Controlling spurious oscillations in high-order methods through deep neural networks

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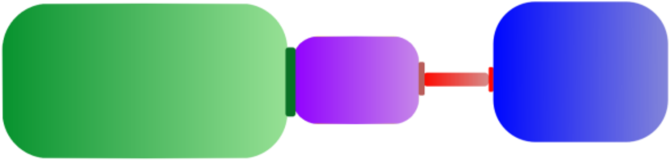
Motivation

Robust numerical machinery developed over the past several decades



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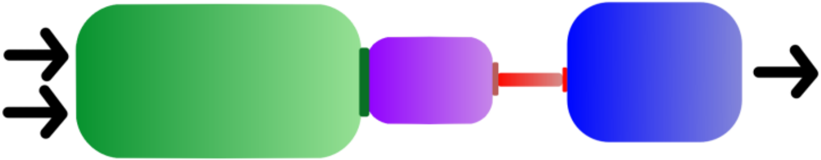
Gives satisfactory results, but ...



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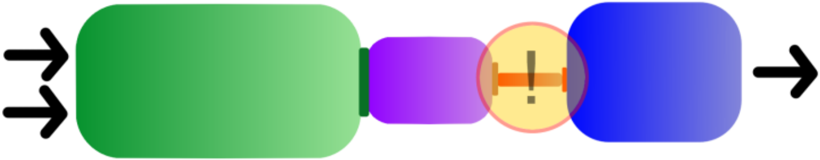
Bottlenecks exist – computationally expensive subcomponents, problem dependent parameters, etc



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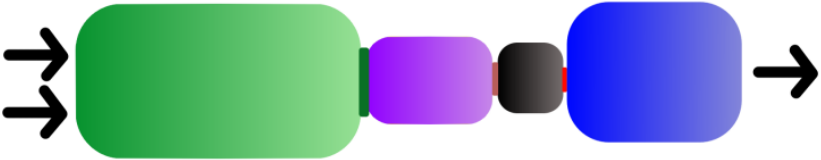
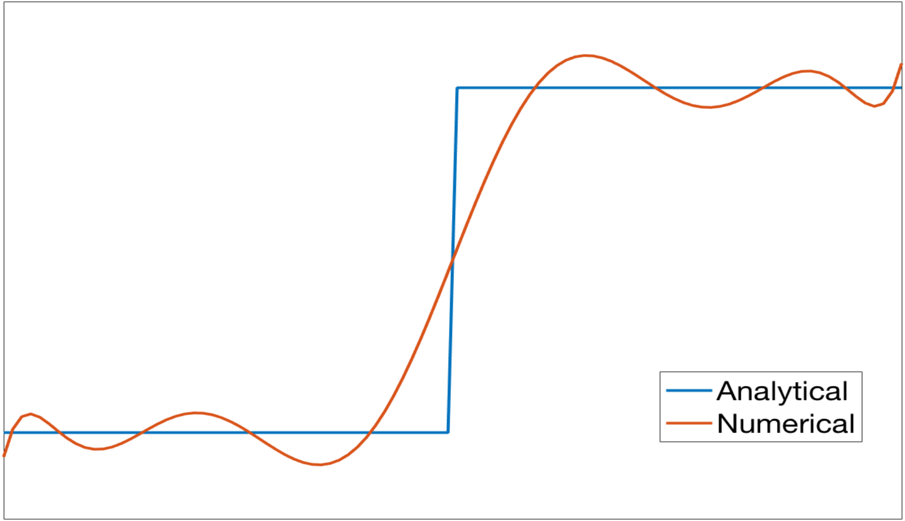


Startegy: Replace (only) the problematic part with Deep Learning black box

The menace of Gibbs oscillations



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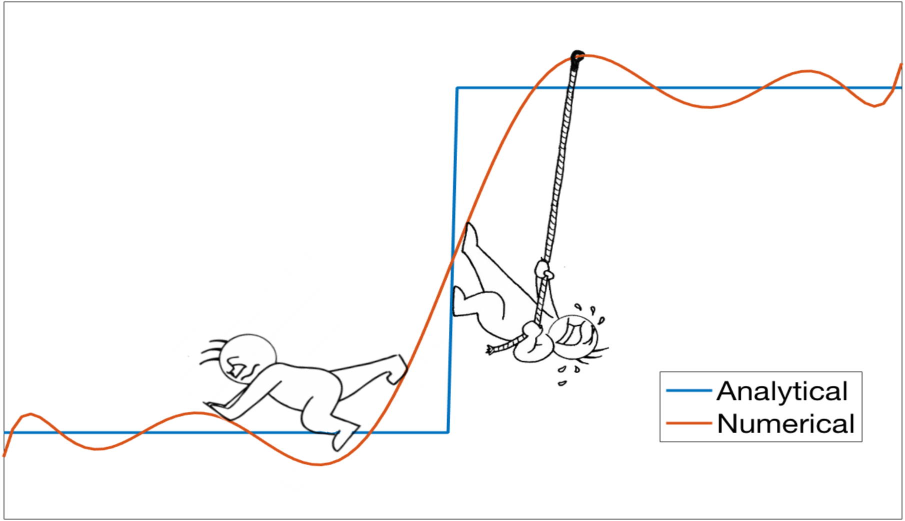

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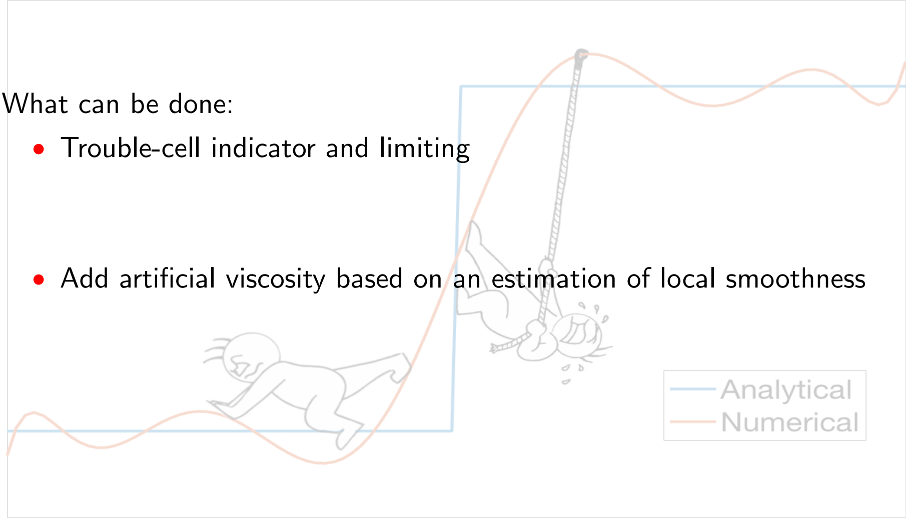
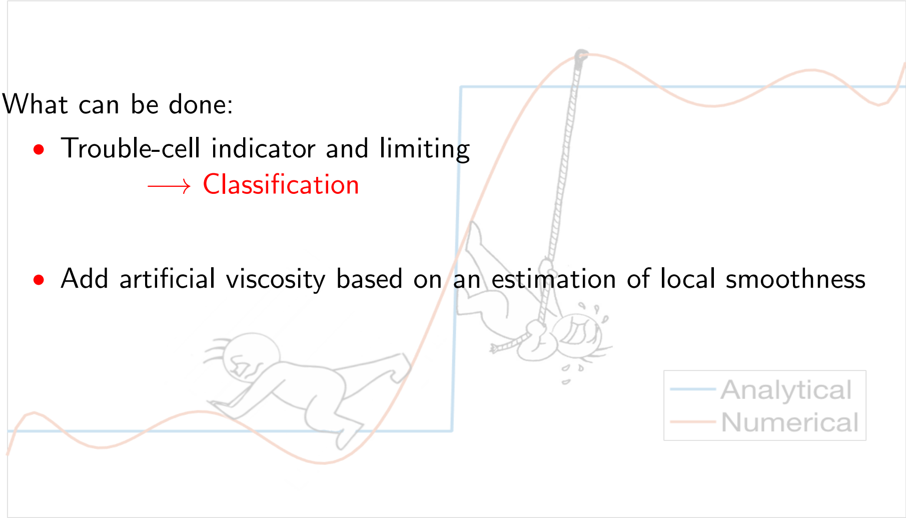


What can be done:

- Trouble-cell indicator and limiting

- Add artificial viscosity based on an estimation of local smoothness

The menace of Gibbs oscillations



What can be done:

