Numerical differentiation: some lessons from blast calculations

Jeffrey Connors

University of Connecticut

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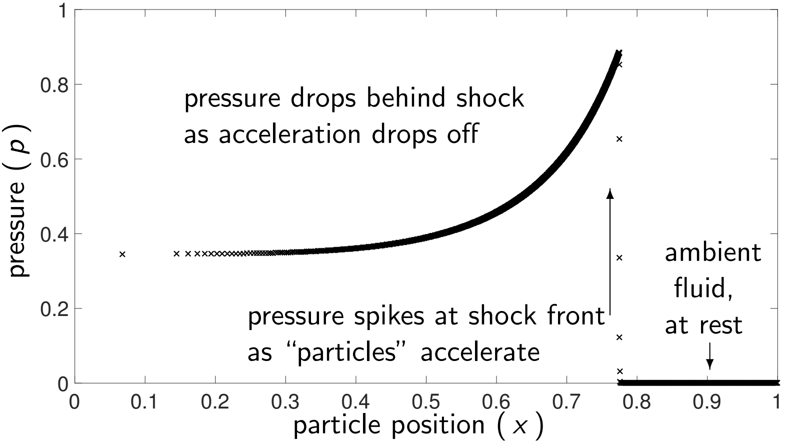
A motivating example: shock (blast wave) calculation. This pressure wave moves left to right over time.



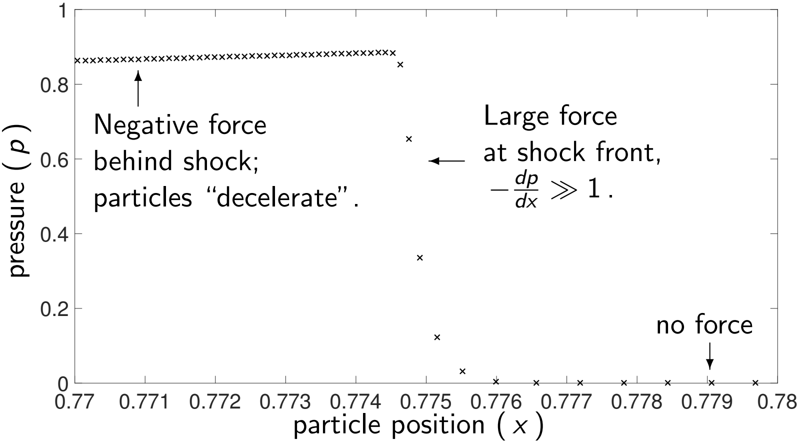
Force on a particle moving with the air is determined by the local pressure change

Force is mass times acceleration.

$$\rho a = -\frac{dp}{dx} \quad \text{(from "Euler equations")}$$

- ρ is mass density.
- a is acceleration.
- p is pressure.
- Other variables (energy, velocity) are involved, but we will focus on just $\frac{dp}{dx}$.

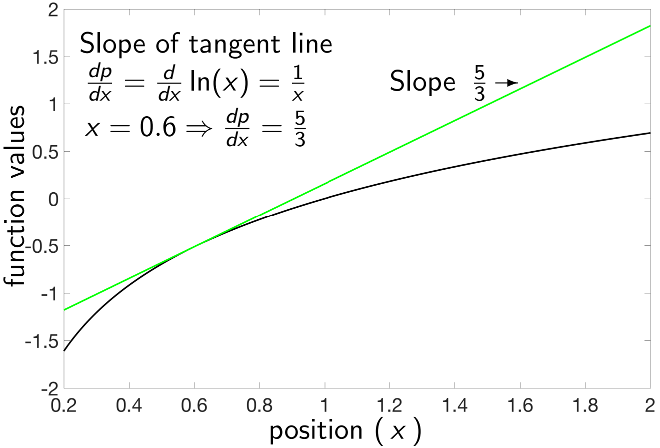
Look at the forces on these particles by studying the pressure derivative (think "slope")...



The fluid states are only computed at specific points (particle locations).

Derivatives do not exist for discrete data, so how does the computer calculate the forces $-\frac{dp}{dx}$?

Two important interpretations of derivatives: algebraic and geometric. Here, $p(x) = \ln(x)$ (black).



