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Efficient Physics-Preserved Neural Network (P^2NN) Methods for Scalar Hyperbolic Conservation Laws

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https://www.math.purdue.edu/~caiz/paper.html

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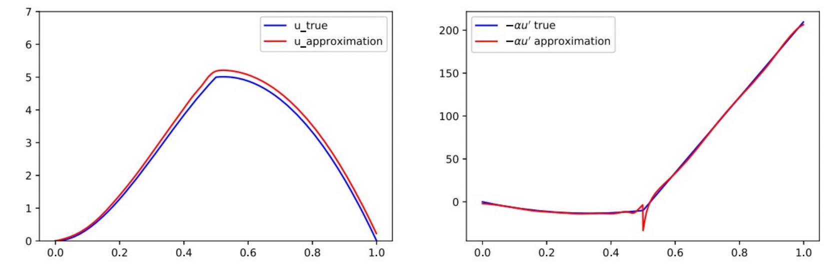
Deep Least-Squares Methods (C.-Chen-Liu-Liu, J. Comput. Phys., 420 (2020) 109707)

Deep least-squares methods: An unsupervised learning-based numerical method for solving elliptic PDEs

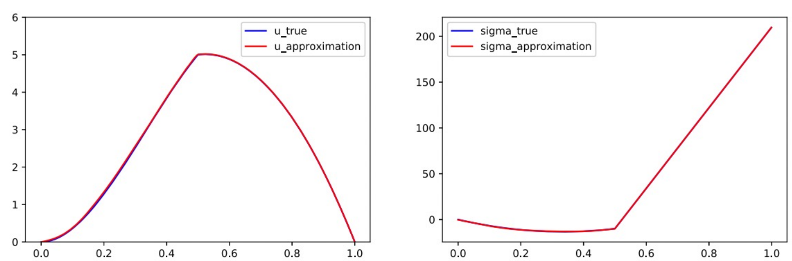
$$\begin{cases} -\left(au'(x)\right)' = f(x), & x \in \Omega = (0, 1), \\ u = 0, & x \in \partial\Omega = \{0, 1\}, \end{cases}$$

1D elliptic interface problem with the jump size 9
1-32-32-24-24-1 NN, 20000 Adam iterations

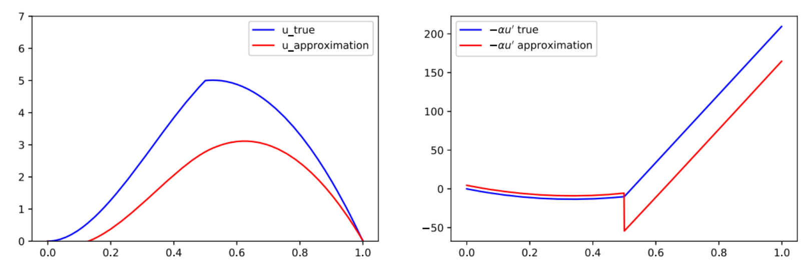


Deep Ritz

Importance of (i) PDE Formulation!



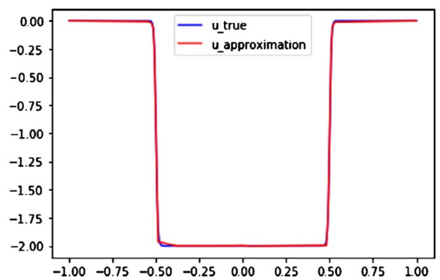
Deep FOSLS



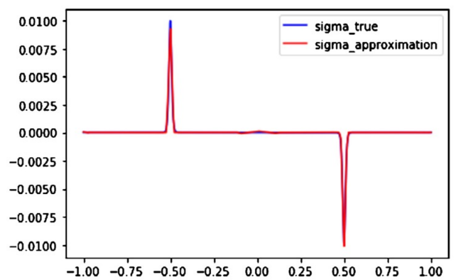
Simplified Bramble-Schatz LS (1970) $\Rightarrow$ PINNs (1994)

1D Interior Layers

- **1D singularly perturbed diffusion-reaction problem**



(a) FOSLS u with Leaky ReLU

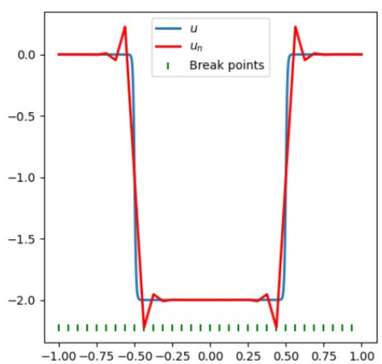


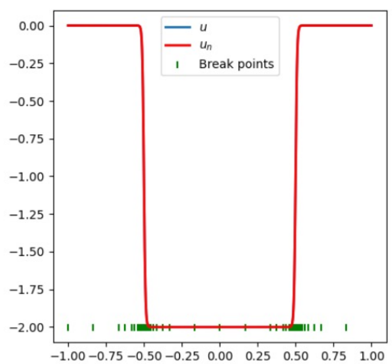
(b) FOSLS σ with Leaky ReLU

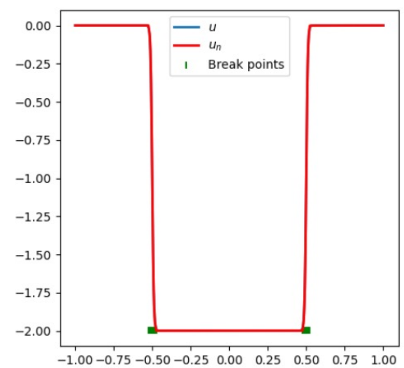
$$\begin{cases} -\varepsilon^2 u''(x) + u(x) = f(x), & x \in \Omega = (-1,\ 1), \\ u = 0, & x \in \partial\Omega = \{-1,\ 1\}. \end{cases}$$

1-32-32-24-24-2, 2962 parameters, about 20 hours

Importance of (ii) NN architecture and efficient (iii) Nonlinear Solver!







Efficient shallow Ritz method
C.-Doktorova-Falgout-Herrera (2024)
1-32-1, 64 parameters, about 70 seconds

Outline

- Why Using ReLU Neural Network?