- Trouble-cell indicator and limiting
  $\longrightarrow$ Classification

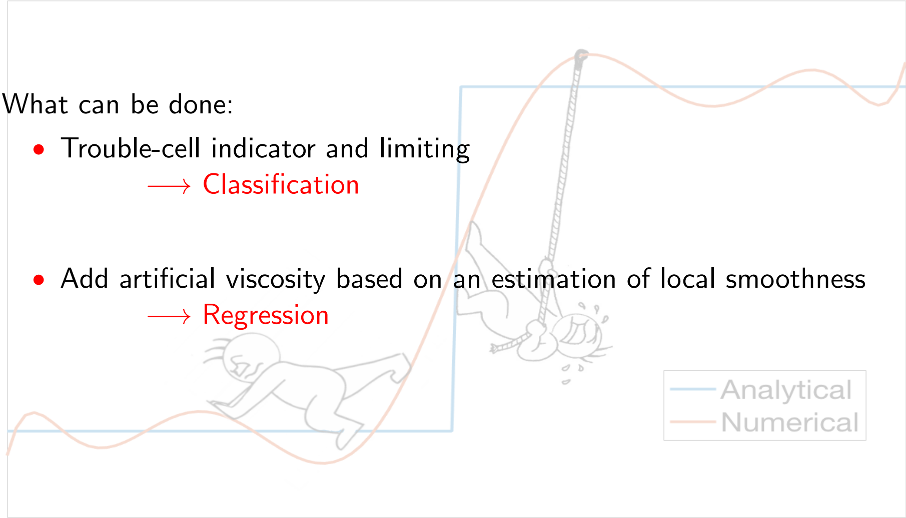
- Add artificial viscosity based on an estimation of local smoothness

The menace of Gibbs oscillations

What can be done:

- Trouble-cell indicator and limiting
  $\longrightarrow$ Classification

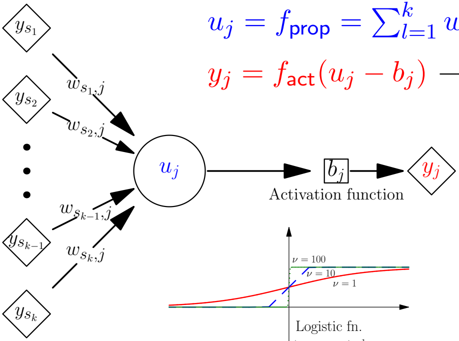
- Add artificial viscosity based on an estimation of local smoothness
  $\longrightarrow$ Regression

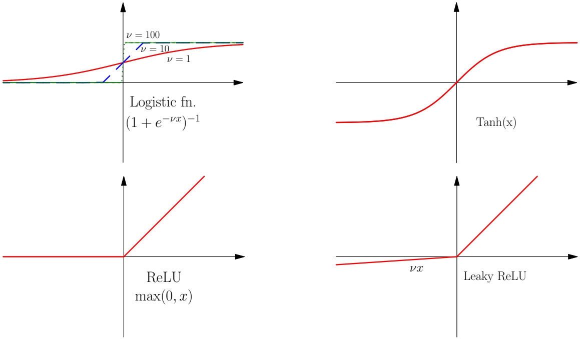


Neural networks

$u_j = f_{\text{prop}} = \sum_{l=1}^{k} w_{s_l,j} y_{s_l} \longrightarrow$ linear

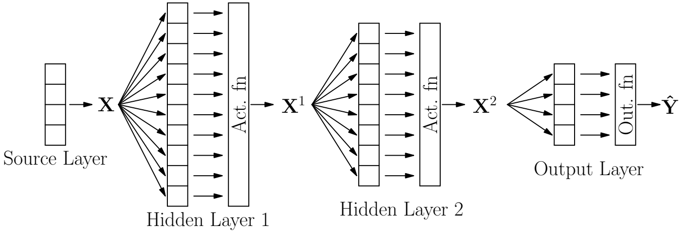
$y_j = f_{\text{act}}(u_j - b_j) \longrightarrow$ introduces non-linearity





Neural networks

Several layers of neurons



Feed forward network - **multilayer perceptron (MLP)**

Weights/biases computed using labeled data $(\mathbf{X}, \mathbf{Y})$

$\longrightarrow$ supervised learning

Choose: architecture, training/validation/test data sets, loss function ...

Part I: ANNs as troubled-cell indicators

Conservation laws

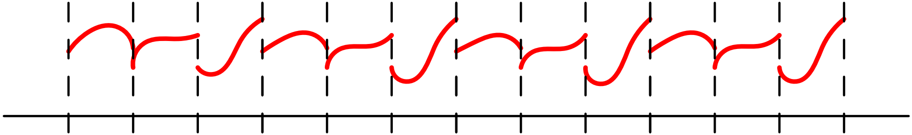
Consider the system of conservation laws

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = 0$$
$$\mathbf{u}(x,0) = \mathbf{u}_0(x)$$

Non-linearity $\Longrightarrow$ Discontinuities in finite time

Solve using DG methods

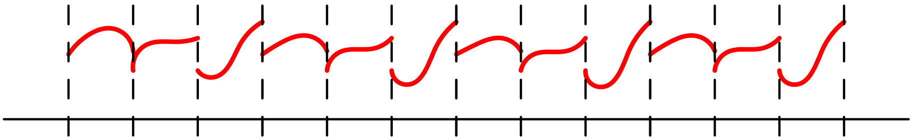
$\longrightarrow$ solution approximated locally using polynomials



Limiting

Strategy for limiting

1. Identify troubled-cells



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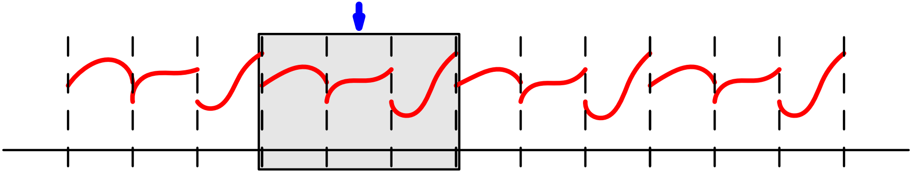

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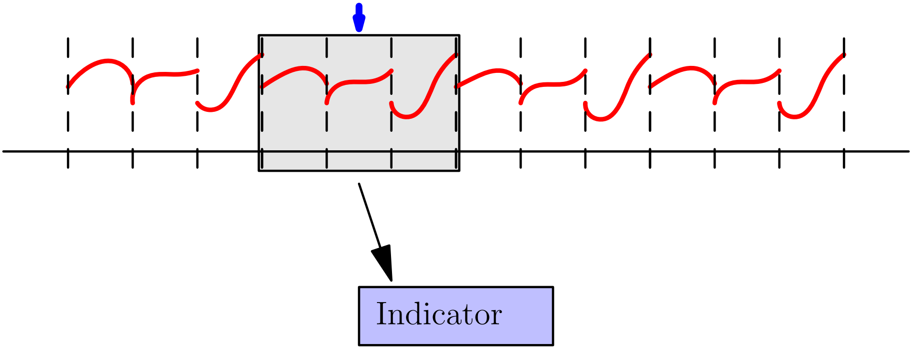

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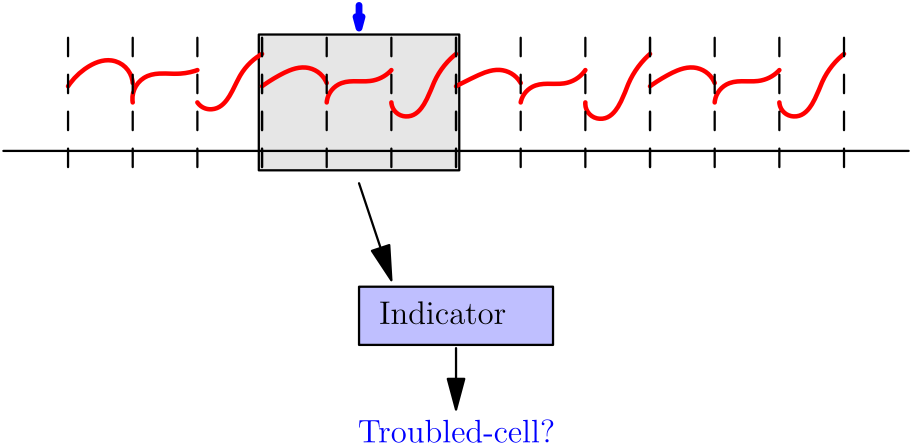