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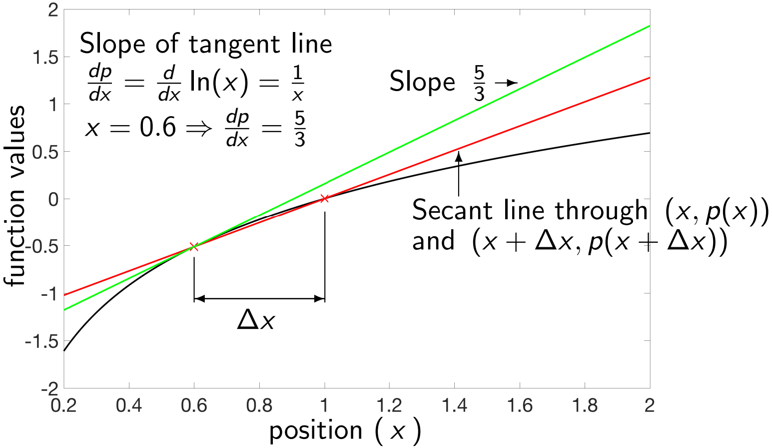

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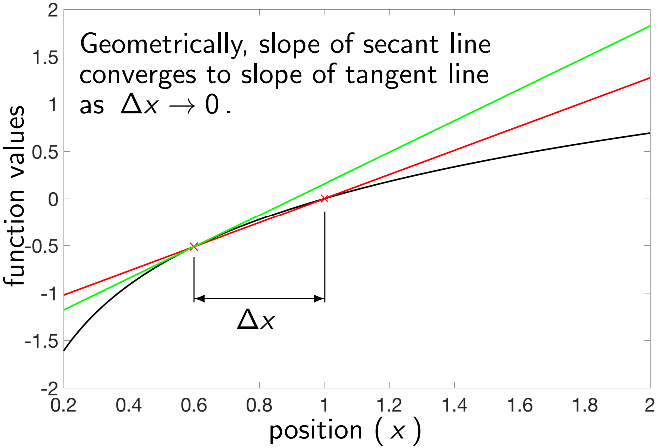

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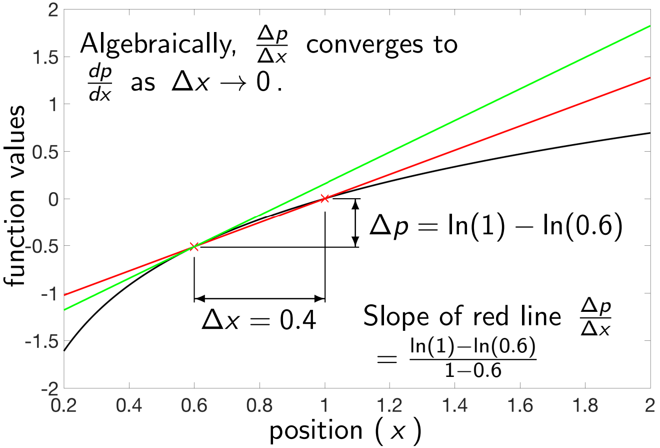

"Numerical differentiation" refers to approximating a derivative using some local function values.

Let $\Delta x > 0$ be given.

- Forward approximation:

$$\frac{d}{dx}p(x) \approx \frac{p(x+\Delta x) - p(x)}{\Delta x}.$$

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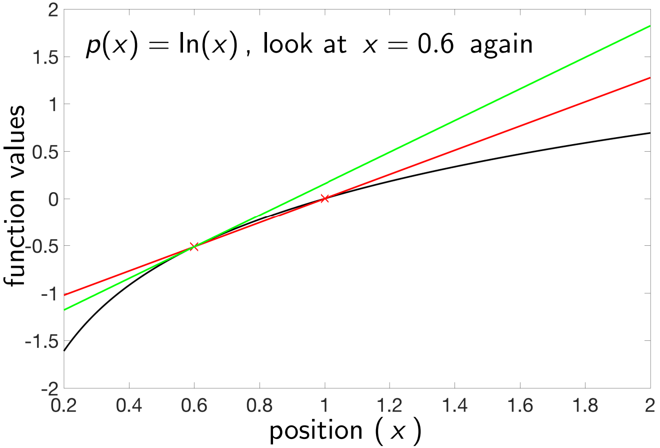
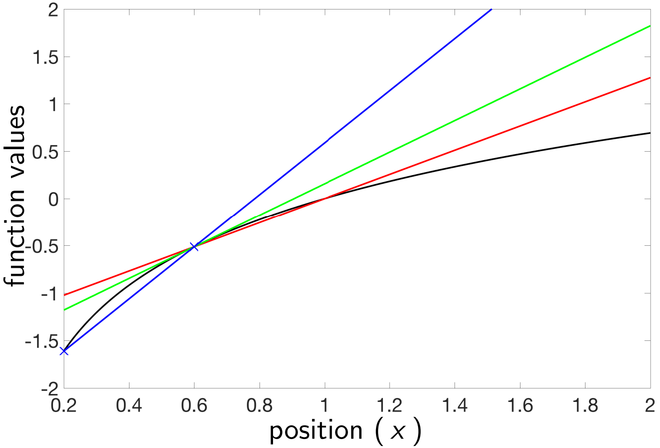
- Centered approximation:

