{(S)} = \gamma_0 f_{k+\frac{1}{2}}^{(0)} + \gamma_1 f_{k+\frac{1}{2}}^{(1)} + \gamma_2 f_{k+\frac{1}{2}}^{(2)} = f\left(x_{k+\frac{1}{2}}\right) + \mathcal{O}(\Delta x^5),$$

How can we maximize our use of information?

We can use all the points in the stencil S to construct a fourth-order interpolant!

$$\begin{array}{ccccc} \text{X} & \text{X} & \text{X} & \circ & \text{X} \\ f_{k-2} & f_{k-1} & f_k & f_{k+1} & f_{k+2} \end{array}$$

$f_{k+\frac{1}{2}}$

There is one fifth-order interpolant of these five points, which we'll denote $f_{k+\frac{1}{2}}^{(S)}$. We can write it as a weighted sum of our third-order interpolants,

$$\boxed{f_{k+\frac{1}{2}}^{(S)} = \gamma_0 f_{k+\frac{1}{2}}^{(0)} + \gamma_1 f_{k+\frac{1}{2}}^{(1)} + \gamma_2 f_{k+\frac{1}{2}}^{(2)}} = f\left(x_{k+\frac{1}{2}}\right) + \mathcal{O}(\Delta x^5),$$

and in general any weighted average $f_{k+\frac{1}{2}}^{(w)}$ such that

$$\boxed{f_{k+\frac{1}{2}}^{(w)} = w_0 f_{k+\frac{1}{2}}^{(0)} + w_1 f_{k+\frac{1}{2}}^{(1)} + w_2 f_{k+\frac{1}{2}}^{(2)}} = f\left(x_{k+\frac{1}{2}}\right) + \mathcal{O}(\Delta x^3),$$

is another third-order interpolant.

WENO Method:

What do we want from our weighting scheme w_i ? What does $w_i \approx \gamma_i$ imply? What does $w_i \approx 0$ imply?

WENO Method:

What do we want from our weighting scheme w_i ? What does $w_i \approx \gamma_i$ imply? What does $w_i \approx 0$ imply?

Given the five-point stencil S , compute the three third-order approximations and sharpness measurements β_j . Introduce the weighting scheme

$$w_i = \frac{W_i}{W_0 + W_1 + W_2}, \quad W_i = \frac{\gamma_i}{(\varepsilon + \beta_i)^2}, \quad \varepsilon = 10^{-6}$$

WENO Method:

What do we want from our weighting scheme w_i ? What does $w_i \approx \gamma_i$ imply? What does $w_i \approx 0$ imply?

Given the five-point stencil S , compute the three third-order approximations and sharpness measurements β_j . Introduce the weighting scheme

$$w_i = \frac{W_i}{W_0 + W_1 + W_2}, \quad W_i = \frac{\gamma_i}{(\varepsilon + \beta_i)^2}, \quad \varepsilon = 10^{-6}$$

Then we let our interpolant be

$$f_{k+\frac{1}{2}} = w_0 f_{k+\frac{1}{2}}^{(0)} + w_1 f_{k+\frac{1}{2}}^{(1)} + w_2 f_{k+\frac{1}{2}}^{(2)},$$

which is fifth-order where f is smooth and third-order near shocks.

The Inviscid Burgers Equations, Non-Linearity, and You.

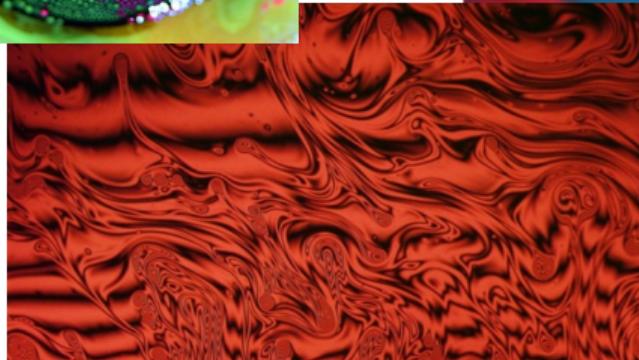
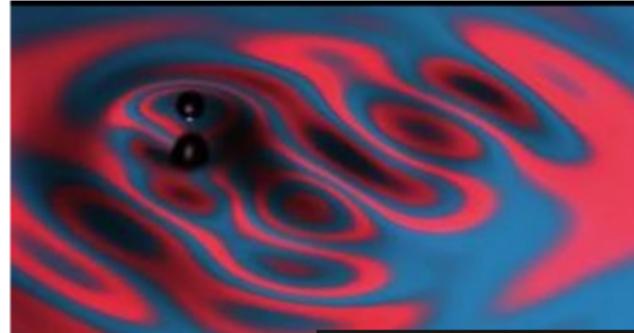
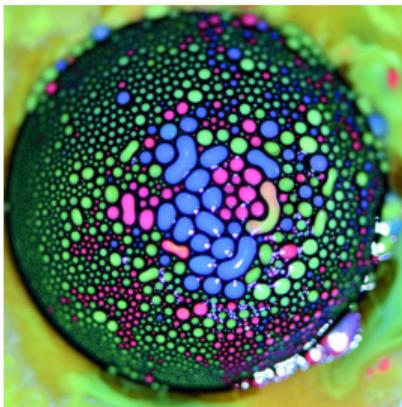
In general, we have assumed a constant velocity c so far. ENO and WENO methods have been able to capture discontinuities in functions whose shapes are not evolving; what happens when we make things more complicated?

Let the velocity be given by $v(x, f) = f/2$, so

$$\frac{\partial f}{\partial t} = -f \frac{\partial f}{\partial x} = -\frac{\partial q}{\partial x}, \quad q = \frac{1}{2}f^2.$$

Let's take a look.

Why do we care? This $f\partial_x f$ term is essentially a 1D version of the $\mathbf{u} \cdot \nabla \mathbf{u}$ advective term in the Navier-Stokes equations.



Another application with shocks: traffic!

Let $f \in [0, 1]$ by the density of cars. A common (dimensionless) approximation to the velocity is

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} (vf), \quad v = 1 - f,$$

i.e. you drive fastest when the road is most open, and you come to a complete stop when everyone is bumper-to-bumper (e.g. at a red light.)

Let's see this one in action!

Group activity write-up:

1. Adapt the code in the notebook to produce a WENO method which upwinds in both directions and use to simulate 1) traffic approaching a red light; and 2) traffic coming out of a green light. Each of these will include a jump condition in the initial condition. Choose the left/right boundary conditions $f = f_l$ and $f = f_r$ on the sides of your domain and explain your choices. How is the behavior different? Is there a shock in both cases? One case? Neither?
2. (Optional) Use the WENO method to simulate 1) a smooth function and 2) a discontinuous function moving to the right with constant velocity. Make a log-log plot showing the convergence of the error at time $T = 1$ as you refine the grid. Do you recover the higher convergence in the smooth case as advertised?

Extra Resources:

- ▶ [WENO methods description](#): the basis of the treatment here
- ▶ [Astrophysical Fluid Dynamics lecture notes](#): excellent treatment of shocks, Rankine-Hugoniot relations, and compressible fluid dynamics more generally.

Thanks a lot, all! Questions?