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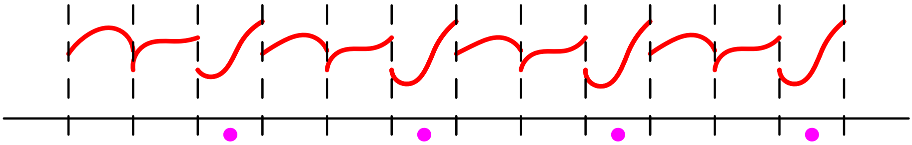
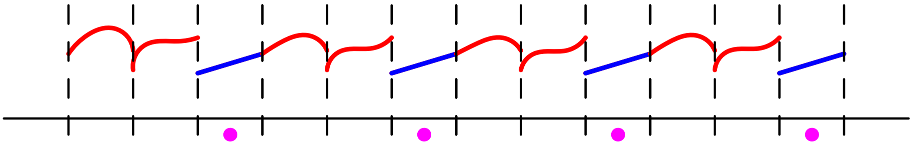


Limiting

Strategy for limiting

1. Identify troubled-cells
2. Limit solution in flagged cells



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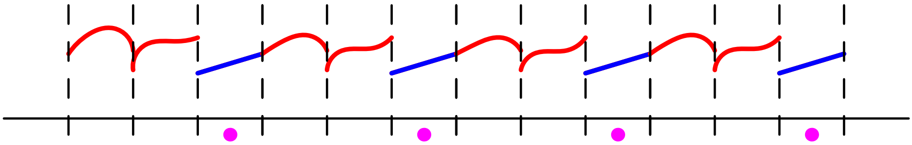

Some issues:

- Problem-dependent parameters
- If insufficient cells marked $\longrightarrow$ re-appearance of Gibbs oscillations
- If excessive cells marked
  - Unnecessary computational cost
  - Loss of accuracy for strong limiters

Available troubled-cell indicators

- Minmod-based TVB limiter (Cockburn and Shu; Math. Comp. '98)
- Moment limiter (Biswas et al.; Appl. Numer. Math. '94)
- Modified moment limiter (Burbeau; JCP '01)
- Monotonicity preserving limiter (Suresh and Huynh; JCP '97)
- Modified MP limiter (Rider and Margolin; JCP '01)
- KXRCF indicator (Krivodonova et al.; App. Numer. Math. '04)
- Polynomial degree based limiter (Fu and Shu; JCP '17)
- Outlier detection using Tukey's boxplot method (Vuik and Ryan; J. Sci. Comp. '16)
- ...

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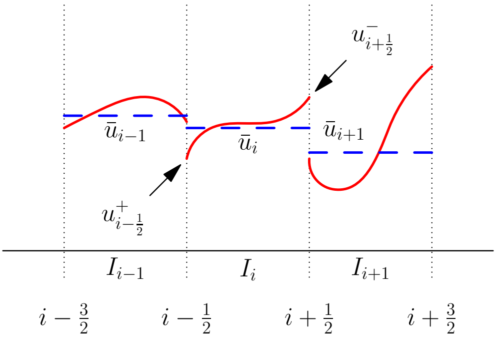
TVB Indicator: Search for the elusive M



- For each cell I_i, get $[\overline{u}_{i-1},\ \overline{u}_i,\ \overline{u}_{i+1},\ u^+_{i-\frac{1}{2}},\ u^-_{i+\frac{1}{2}}]$.
- Evaluate divided difference.
- Choose $M \longrightarrow$ problem dependent!!

Objective: Find a troubled-cell indicator which is:

- independent of problem-dependent parameters
- does not flag smooth extrema
- relatively inexpensive

An MLP-based indicator

- Input $\mathbf{X} = [\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}] \in \mathbb{R}^5$
- 5 Hidden Layers with width 256, 128, 64, 32, 16
- Leaky ReLU activation function with $\nu = 10^{-3}$
- Softmax output function

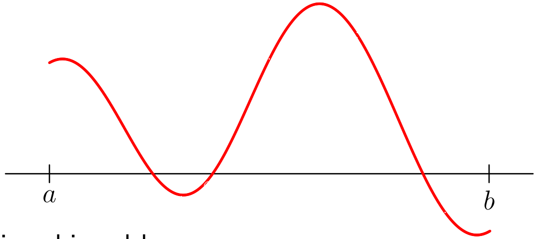
$$\hat{Y}^{(k)} = \frac{e^{\hat{Y}^{(k)}}}{\sum_j e^{\hat{Y}^{(j)}}} \quad \in \quad [0,1] \quad \longrightarrow \quad \text{probabilities/classification}$$

  Output $\hat{Y} = [\hat{Y}^{(0)}, \hat{Y}^{(1)}] \in [0,1]^2$

- Cost functional: cross-entropy

$$C = -\sum_{i=1}^{N} \left[Y_i^{(0)} \log\left(\hat{Y}_i^{(0)}\right) + Y_i^{(1)} \log\left(\hat{Y}_i^{(1)}\right) \right]$$

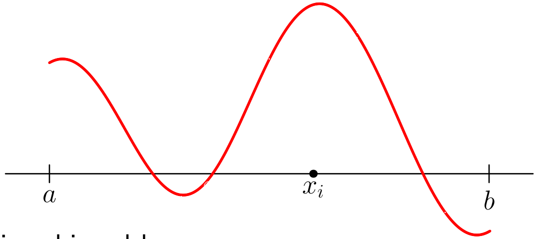
Generating the training data



Data sampling is achieved by

- Choose a known function $u(x)$

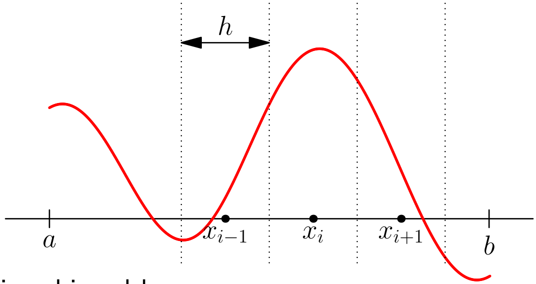
Generating the training data



Data sampling is achieved by

- Choose a known function $u(x)$
- Pick a point x_i

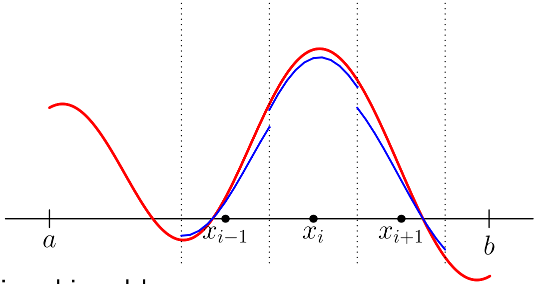
Generating the training data



Data sampling is achieved by

- Choose a known function $u(x)$
- Pick a point x_i
- Pick a cell size h and make stencil

Generating the training data



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- Choose a known function $u(x)$
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- Pick a degree r and approximate

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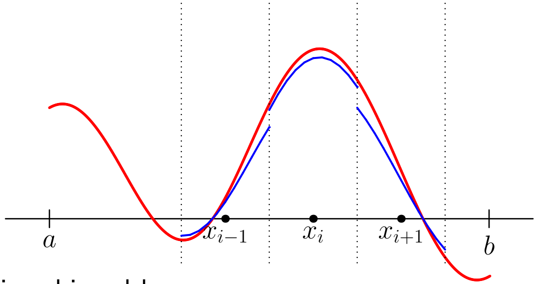

Data sampling is achieved by

- Choose a known function $u(x)$
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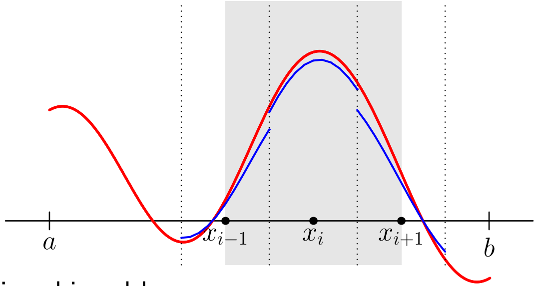
- Pick a degree r and approximate
- Extract needed data $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$

Generating the training data



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- Extract needed data $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$
- Flag cell if discontinuity in $[x_{i-\frac{1}{2}} - h/2, x_{i+\frac{1}{2}} + h/2]$

Generating the training data

$\mathbf{u(x)}$	**Domain**	**Additional parameters varied**	**Good cells**	**Troubled cells**
$\sin(4\pi x)$	$[0,1]$	–	4470	0
ax	$[-1,1]$	$a \in \mathbb{R}$	10000	0
$a\|x\|$	$[-1,1]$	$a \in \mathbb{R}$	800	3200
$ul.(x < x_0) + ur.(x > x_0)$ (only troubled-cells selected)	$[-1,1]$	$(u_l, u_r) \in [-1,1]^2$ $x_0 \in [-0.76, 0.76]$	0	19800
			15270	**23000**

(a) Functions used to create $\mathbb{T}$.