$$\frac{d}{dx}p(x) \approx \frac{p(x+\Delta x) - p(x-\Delta x)}{2\Delta x}.$$

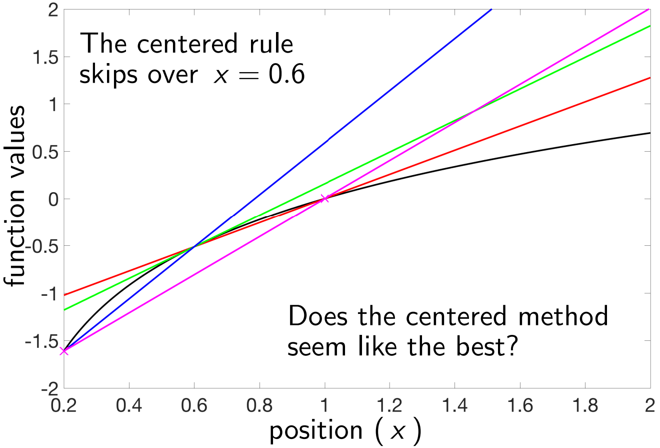
Forward approximation means calculates the slope of the red line, as before.



Backward approximation means calculating the slope of the blue line.



A centered approximation means calculating the slope of the magenta line.



Note that the centered slope is the average of the forward and backward slopes:

$$
\begin{aligned}
&\frac{1}{2}\left(\frac{p(x+\Delta x)-p(x)}{\Delta x}\right)+\frac{1}{2}\left(\frac{p(x)-p(x-\Delta x)}{\Delta x}\right)\\
&=\frac{1}{2}\frac{p(x+\Delta x)-p(x)+p(x)-p(x-\Delta x)}{\Delta x}\\
&=\frac{p(x+\Delta x)-p(x-\Delta x)}{2\Delta x}
\end{aligned}
$$

The centered method is usually the most accurate, because it averages the errors.

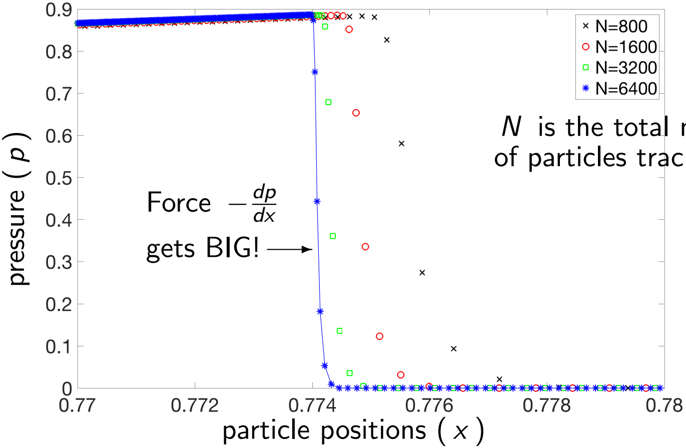
$$
\begin{aligned}
&\frac{p(x+\Delta x)-p(x-\Delta x)}{2\Delta x}-\frac{dp}{dx}\\
&=\frac{1}{2}\left\{\left(\frac{p(x+\Delta x)-p(x)}{\Delta x}\right)-\frac{dp}{dx}\right\}\\
&+\frac{1}{2}\left\{\left(\frac{p(x)-p(x-\Delta x)}{\Delta x}\right)-\frac{dp}{dx}\right\}
\end{aligned}
$$

In fact, look at errors in $\frac{dp}{dx}$ at $x = 0.6$ using these three methods (with $p(x) = \ln(x)$ again)...