- Physics-Preserved Neural Network (P^2NN) Methods for HCLs

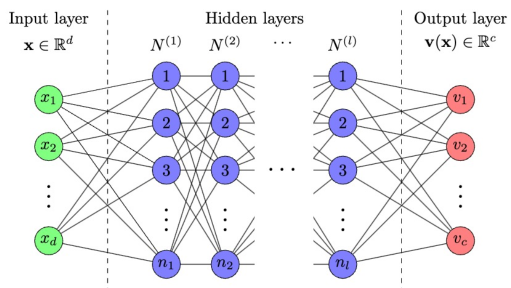
  (i) Least-squares neural network (LSNN) method (a space-time approach)

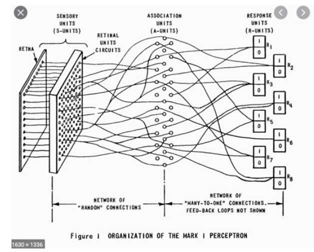
  (ii) Evolving neural network (ENN) method (an approach emulating physics)

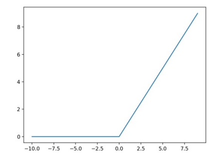
- Efficient Nonlinear Solver

ReLU Neural Networks (NNs)

- **Fully-connected (Multi-Layer Perceptron) NN (Rosenblatt 1958)**







$$\sigma(t) = \begin{cases} t, & t > 0, \\ 0, & t \le 0. \end{cases}$$

- **A class of approximating functions (ReLU NN)** ⇒ **C^0 piecewise linear functions**

$$\mathcal{M}_N(d,l) = \left\{ c_0 + \sum_{j=1}^{n_l} c_j x_j^{(l)}(\mathbf{x}) : \mathbf{c} \in \mathcal{R}^{n_l+1}, \boldsymbol{\omega}^{(k)} \in \mathcal{R}^{n_{k-1}\times n_k}, \mathbf{b}^{(k)} \in \mathcal{R}^{n_k} \right\}$$

where $\mathbf{x}^{(0)} = \mathbf{x}$ and $x_i^{(k)}(\mathbf{x}) = \sigma\left(\boldsymbol{\omega}_i^{(k)} \mathbf{x}^{(k-1)} + b_i^{(k)}\right)$

Why Using Neural Networks instead of Finite Elements?

Scalar Nonlinear Hyperbolic Conservation Laws

- **Scalar Nonlinear Hyperbolic Conservation Laws**

$$\begin{cases} \dfrac{\partial}{\partial t}u(\mathbf{x},t) + \displaystyle\sum_{i=1}^{d} \dfrac{\partial}{\partial x_i} f_i(u(\mathbf{x},t)) & = & 0, & \text{in } \mathcal{R}^d \times (0,T), \\ u(\mathbf{x},0) & = & u_0(\mathbf{x}), & \text{in } \mathcal{R}^d \end{cases}$$

- **The Rankine-Hugoniot jump condition**

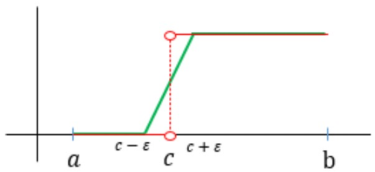
$$\left(\mathbf{f}(u^+), u^+\right) \cdot \mathbf{n}^+\Big|_\Gamma + \left(\mathbf{f}(u^-), u^-\right) \cdot \mathbf{n}^-\Big|_\Gamma = 0.$$

- **Numerical and Theoretical Difficulties**
  - discontinuous solution with unknown interfaces
  - formulation, theory, ...

1-Dimensional Unit Step Function with Unknown Interface

- Unit step function and its CPWL approximation

$$f_c(x) = \begin{cases} 0, & a < x < c, \\ 1, & c < x < b \end{cases}$$



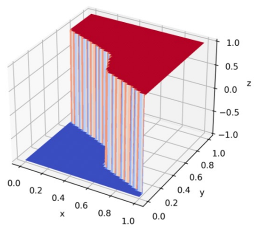
$$p_c(x) = \begin{cases} 0, & a < x \le c - \varepsilon, \\ \dfrac{x - (c-\varepsilon)}{2\varepsilon}, & c - \varepsilon \le x \le c + \varepsilon, \\ 1, & c + \varepsilon \le x < b \end{cases}$$

$$\|f_c - p_c\|_{L^\infty(I)} = \frac{1}{2} \quad \text{and} \quad \|f_c - p_c\|_{L^r(I)} = \frac{\varepsilon^{1/r}}{2^{1-1/r}(1+r)^{1/r}}$$

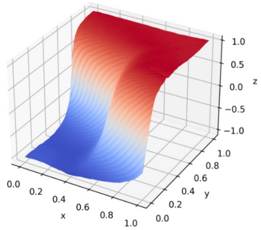
- **Finite element approximation on a quasi-uniform mesh**
  - **- very fine mesh-size:** $h = \varepsilon$
  - **- overshooting, oscillation, etc.**
- **Neural Network approximation**

$$p_c(x) = \frac{1}{2\varepsilon}\left[\sigma(x - c + \varepsilon) - \sigma(x - c - \varepsilon)\right] \in \mathcal{M}_2(1,1)$$

d-Dimensional Unit Step Function with Unknown Interface

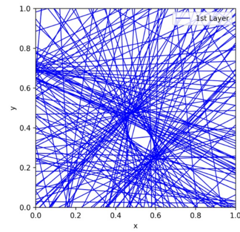


(b) Exact solution

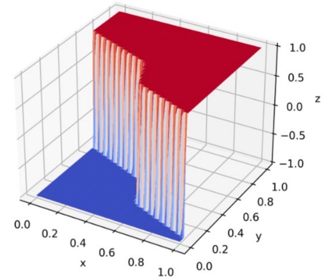


(c) 2 layer NN approximation

2-300-1

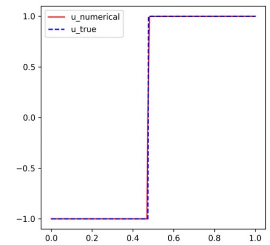


(g) 2 layer NN breaking lines

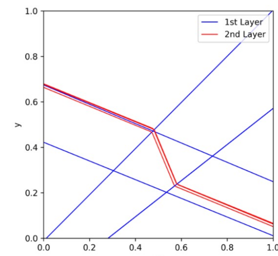


(d) 3 layer NN approximation

2-5-5-1



(f) 3 layer NN trace on $y = x$



(h) 3 layer NN breaking lines

Let $\chi(\mathbf{x})$ be the unit step function with unknown C^0 interface and let $l = \lceil \log_2(d+1) \rceil$). For any given $\varepsilon > 0$, we have