$\mathbf{u(x)}$	**Domain**	**Additional parameters varied**	**Good cells**	**Troubled cells**
$\sum_{p=1}^{5} \sin(p\pi x)$	$[0,2]$	–	3740	0
$\sin(2\pi x)\cos(3\pi x)\sin(4\pi x)$	$[0,2]$	–	3740	0
$\sin(\pi x) + e^x$	$[-1,1]$	–	3740	0
$ul.(x < x_0) + ur.(x > x_0)$ (only troubled-cells selected)	$[-1,1]$	$(u_l, u_r) \in [-20,20]^2$ $x_0 \in [-0.76, 0.76]$	0	13060
			11220	**13060**

(b) Functions used to create $\mathbb{V}$.

Parameters varied:

- Mesh size h
- Approximating polynomial degree r

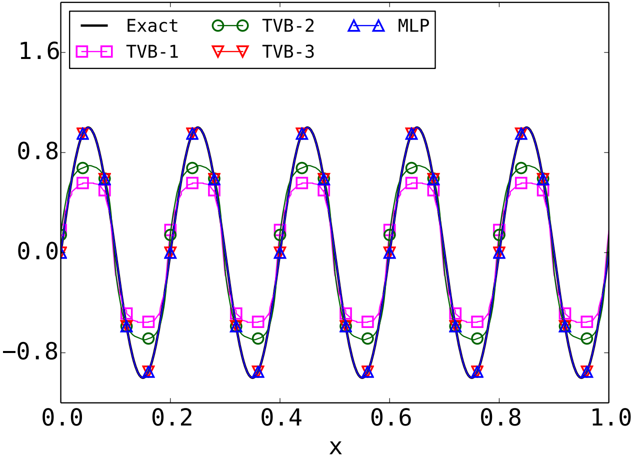
An artificial neural network as a troubled-cell indicator by D. Ray and J. S. Hesthaven; J. Comp. Phy., vol. 367(15), 2018.

So how well does the trained MLP really work?

Linear advection: $u_t + u_x = 0$

$$u_0(x) = \sin(10\pi x), \quad x \in [0,1], \quad T_f = 1, \quad N = 100, \quad r = 4$$

TVB-1 $\longrightarrow$ M=10
TVB-2 $\longrightarrow$ M=100
TVB-3 $\longrightarrow$ M=1000



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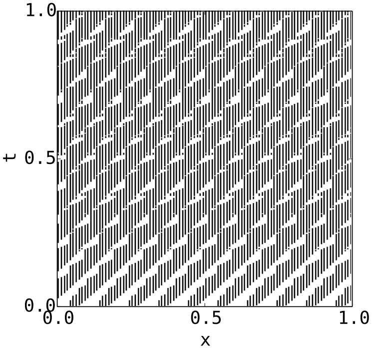
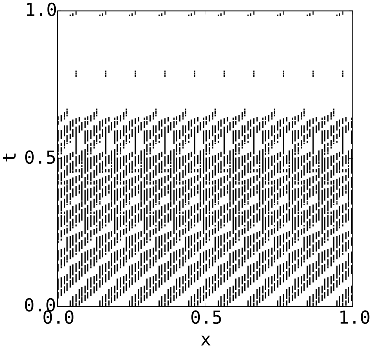


TVB-1

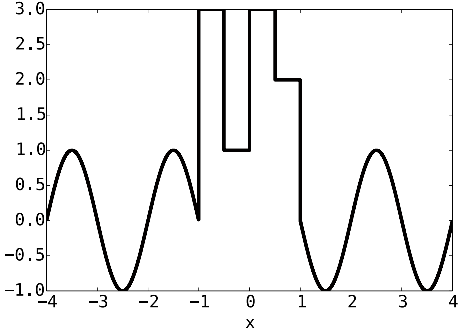


TVB-2

MLP and TVB-3 do not flag any cell

Burgers equation: $u_t + (u^2/2)_x = 0$

$$x \in [-4, 4], \quad T_f = 0.4, \quad N = 200, \quad r = 4$$



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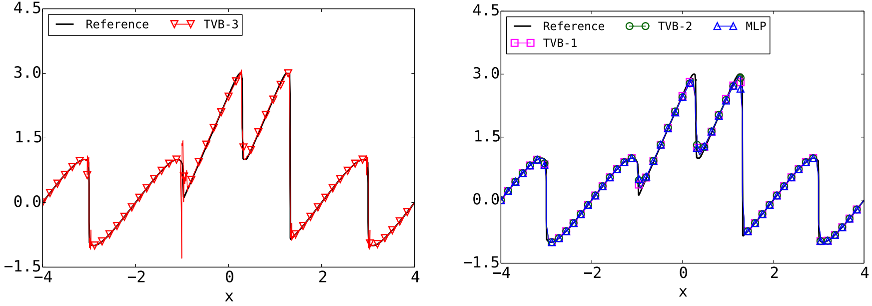

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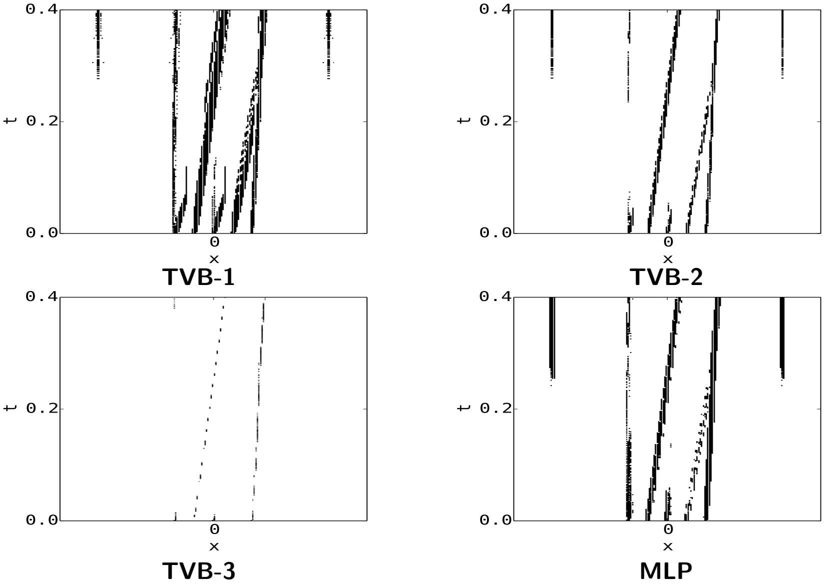
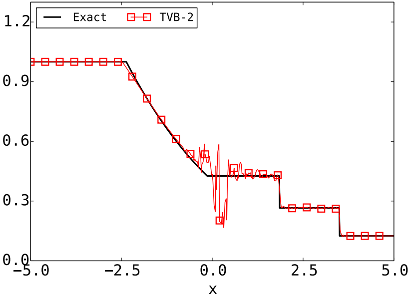
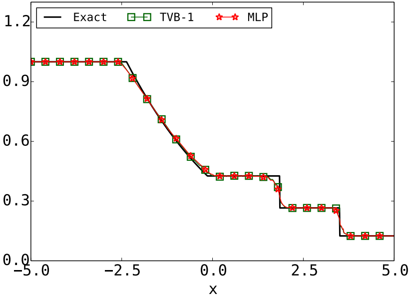


Euler equations: Sod shock tube

$$(\rho,\ u,\ p) = \begin{cases} (1,\ 0,\ 1) & \text{if } x < 0 \\ (0.125,\ 0,\ 0.1) & \text{if } x > 0 \end{cases}, \qquad x \in [-1, 1]$$