The centered method benefits from error cancellation!

Δx	forward	backward	centered
0.4	-0.3896	1.0799	0.3451
0.04	-0.0532	0.0582	0.0025
0.004	-0.0055	0.0056	2.5×10^{-5}
0.0004	-0.0006	0.0006	2.5×10^{-7}

As more particles are used in our shock calculation, the resolution of the front improves.



N is the total number of particles tracked.

The standard centered approximation for $-\frac{dp}{dx}$ is our shock calculation FAILS!

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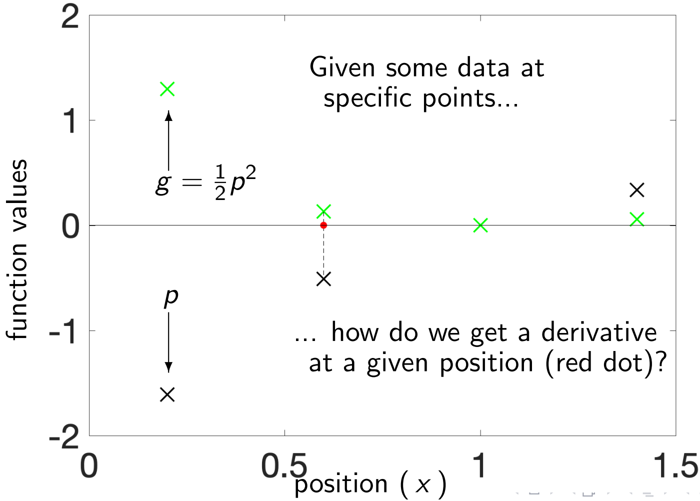
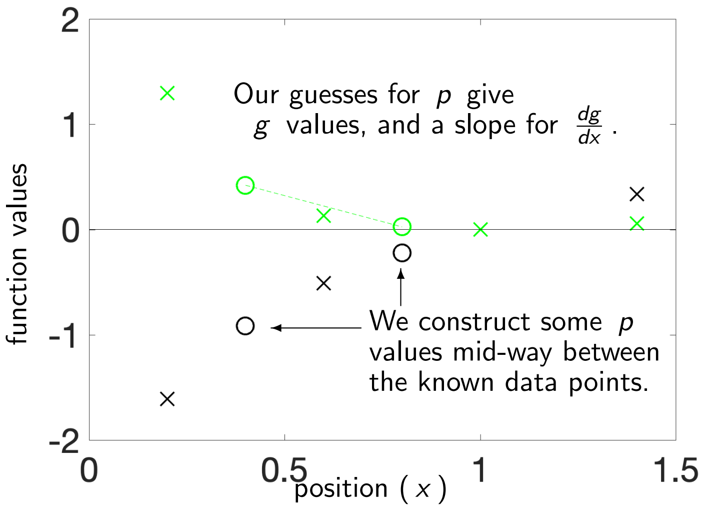
- In other words, set $g(x) = \frac{1}{2}p(x)^2$ and it reduces to

$$-\frac{d}{dx}g(x).$$

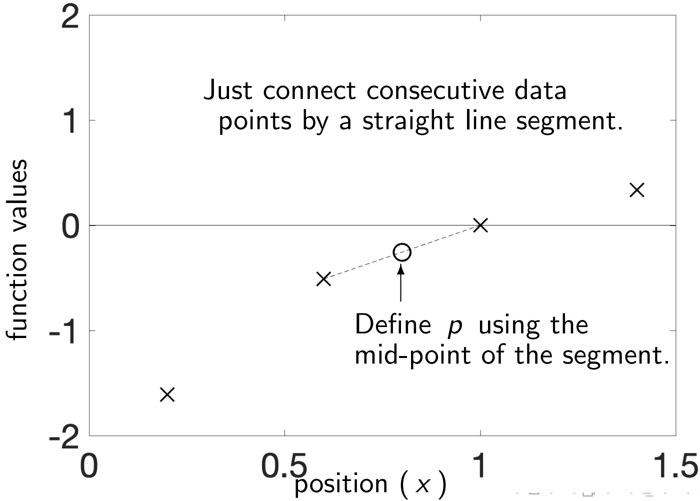
The first step is to generalize our thinking about how to compute the derivative.