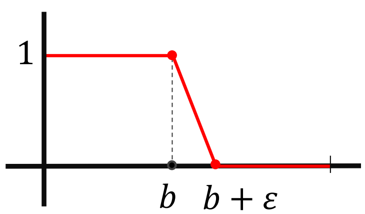
$$\min_{v \in \mathcal{M}_N(d,l)} \|\chi - v\|_{L^r(\Omega)} = \mathcal{O}(\varepsilon^{1/r}).$$

C., J. Choi, and M. Liu, SISC (2024) (d=2, 3, l=2; d=4,...,8, l=3)

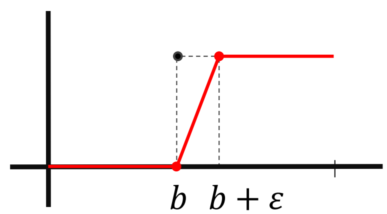
A New Result in R^d (C.-Choi-Liu, 2024)

Let $\chi(\mathbf{x})$ be the unit step function with unknown C^0 interface. For any given $\varepsilon > 0$, we have

$$\min_{v \in \mathcal{M}_N(d,2)} \|\chi - v\|_{L^r(\Omega)} = \mathcal{O}(\varepsilon^{1/r}).$$



$\sigma\left(1 - \frac{1}{\varepsilon}\sigma(\vec{a} \cdot \vec{x} - b)\right)$



$1 - \sigma\left(1 - \frac{1}{\varepsilon}\sigma(\vec{a} \cdot \vec{x} - b)\right)$

The P^2NN Method (C.-Chen-Liu, J. Comput. Appl. Math., 433 (2023) 115298)

- **Scalar Nonlinear Hyperbolic Conservation Laws**

$$\begin{cases} \dfrac{\partial}{\partial t}u(\mathbf{x},t) + \displaystyle\sum_{i=1}^{d}\dfrac{\partial}{\partial x_i}f_i(u(\mathbf{x},t)) &= 0, \\ u(\mathbf{x},0) &= u_0(\mathbf{x}), \quad \text{in } \mathcal{R}^d \end{cases}$$

$$\left(\mathbf{f}(u^+), u^+\right)\cdot\mathbf{n}^+\Big|_\Gamma + \left(\mathbf{f}(u^-), u^-\right)\cdot\mathbf{n}^-\Big|_\Gamma = 0.$$

- **The Rankine-Hugoniot jump condition**

$$\left(\mathbf{f}(u^+), u^+\right)\cdot\mathbf{n}^+\Big|_\Gamma + \left(\mathbf{f}(u^-), u^-\right)\cdot\mathbf{n}^-\Big|_\Gamma = 0.$$

- **The total flux** $\mathbf{F}(u) = (\mathbf{f}(u), u)$

$$\nabla\cdot\mathbf{F}(u) = 0, \quad \text{in} \quad (\mathcal{R}^d \times I)\setminus\Gamma \quad \text{and} \quad [\![\mathbf{F}(u)\cdot\mathbf{n}]\!]_\Gamma = 0$$

Equivalent Least-Squares Minimization Formulation

$$\nabla \cdot \mathbf{F}(u) = 0, \quad \text{in} \quad (\mathcal{R}^d \times I) \setminus \Gamma \quad \text{and} \quad [\![\mathbf{F}(u) \cdot \mathbf{n}]\!]_{\Gamma} = 0$$

- **Solution set**

$$V_{\mathbf{f}}(u_0) = \{v \in L^2(\mathcal{R}^d \times I) : \mathbf{F}(v) \in H(\text{div}; \mathcal{R}^d \times I),\ v(\mathbf{x}, 0) = u_0(\mathbf{x})\}$$

- **Least-squares functional**

$$\mathcal{L}(v; \mathbf{f}) = \|\text{div}\, \mathbf{F}(v)\|^2_{0,\mathcal{R}^d \times I}$$

- **Equivalent Least-squares formulation**

$$\text{Find } u \in V_{\mathbf{f}}(u_0) \text{ such that } \qquad u = \operatorname*{arg\,min}_{v \in V_{\mathbf{f}}(u_0)} \mathcal{L}(v; \mathbf{f})$$

- **Divergence operator**

$$\text{div}\, \mathbf{F}(u(\mathbf{x}, t)) = \lim_{\epsilon \to 0} \frac{1}{|B_\epsilon(\mathbf{x}, t)|} \int_{\partial B_\epsilon(\mathbf{x}, t)} \mathbf{F}(u) \cdot \mathbf{n}\, dS,$$

Physics-Preserved Neural Network (P^2NN) Discretization

- **Physics-Preserved** **discrete divergence operator** (C.-Chen-Liu, J Comput Appl Math (2023))

Let $\mathcal{T}$ be a partition of the domain $\Omega \subset \mathbb{R}^{d+1}$. For any $K \in \mathcal{T}$, let $\mathbf{z}_K$ be the centroid of K.

$$\mathbf{div}_{\mathcal{T}} \mathbf{F}\big(u(\mathbf{z}_{_K})\big) \approx \text{avg}_K \mathbf{div}\, \mathbf{f}(u) = \frac{1}{|K|} \int_{\partial K} \mathbf{F}(u) \cdot \mathbf{n}\, dS$$