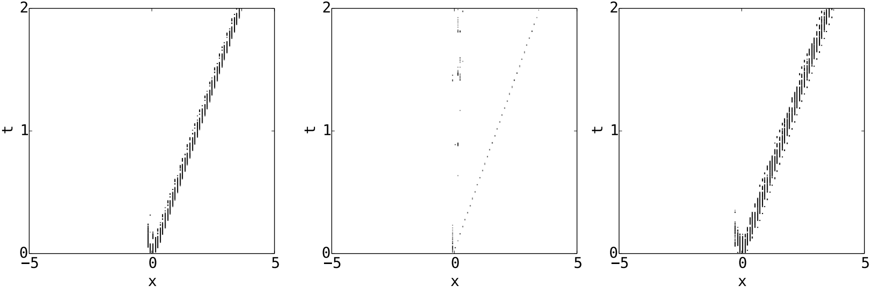
$$T_f = 2, \quad N = 100, \quad r = 4$$





Loss of positivity with TVB-3

Euler equations: Sod shock tube

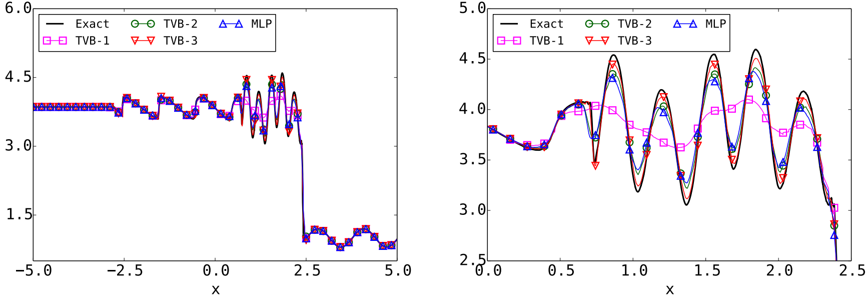


TVB-1 **TVB-2** **MLP**

Euler equations: Shock-entropy problem

$$(\rho,\ u,\ p) = \begin{cases} (3.857143,\ 2.629369,\ 10.33333) & \text{if } x < -4 \\ (1 + 0.2\sin(5x),\ 0,\ 1) & \text{if } x > -4 \end{cases}$$

$$T_f = 1.8, \quad N = 256, \quad r = 4$$



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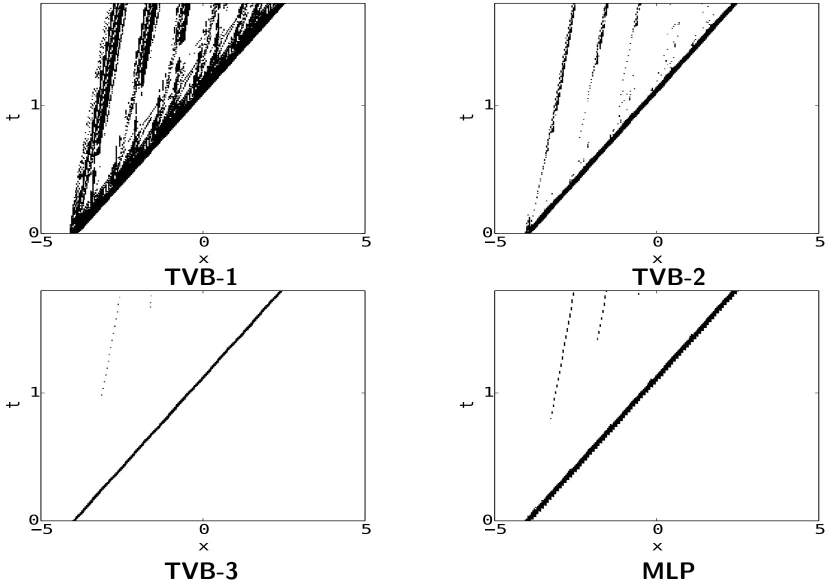
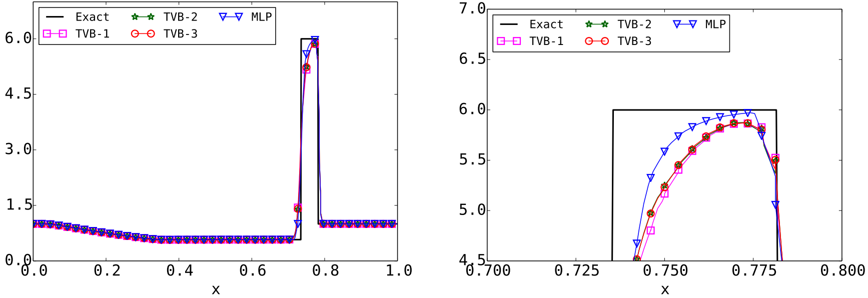


Euler equations: Left half of blast-wave

$$(\rho,\ u,\ p) = \begin{cases} (1,\ 0,\ 1000) & \text{if } x < 0.5 \\ (1,\ 0,\ 0.01) & \text{if } x > 0.5 \end{cases}, \qquad x \in [0, 1],$$

$$T_f = 0.012, \quad N = 256, \quad r = 4$$



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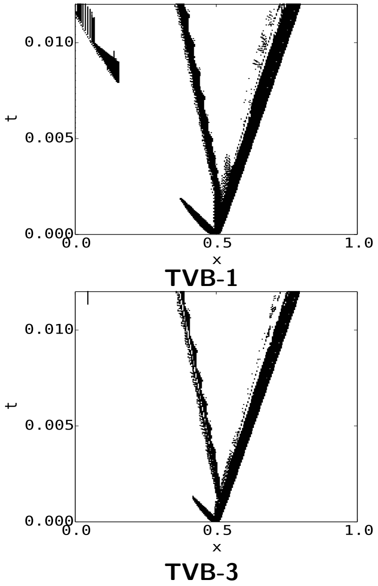
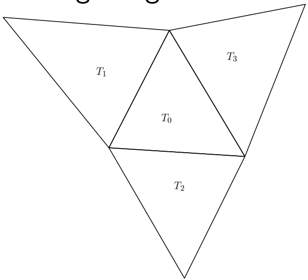


Extension to 2D

We consider unstructured triangular grids



Training data constructed by:

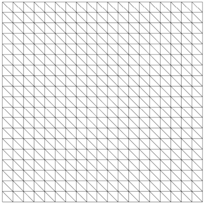
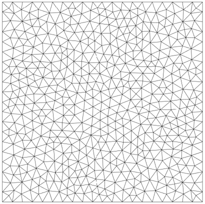
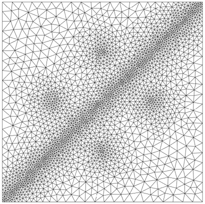
- Interpolating functions to patch of 4 triangles.
- Extracting linear components, with $\mathbf{X} \in \mathbb{R}^{12}$.
- Label cell as troubled-cell if discontinuity present within circumscribed circle.

Extension to 2D

Training functions

$\mathbf{u}(\mathbf{x})$	Parameters	Good cells	Troubled cells
$ax + by$	$a, b \in \mathcal{U}[-10, 10]$	34,776	0
$\sum_{k=1}^{N_f} a_k \sin(k\pi x) + b_k \cos(k\pi y)$	$a_k, b_k \in \mathcal{U}[-1, 1], \quad N_f = 1, 2, 3$	202,980	0
$\exp(a_1[(x-a_2)^2 + (y-a_3)^2])$ $+\exp(a_4[(x-a_5)^2 + (y-a_6)^2])$	$a_i \in \mathcal{U}[-1, 1]$	135,320	0
4 values u_1, u_2, u_3, u_4 in 4 sections created by the lines $y - y_0 = m(x - x_0)$ and $y - y_0 = -1/m(x - x_0)$ (only troubled-cells selected)	$u_i \in \mathcal{U}[-1, 1], \quad m \in \mathcal{U}[0, 20]$, $x_0, y_0 \in \mathcal{U}[-0.5, 0.5]$	0	337,976
$a\lvert(y - y_0) - m(x - x_0)\rvert$ (only troubled-cells selected)	$a \in \mathcal{U}[-100, 100], \quad m \in \mathcal{U}[-1, 1]$, $x_0, y_0 \in \mathcal{U}[-0.5, 0.5]$	0	60,182
		373,076	**398,158**

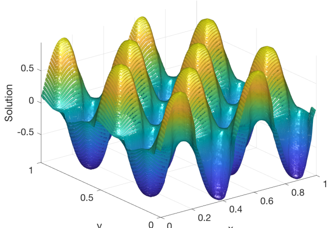
MLP with:
- 5 hidden layer
- 20 neurons each

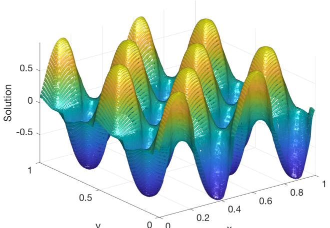
2D Linear advection: $u_t + u_x + u_y = 0$

$$u_0(x) = \sin(4\pi x)\sin(4\pi y), \quad r = 3$$

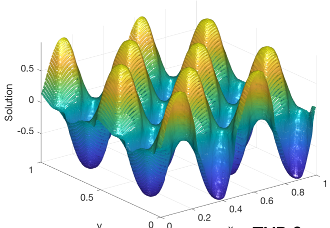
Mesh S-150:



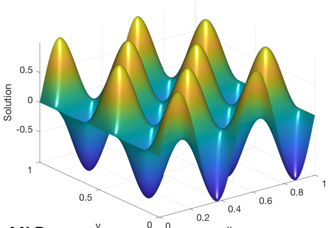
TVB-1



TVB-2



TVB-3

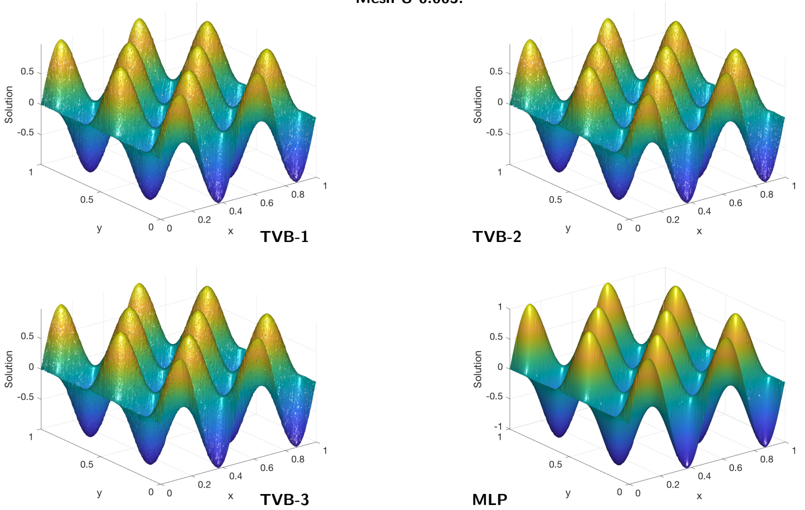


MLP

2D Linear advection: $u_t + u_x + u_y = 0$

$$u_0(x) = \sin(4\pi x)\sin(4\pi y), \quad r = 3$$

Mesh U-0.005:

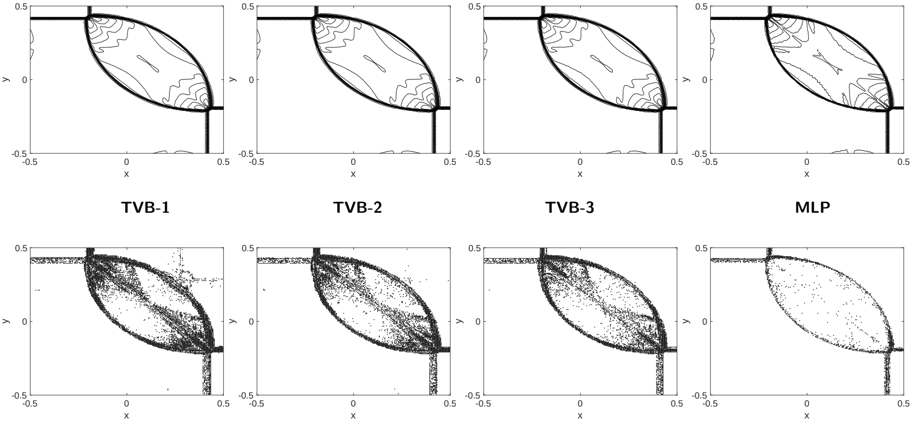


2D Linear advection: $u_t + u_x + u_y = 0$

Indicator	Mesh	$p = 1$		$p = 2$		$p = 3$	
		Max. % cells flagged	Avg. % cells flagged	Max. % cells flagged	Avg. % cells flagged	Max. % cells flagged	Avg. % cells flagged
TVB-1	S-100	31.71	29.51	32.10	28.57	33.78	29.91
	S-150	20.46	18.90	24.85	21.98	27.01	24.00
	U-0.01	29.67	28.33	33.15	31.23	32.29	30.35
	U-0.005	19.43	18.46	28.20	26.54	28.39	26.79
TVB-2	S-100	28.06	26.40	28.20	25.11	30.80	26.90
	S-150	17.35	16.41	22.10	19.73	25.51	22.30
	U-0.01	25.00	23.85	28.85	26.97	27.83	25.71
	U-0.005	16.30	15.40	25.44	23.87	25.32	23.72
TVB-3	S-100	23.86	22.66	24.48	22.13	26.34	23.63
	S-150	14.77	13.95	19.08	17.44	21.54	19.65
	U-0.01	20.88	19.99	25.34	23.46	24.12	22.27
	U-0.005	13.47	12.67	23.36	21.66	23.20	21.50
MLP	S-100	1.33	0.74	1.04	0.23	0.92	0.33
	S-150	0.24	0.12	0.23	0.02	0.18	0.01
	U-0.01	0.71	0.56	0.81	0.60	1.08	0.76
	U-0.005	0.13	0.11	0.19	0.13	0.18	0.13

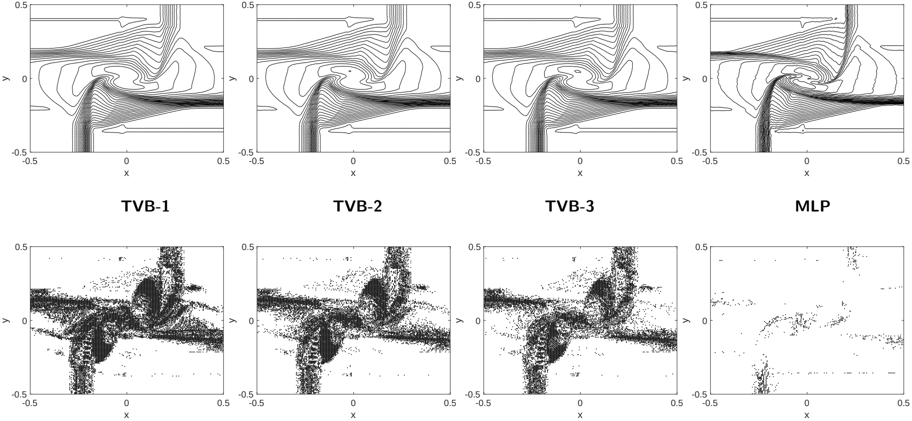
2D Euler equations

2D Riemann problem (config. 4), r=3

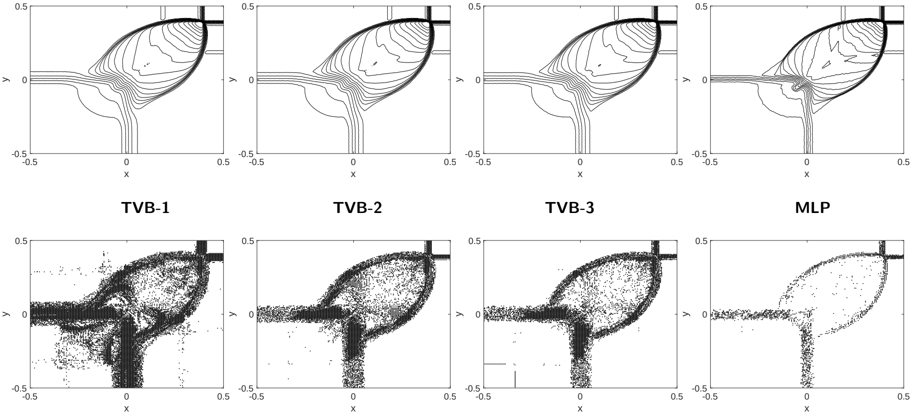


2D Euler equations

2D Riemann problem (config. 6), r=3



2D Riemann problem (config. 12), r=3



Detecting troubled-cells on two-dimensional unstructured grids using a neural network by D. Ray and J. S. Hesthaven (submitted, 2018)

Part II: ANNs predicting artificial viscosity

Shock capturing techniques

Now consider the problem

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \nabla \cdot \mathbf{g}, \quad \mathbf{g} = \mu \mathbf{w}, \quad \mathbf{w} = \nabla \mathbf{u}$$

Viscosity depends on $\mathbf{u}$ and locally controls oscillations.

$$\mu \sim h|\mathbf{f}'(\mathbf{u})|$$

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Viscosity depends on $\mathbf{u}$ and locally controls oscillations.