Use a centered approximation from fictitious points nearby.

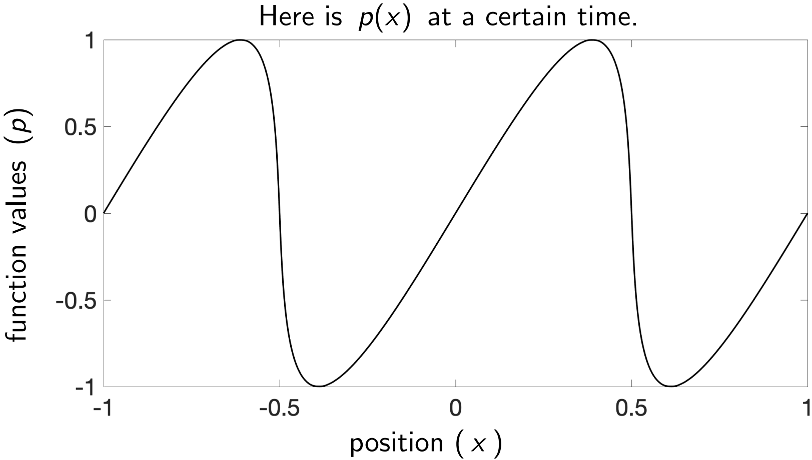


The problem reduces to constructing p at midpoints. Again, a seemingly intuitive approach may fail.



This approach fails...

A lesson: numerics must generally be tailored to the solution behavior. We apply the idea of “upwinding”.



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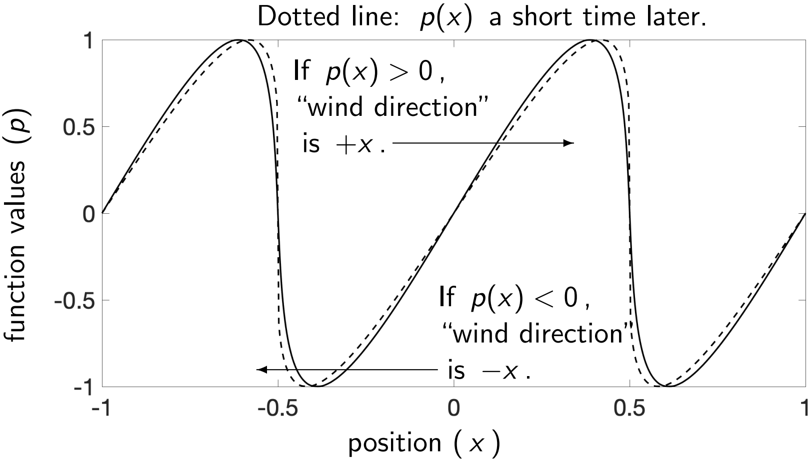

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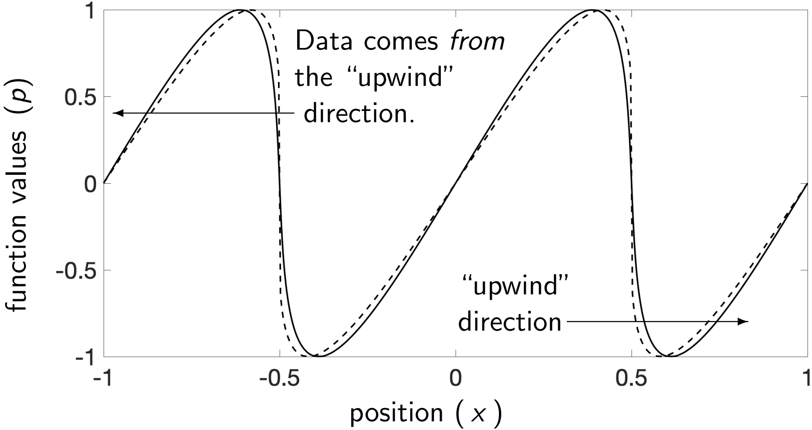
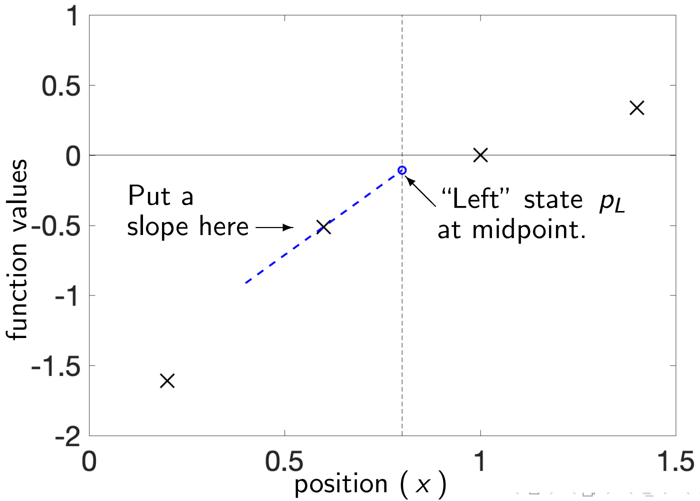