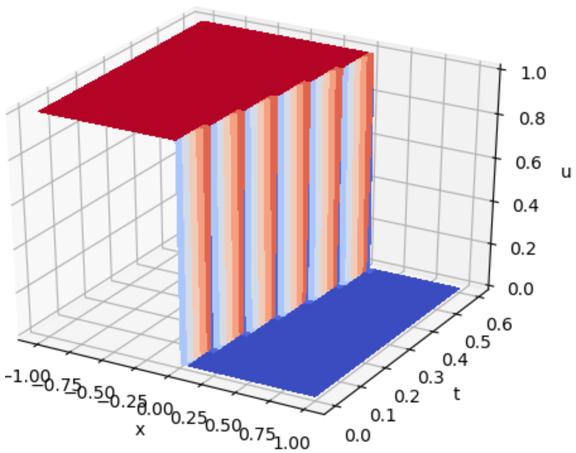
- **Least-squares neural network (LSNN) method**

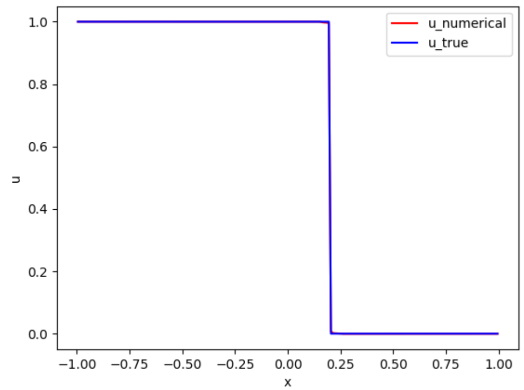
Find $u_n \in \mathcal{M}(l,n) \subset V_{\mathbf{f}}$ such that $\quad u_n = \underset{v \in \mathcal{M}(l,n)}{\arg\min}\, \mathcal{L}_{\mathcal{T}}(v;\mathbf{f})$,

where $\mathcal{L}_{\mathcal{T}}(v;\mathbf{f})$ is a discrete LS functional based on $\mathcal{L}(v;\mathbf{f})$.

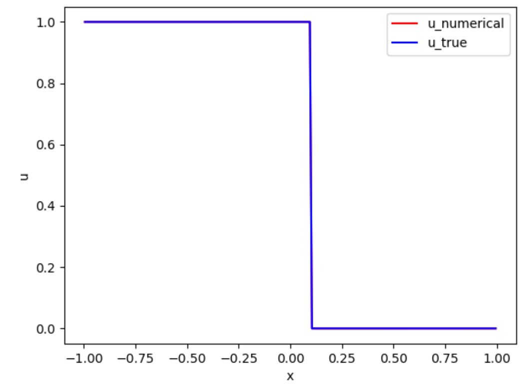
Inviscid Burger Equation $f(u) = \frac{1}{2}u^2$

Riemann Problem Shock formation: exact solution

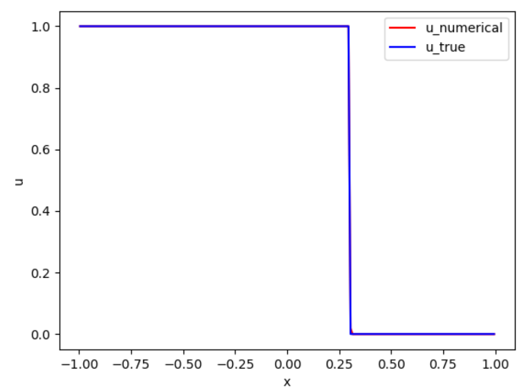




t=0.2



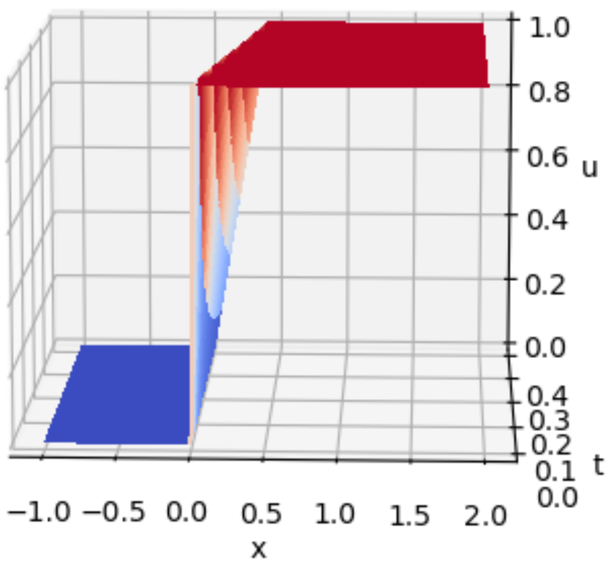
t=0.4

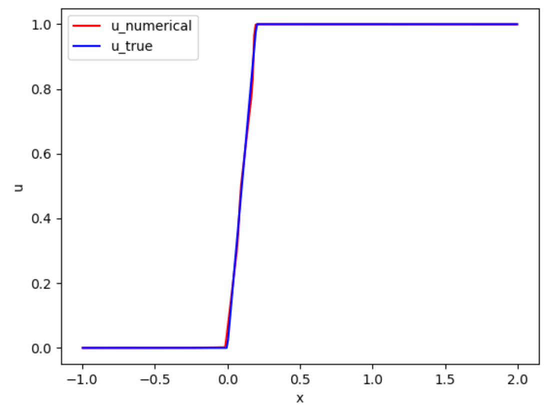


t=0.6 (2-10-10-1)

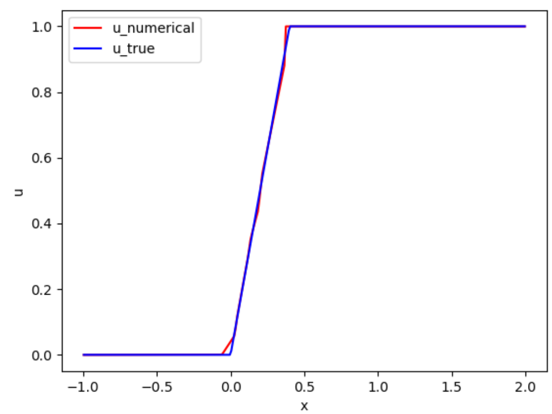
C.-Chen-Liu, arXiv: 2110.10895 [math.NA]