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Several artificial viscosity models exist

- Derivative-based model (DB)
- Highest Modal Decay (MDH)
- Averaged Modal Decay (MDA)
- Entropy Viscosity (EV)

Dependent on problem specific parameters

Training the 1D network

$$\boxed{\mathbf{u}} \xrightarrow{\text{scale}} \boxed{\frac{\mathbf{u}}{\max\{u^i\}}} \xrightarrow{\text{NN}} \boxed{\frac{\mu}{h\Lambda}} \xrightarrow{\text{rescale}} \boxed{\mu}$$

$$\Lambda = \max|\mathbf{f}'(\mathbf{u})|$$

Network architecture:

- Input: $(r+1)$ solution point values of cell (in 1D)
- Output: μ in cell
- 5 hidden layers of width 10 each
- Leaky ReLU activation
- Softplus output function, i.e., $f(x) = \log(1+e^x)$
- Mean Squared Error cost function

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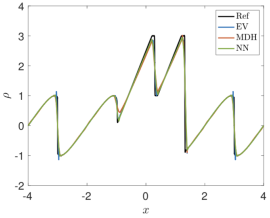
- Mean Squared Error cost function

Training/validation sets:

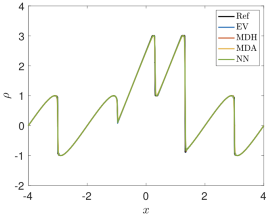
- Using numerical solution of conservation laws
- Only linear advection and Burgers equations
- Target viscosity: viscosity corresponding to "best" model

Burgers equation: $u_t + (u^2/2)_x = 0$

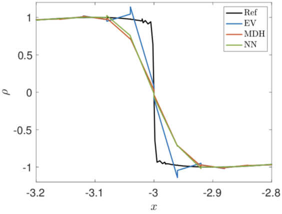
$x \in [-4, 4]$, $T_f = 0.4$, $h = 8/200$ (not in training set)



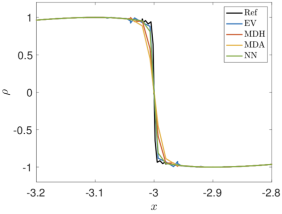
(a) Overall result, $m = 1$.



(b) Overall result, $m = 4$.



(c) Zoom close to the first shock, $m = 1$.



(d) Zoom close to the first shock, $m = 4$.

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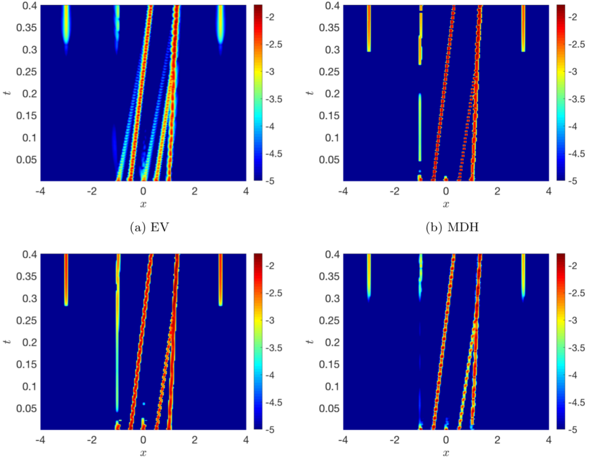


(a) EV

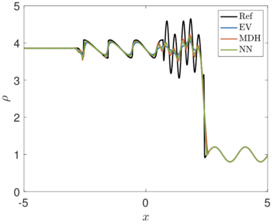
(b) MDH

(c) MDA

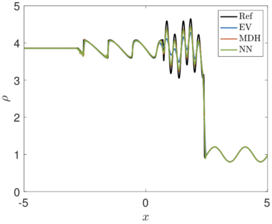
(d) NN

1D Euler equations: Shock-Entropy

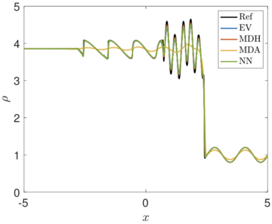
$x \in [-5, 5], \quad T_f = 1.8, \quad h = 10/200$



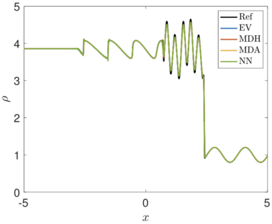
(a) Overall result, $m = 1$.



(b) Overall result, $m = 2$.



(c) Overall result, $m = 3$.



(d) Overall result, $m = 4$.

1D Euler equations: Shock-Entropy

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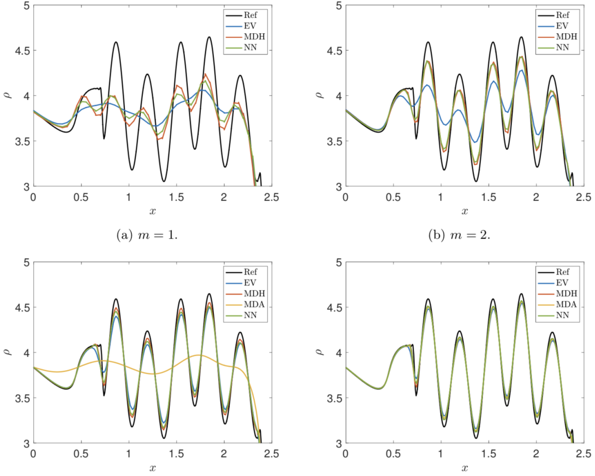


(a) $m = 1$.

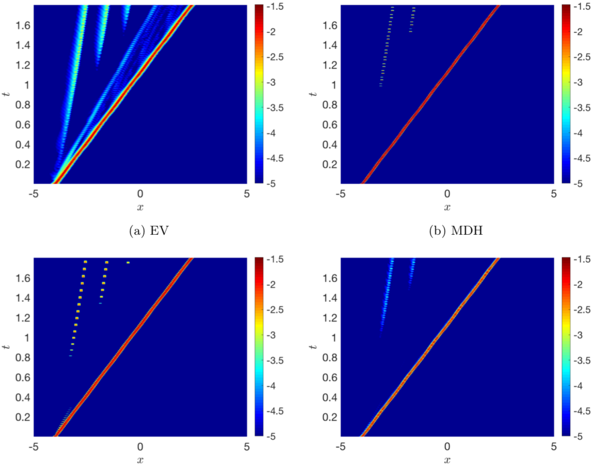
(b) $m = 2$.

(c) $m = 3$.

(d) $m = 4$.

1D Euler equations: Shock-Entropy

$x \in [-5, 5], \quad T_f = 1.8, \quad h = 10/200$



(a) EV

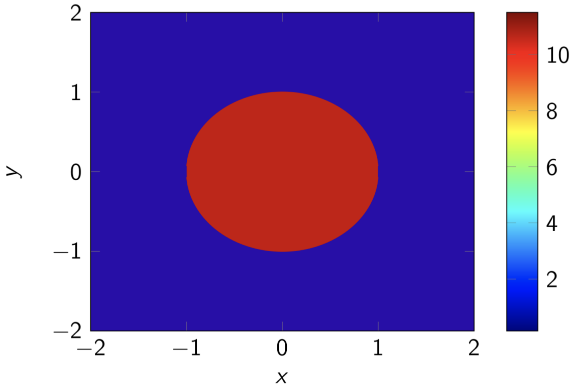
(b) MDH

(c) MDA

(d) NN

2D KPP equations: Rotating wave

$\mathbf{f}(u) = (\sin u, \cos u), \quad T_f = 1, \quad h = 4\sqrt{2}/120, \quad r = 4$



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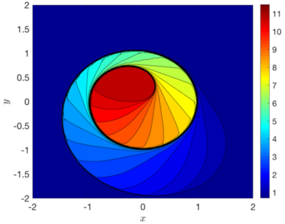
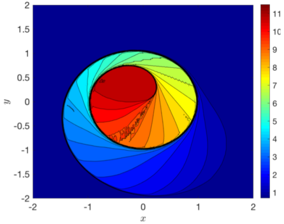
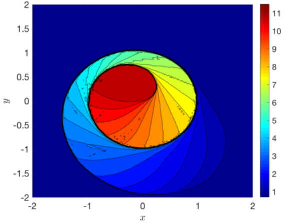