Upwinding: construct "left" and "right" states, then choose the result from the upwind direction.



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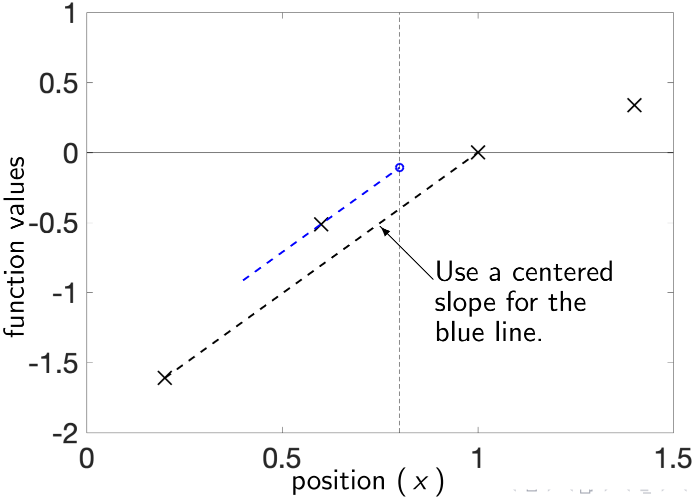

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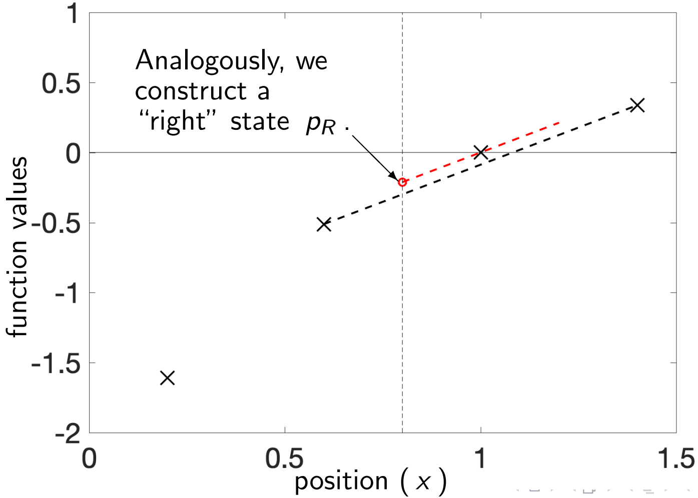