Riemann Problem
Rarefaction wave: exact solution





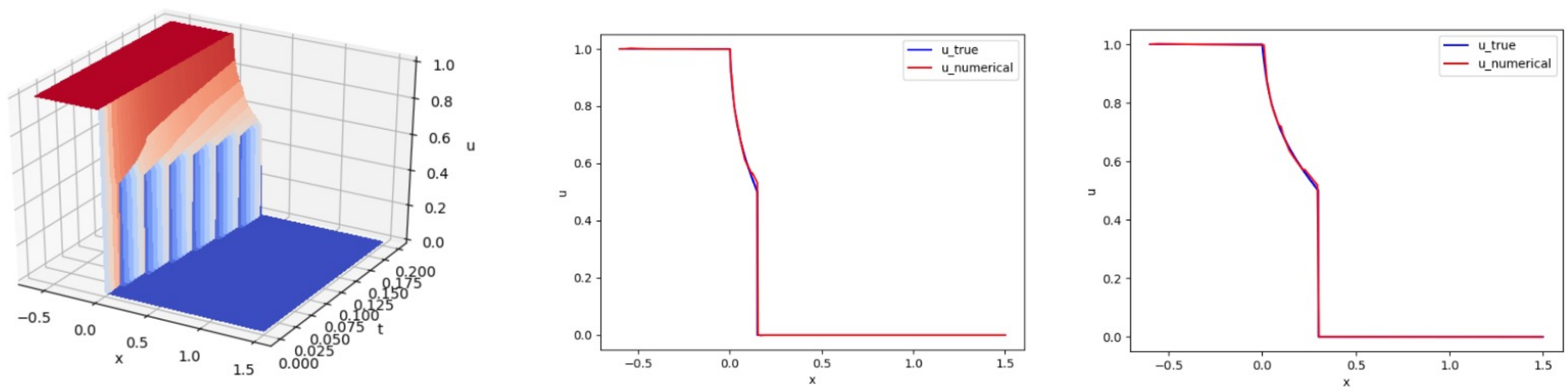
t=0.2



t=0.4

(2-10-10-1)

Buckley-Leverett Problem $f(u) = u(1-u)/[u^2 + a(1-u)^2]$

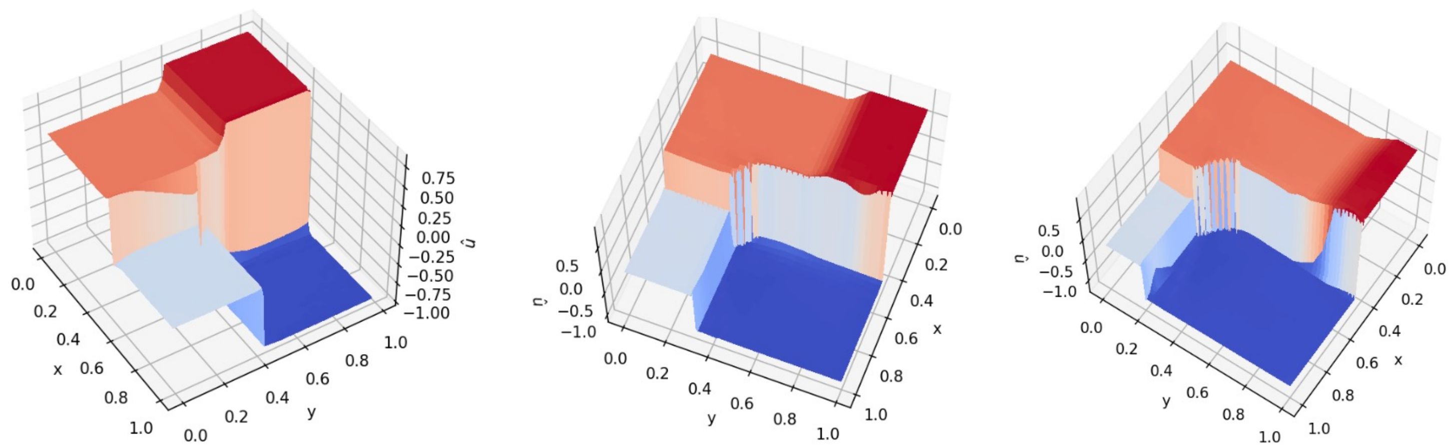


(a) Numerical solution u_N on Ω (b) Traces at $t = 0.1$ (c) Traces at $t = 0.2$

FIG. 6. *Numerical results of Buckley-Leverett Riemann problem*

2D Inviscid Burger Equation $f(u) = \frac{1}{2}(u^2, u^2)$

Network structure	Block	$\frac{\|u^k - u^k_{\mathcal{T}}\|_0}{\|u^k\|_0}$
3-48-48-48-1	$\Omega_{0,1}$	0.093679
	$\Omega_{1,2}$	0.121375
	$\Omega_{2,3}$	0.163755
	$\Omega_{3,4}$	0.190460
	$\Omega_{4,5}$	0.213013



(a) $t = 0.1$ (b) $t = 0.3$ (c) $t = 0.5$

Evolving Neural Network (ENN) Method (C. and B. Hejnal)

- **One-Dimensional Scalar Nonlinear Hyperbolic Conservation Laws**

$$\begin{cases} \frac{\partial}{\partial t}u(x,t) + \frac{\partial}{\partial x}f\big(u(x,t)\big) &= 0, & \text{in } \Omega\times(0,T), \\ u(x,t) &= g(t), & \text{on } \Gamma_-, \\ u(x,0) &= u_0(x), & \text{in } \Omega \end{cases}$$