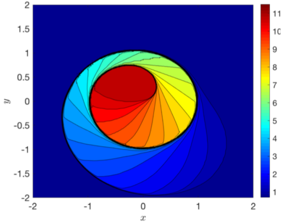
(a) EV



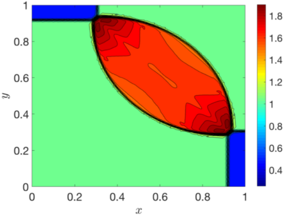
(b) MDH



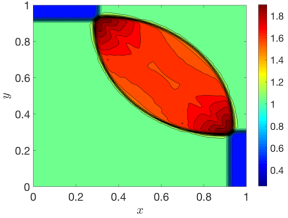
(c) MDA



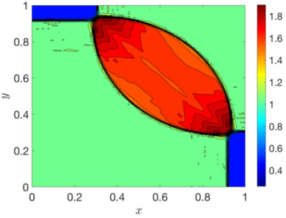
(d) NN



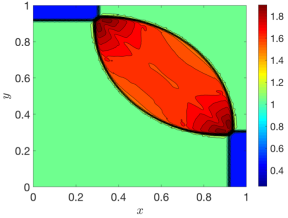
(a) EV



(b) MDH

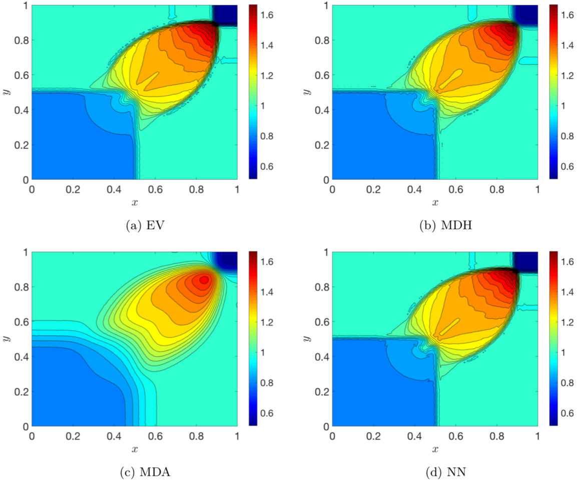


(c) MDA

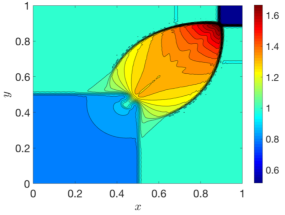


(d) NN

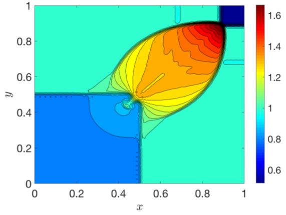
2D Euler equations: Riemann Problem 12, r=3



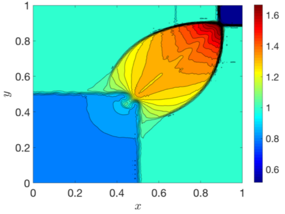
2D Euler equations: Riemann Problem 12, r=4



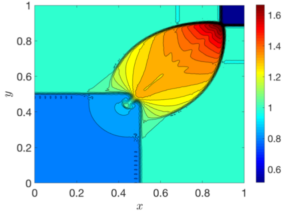
(a) EV



(b) MDH



(c) MDA



(d) NN

Summarizing

- When trained properly, ANN's work well for classification and regression
- Only needs to be trained once offline
- Parameter free
- Improves computational cost
- Can be easily extended to 3D (in principle)

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Thank you

RKDG and limiting

RKDG solver

```
Initialize U[0]
n = 1
while t .lte. Tf do
    U[n] = U[n-1]
    for r = 1 to 3 do
        L = FindRHS(U[n])
        U[n] = RK_update(U[n-1], U[n], L, r)
        U[n] = Limit(U[n])
    end for
    n++, t+=dt
end while
```

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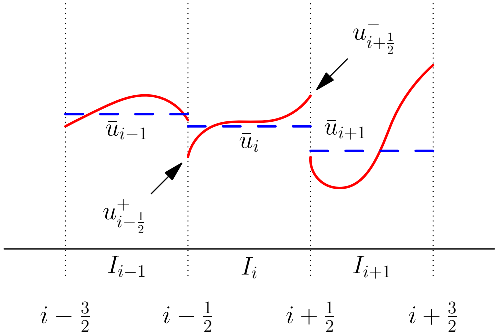
```

Bottleneck step!!

Identification: For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$



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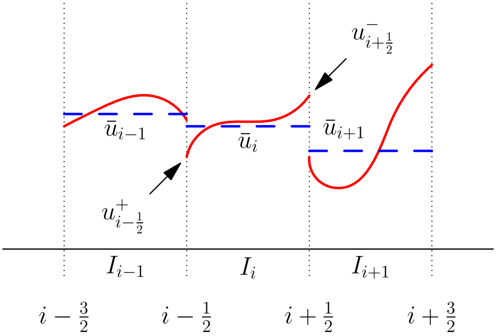
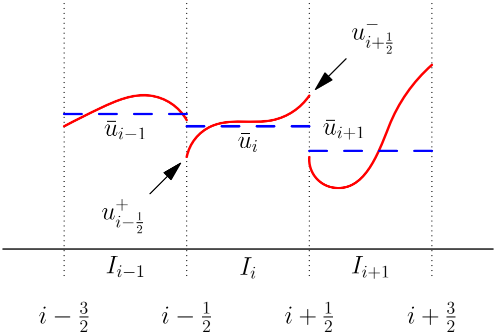


Evaluate 4 differences

$$\Delta^- u_i = \overline{u}_i - \overline{u}_{i-1}, \qquad \Delta^+ u_i = \overline{u}_{i+1} - \overline{u}_i,$$
$$\check{u}_i = \overline{u}_i - u^+_{i-\frac{1}{2}}, \qquad \hat{u}_i = u^-_{i+\frac{1}{2}} - \overline{u}_i$$

TVB Limiter (Qiu and Shu, 2005)

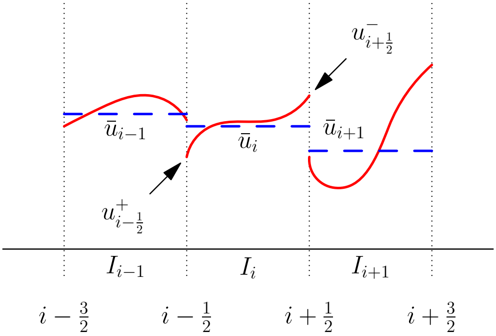
Identification: For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$



Modify interface values

$$\widetilde{u}^+_{i-\frac{1}{2}} = \overline{u}_i + \mathcal{F}\left(\check{u}_i, \Delta^- u_i, \Delta^+ u_i\right)$$
$$\widetilde{u}^-_{i+\frac{1}{2}} = \overline{u}_i - \mathcal{F}\left(\hat{u}_i, \Delta^- u_i, \Delta^+ u_i\right)$$

Identification: For each cell I_i, get $[\overline{u}_{i-1}, \overline{u}_i, \overline{u}_{i+1}, u^+_{i-\frac{1}{2}}, u^-_{i+\frac{1}{2}}]$



Flag I_i as troubled-cell if

$$\widetilde{u}^+_{i-\frac{1}{2}} \neq u^+_{i-\frac{1}{2}} \quad \text{or} \quad \widetilde{u}^-_{i+\frac{1}{2}} \neq u^-_{i+\frac{1}{2}}$$

Search for the elusive M

We consider the following limiter-based indicators $\mathcal{F}$:

- Minmod limiter:

$$\mathcal{F}^{\mathsf{mm}}(a,b,c) = \begin{cases} s.\min(|a|,|b|,|c|), & \text{if } s = \mathsf{sign}(a) = \mathsf{sign}(b) = \mathsf{sign}(c) \\ 0, & \text{otherwise} \end{cases}$$

Disadvantage: Flags cell with smooth extrema

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  Disadvantage: Flags cell with smooth extrema

- TVB limiter: Depends on h and tunable parameter M

$$\mathcal{F}^{\mathsf{tvb}}(a,b,c,h,M) = \begin{cases} a, & \text{if } |a| \le Mh^2 \\ \mathcal{F}^{\mathsf{mm}}(a,b,c), & \text{otherwise} \end{cases}$$

  M is proportional to second derivative at smooth extreme

  Disadvantage: M is problem dependent

Limiting the solution (Qiu and Shu, 2005)

Limited reconstruction: In troubled cells:

- Project u_h to $\mathbb{P}_1$

$$u_h = \overline{u}_i + \left(\frac{x - x_i}{\frac{1}{2}\Delta x_i}\right) s_i + \text{ H.O.T.}$$

Limiting the solution (Qiu and Shu, 2005)

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- Limit slope

$$\widetilde{u}_h^{(m)} = \overline{u}_i + \left(\frac{x - x_i}{\frac{1}{2}\Delta x_i} \right) \widetilde{s}_i$$

where

$$\widetilde{s}_i = \mathcal{Q}(s_i, \overline{u}_i - \overline{u}_{i-1}, \overline{u}_{i+1} - \overline{u}_i)$$