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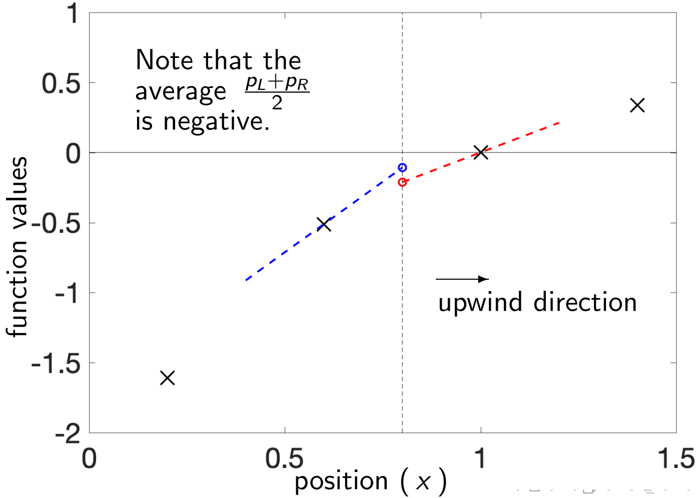
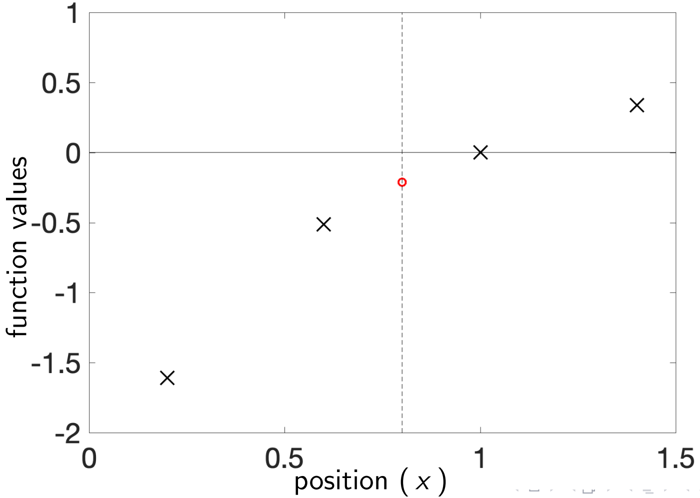
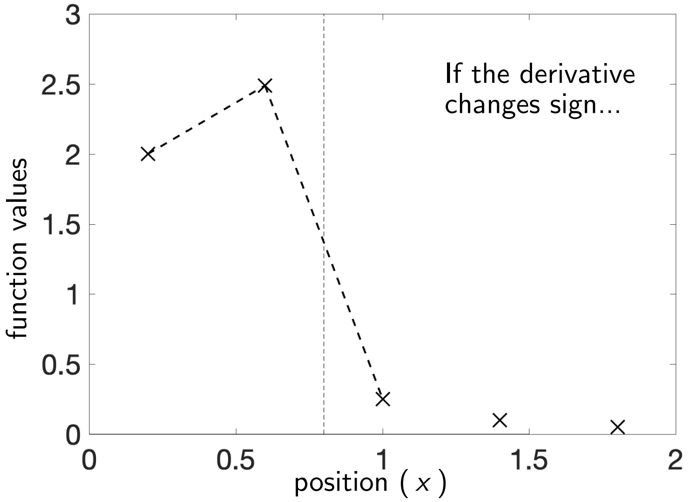


The “right” state is used in this example since it comes from the upwind direction.



This approach works better...

We use “slope limiting” to get better accuracy at a front.



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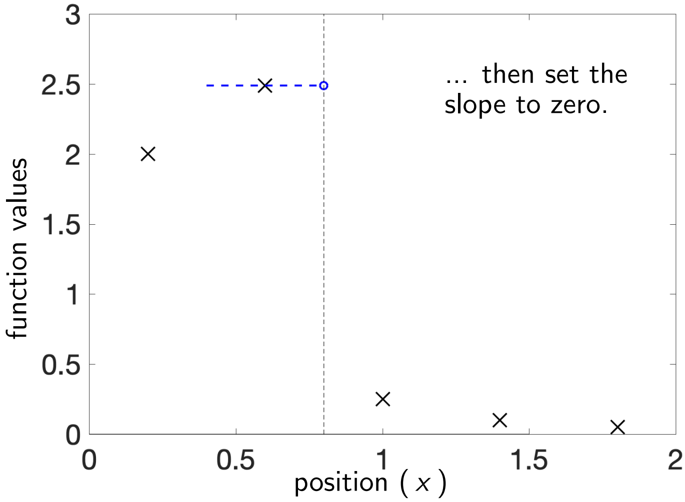
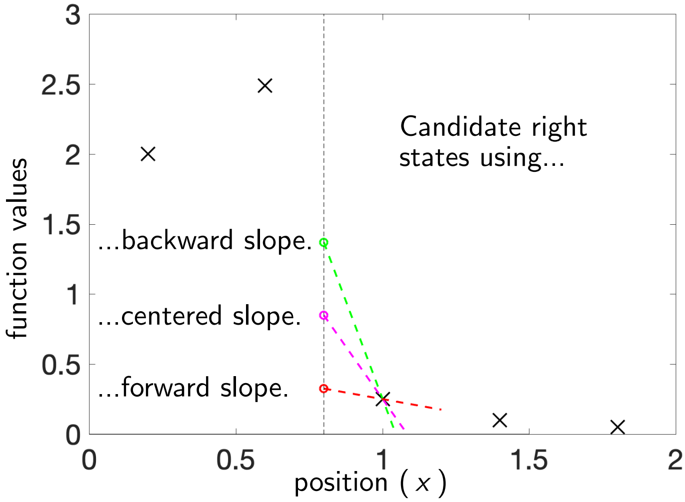
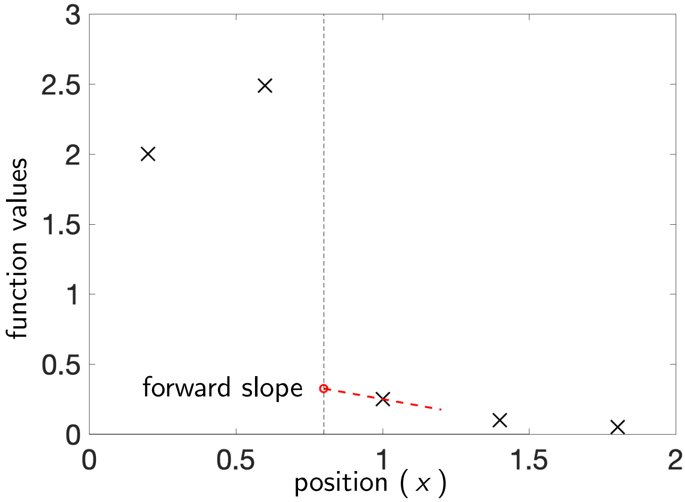