- **Two features of HCLs (characteristic line and shock formation)**

$$\begin{cases} \frac{d}{dt}x(t) &= f'\big(u(x(t),t)\big) \\ x(t_0) &= x_0 \end{cases}$$

$$x(t) = x_0 + (t - t_0)\, f'\big(u(x_0, t_0)\big)$$

$$\frac{d}{dt}u(x(t), t) = 0$$

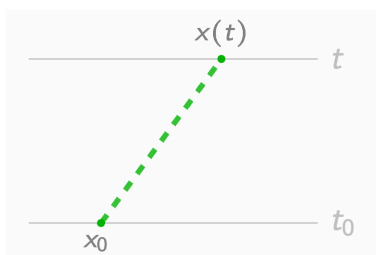
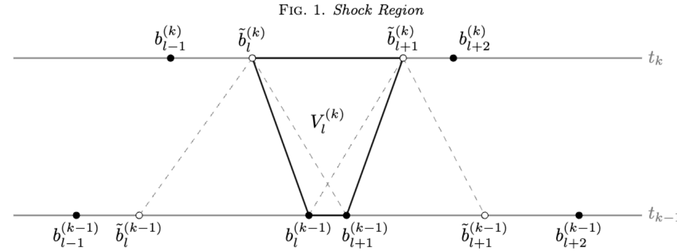
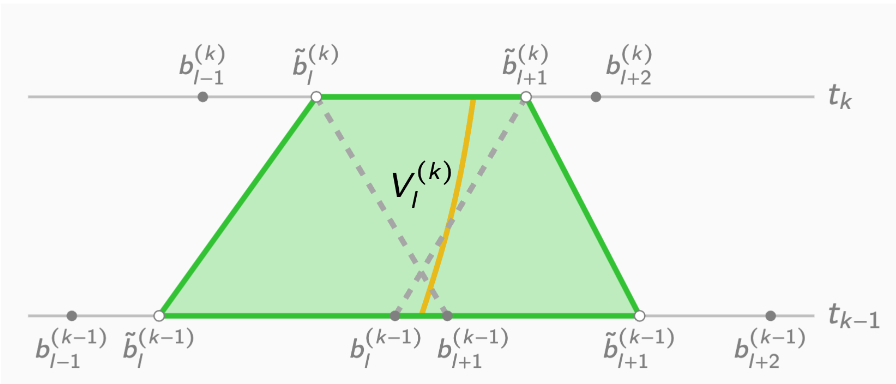


FIG. 1. *Shock Region*



Finite Volume Characteristic Scheme



$$\int_{\partial V_l^{(k)}} \begin{pmatrix} \boldsymbol{f(u)} \\ \boldsymbol{u} \end{pmatrix} \cdot \hat{\boldsymbol{n}}\, ds = 0$$

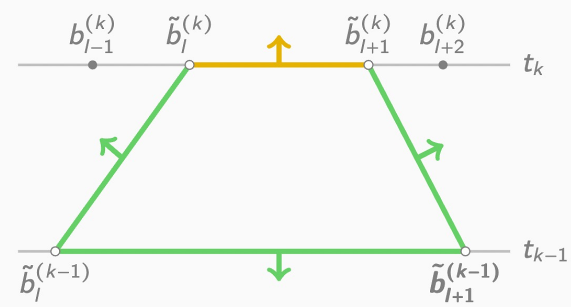
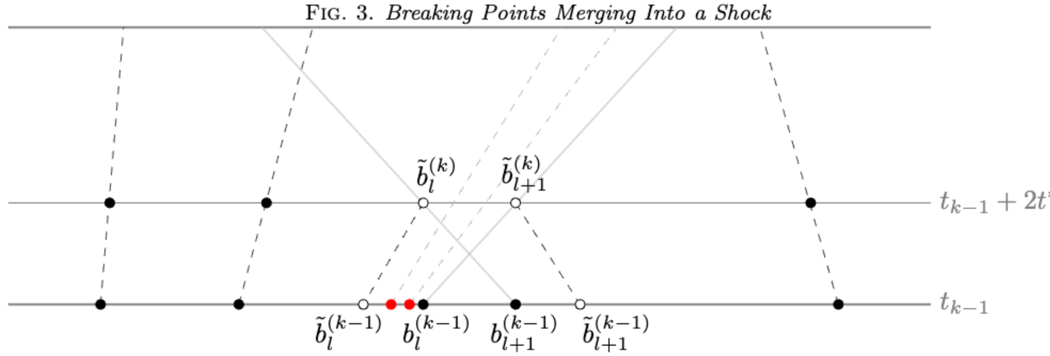
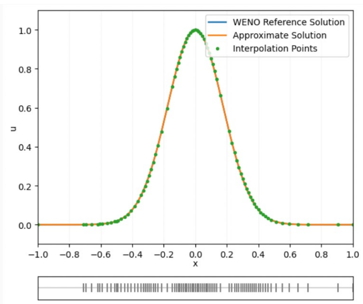


FIG. 3. *Breaking Points Merging Into a Shock*

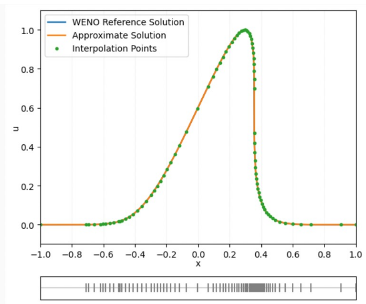


Shock Formation (exponential initial profile)

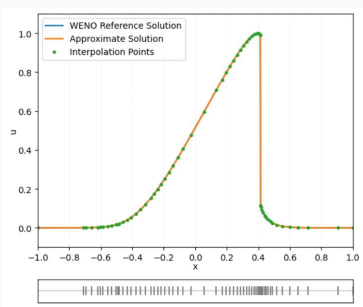
Inviscid Burgers' Equation



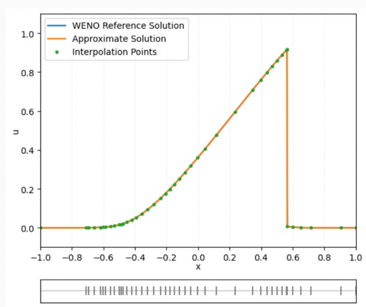
Initial data



$t = 0.3$



$t = 0.4$



$t = 0.7$

Time	$\frac{\|\tilde{u}(\cdot,t_k)-u_N^{(k)}\|_{L^2(\Omega)}}{\|\tilde{u}(\cdot,t_k)\|_{L^2(\Omega)}}$	n_k
0.0	6.6207×10^{-4}	83
0.2	7.2902×10^{-4}	83
0.4	1.2718×10^{-2}	61
0.6	2.1803×10^{-2}	47
0.8	2.0423×10^{-2}	40
1.0	1.4822×10^{-2}	37

ENN

- **83** breaking points
- **418** time steps

WENO

- **2000** mesh points
- **5000** time steps

Shock Formation (sinusoidal initial profile)

Inviscid Burgers' Equation

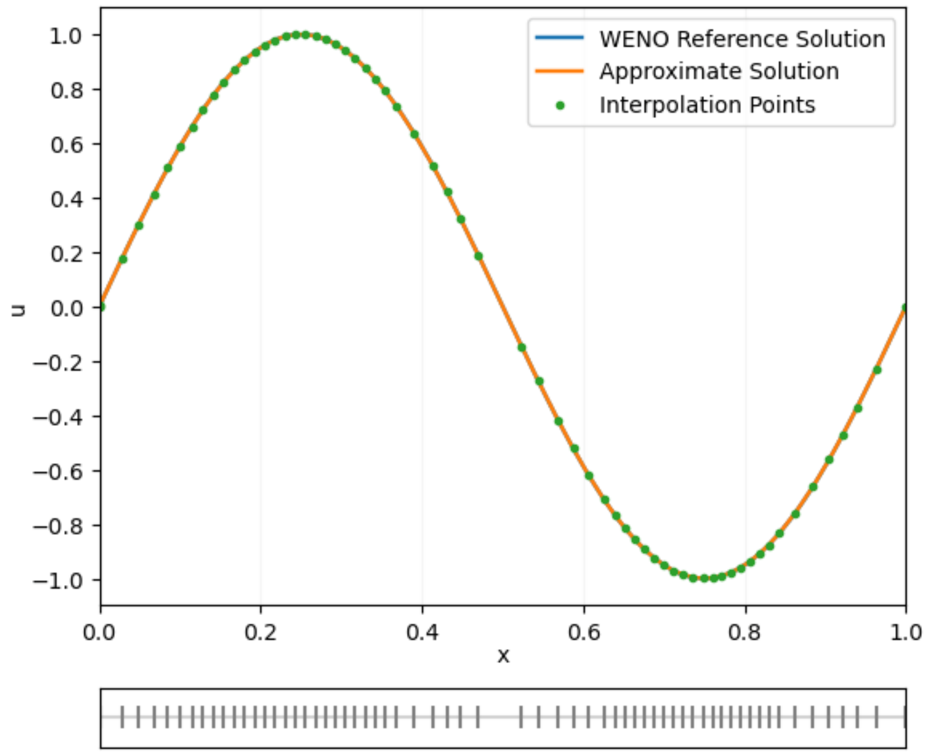
Time	$\frac{\|\tilde{u}(\cdot,t_k)-u_N^{(k)}\|_{L^2(\Omega)}}{\|\tilde{u}(\cdot,t_k)\|_{L^2(\Omega)}}$	n_k
0.0	6.6923×10^{-4}	78
0.1	7.8352×10^{-4}	78
0.2	4.0166×10^{-2}	56
0.3	5.1491×10^{-2}	38
0.4	5.3515×10^{-2}	30
0.5	5.4162×10^{-2}	25

ENN

- **78** breaking points
- **587** time steps

WENO

- **1000** mesh points
- **2500** time steps

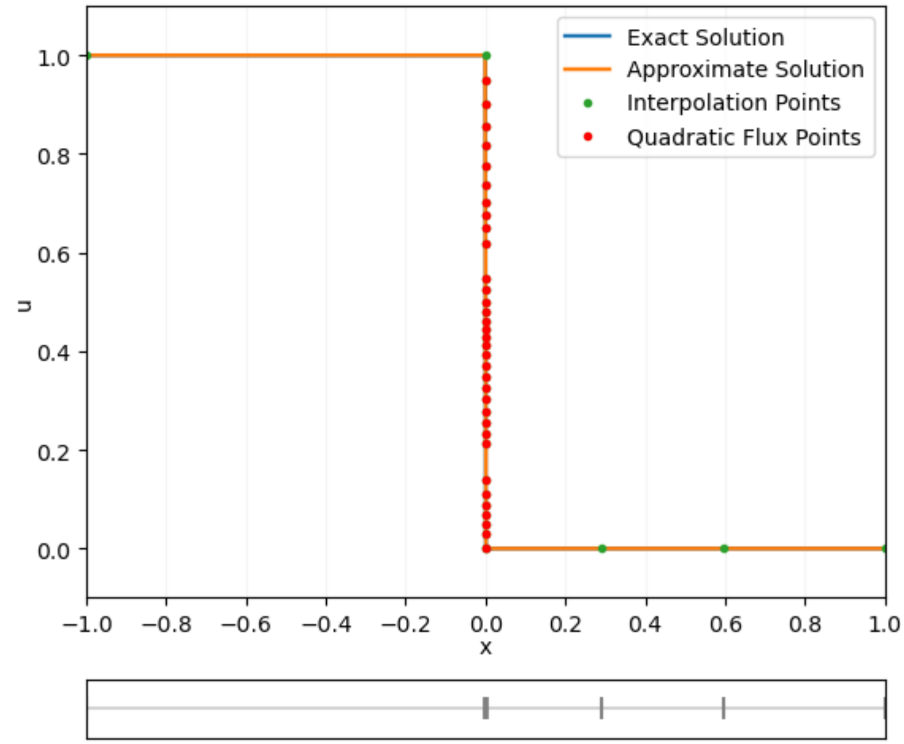


Compound Wave

Buckley-Leverett Equation

$$f(u) = \frac{u^2}{u^2 + \frac{1}{2}(1-u)^2}$$

Time	$\frac{\|u(\cdot,t_k)-u_N^{(k)}\|_{L^2(\Omega)}}{\|u(\cdot,t_k)\|_{L^2(\Omega)}}$	n_k
0.00	1.3732×10^{-2}	40
0.25	6.9084×10^{-3}	16
0.50	5.8335×10^{-3}	15



Efficient Nonlinear Solver

- **1D Diffusion problem**

$$\begin{cases} -(a(x)u'(x))' = f(x), \quad x \in I = (0,1), \\ u(0) = \alpha, \quad u(1) = \beta, \end{cases}$$