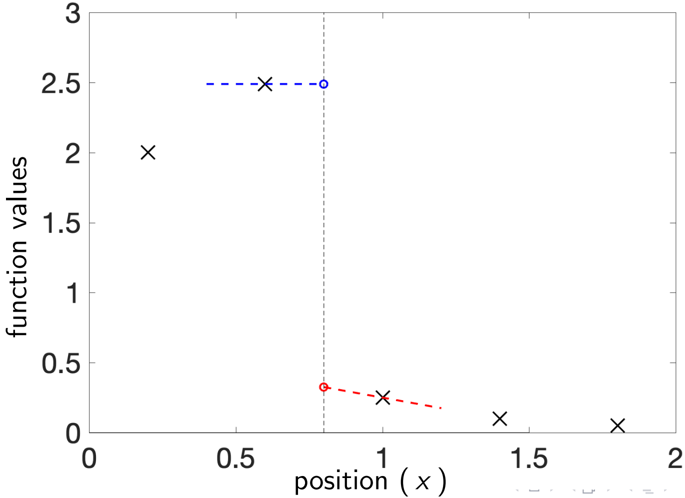
If the slope does not change sign, the limiting is less severe.



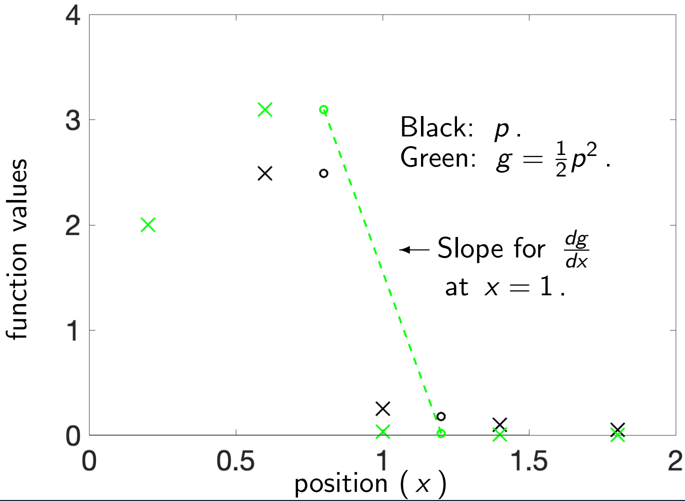
We "limit" by using the slope with the smallest size.



Here, the "left" state (blue) would be chosen, being the upwind value.



Summary: use slope-limiting and upwinding to construct p at midpoint. Use a centered slope for $\frac{dg}{dx}$.



This approach yields a reasonable result...

THANK YOU!