- **Shallow Ritz method**

$$\text{find } u_n \in \mathcal{M}_n(\Omega) = \left\{ \alpha + \sum_{i=1}^{n} c_i \sigma(x - b_i) : c_i \in \mathbb{R}, 0 = b_0 \le b_1 < \cdots < b_n < b_{n+1} = 1 \right\} \text{ s.t.}$$

$$J(u_n) = \min_{v \in \mathcal{M}_n(\Omega)} J(v)$$

$$J(v) = \frac{1}{2} \int_0^1 a(x)(v'(x))^2 dx - \int_0^1 f(x)v(x)dx + \frac{\gamma}{2}(v(1) - \beta)^2.$$

- **Error estimate for non-smooth solution in H^{1+a}**

$$\|u - u_n\|_a \le C \left(n^{-1} + \gamma^{-1/2} \right)$$

Algebraic Structure

- **Optimality conditions for critical points**

$$\mathbf{0} = \nabla_{\mathbf{c}} J(u_n) = \mathcal{A}(\mathbf{b})\,\mathbf{c} - \mathcal{F}(\mathbf{b}) \quad \text{and} \quad \mathbf{0} = \nabla_{\mathbf{b}} J(u_n) = \mathbf{D}(\mathbf{c})\,\{\mathbf{g} - \gamma(u_n(1) - \beta)\mathbf{1}\}$$

- **Coefficient and Hessian matrices**

$$\mathcal{A}(\mathbf{b}) = A(\mathbf{b}) + \gamma \mathbf{d}\mathbf{d}^T \quad \text{and} \quad \nabla^2_{\mathbf{b}} J(u_n) \equiv \mathcal{H}(\mathbf{c}, \mathbf{b}) = \mathbf{D}(\mathbf{c})\left(\mathbf{B}(\mathbf{b}) + \gamma \mathbf{c}\,\mathbf{1}^T\right)$$

where A(**b**) is symmetric positive definite and **B**(**b**) is diagonal

- **Condition number**

$$\kappa(A) = \mathcal{O}\left(n\,h_{\min}^{-1}\right) \quad \text{and} \quad \kappa(M) = \mathcal{O}\left(n\,h_{\min}^{-3}\right)$$

where A(**b**) and M(**b**) are ill-conditioned, but their inverses are tri-diagonal

damped Block Newton (dBN) Method

Algorithm 5.1 A damped block Newton (dBN) method for (3.4)

Input: Initial network parameters $\mathbf{b}^{(0)}$, coefficient function $a(x)$, the right-hand side function $f(x)$, boundary data α and β.
Output: Network parameters $\mathbf{c}$, $\mathbf{b}$

for $k = 0, 1 \ldots$ **do**

▷ *Linear parameters*

$\mathbf{c}^{(k+1)} \leftarrow \mathcal{A}\left(\mathbf{b}^{(k)}\right)^{-1} \mathcal{F}\left(\mathbf{b}^{(k)}\right)$

▷ *Non-linear parameters*

Compute the search direction $\mathbf{p}^{(k)}$ *as in* (5.7)

$\eta_k \leftarrow \underset{\eta \in \mathbb{R}^+}{\operatorname{argmin}}\, J(u_n(x; \mathbf{c}^{(k+1)}, \mathbf{b}^{(k)} + \eta \mathbf{p}^{(k)}))$

$\mathbf{b}^{(k+1)} \leftarrow \mathbf{b}^{(k)} + \eta_k \mathbf{p}^{(k)}$

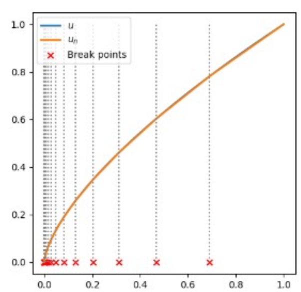
▷ *Redistribute non-contributing neurons and sort* $\mathbf{b}^{(k+1)}$

end for

C.-*Dokotorova-Falgout-Herrera,* Efficient shallow Ritz method for 1D diffusion problems, arXiv:2404.17750[math.NA]

1D Non-Smooth Solution

- **1D diffusion problem with non-smooth solution** $u(x)=x^{2/3}$ **in** $H^{1+1/6}$



Method (n breakpoints)	e_n	ξ_n	r
dBN (10)	1.41×10^{-1}	0.173	0.849
dBN (14)	1.08×10^{-1}	0.129	0.844
dBN (19)	8.16×10^{-2}	0.095	0.851
dBN (24)	6.71×10^{-2}	0.077	0.850
AdBN (14)	9.22×10^{-2}	0.106	0.903
AdBN (19)	7.05×10^{-2}	0.079	0.901
AdBN (24)	5.75×10^{-2}	0.063	0.899
aFEM (10)	3.39×10^{-1}	0.103	0.451
aFEM (27)	1.54×10^{-1}	0.049	0.570
aFEM (82)	6.88×10^{-2}	0.022	0.607
aFEM (122)	5.45×10^{-2}	0.017	0.606

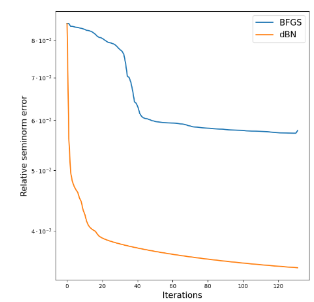


Table 3: Comparison of dBN, AdBN and aFEM for relative errors e_n, estimator errors ξ_n and powers r. The initial number of breakpoints for AdBN and aFEM is 10.

Summary

- **ReLU NN as a new class of approximating functions**

  Remarkable approximation property for non-smooth functions

- **NN discretization for interface problems**

  LSNN (a P^2NN approach) for HCLs

  No numerical artifacts such as overshooting, oscillation, or smearing

  Complicated and expensive iterative solvers

  ENN (an approach from physics to computation)

  Super accurate and efficient for 1D scalar HCLs comparing with existing methods

  Extension to multi-dimension?

- **Nonlinear iterative solvers for NN approximations**

  Structure-guided Gauss-Newton and Newton for shallow ReLU NN

THANK YOU

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https://www.math.purdue.edu/~caiz/paper.html