NEURAL NETWORKS IN SCIENTIFIC COMPUTING

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Outline

- **ReLU Neural Network (as a "new" class of approximating functions)**

- **Scalar Hyperbolic Conservation Laws**

  Least-Squares Neural Network (LSNN) Method (J. Chen, J. Choi, and M. Liu)

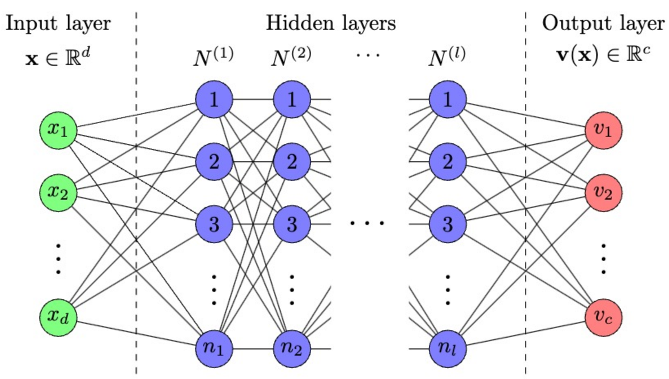
  Evolving Neural Network (ENN) Method (B. Hejnal)

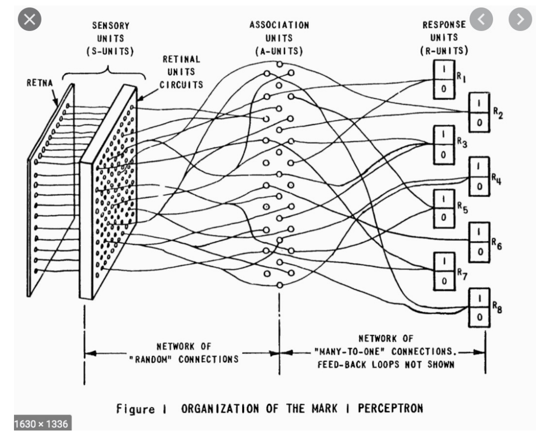
- **A Structure-guided Gauss-Newton Method**

  (T. Ding, M. Liu, X. Liu, and J. Xia)

Neural Network (NN)

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





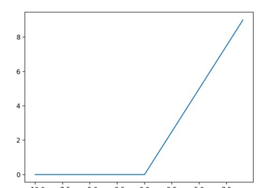
NN function

$$v(\mathbf{x}) = c_0 + \sum_{j=1}^{n_l} c_j \, x_j^{(l)}(\mathbf{x})$$

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

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

for $i = 1, \ldots, n_k$ and $k = 1, \ldots, l$



Free Knot Spline

- C^0 Linear spline (finite element) on a **fixed** mesh

$$\mathcal{S}_1^0(\Delta) = \text{span}\,\{\phi_i(x)\}_{i=0}^n = \left\{\sum_{i=0}^n c_i\phi_i(x) : c_i \in \mathcal{R}\right\} \qquad \phi_i(x) = \begin{cases} \dfrac{x - x_{i-1}}{x_i - x_{i-1}}, & x \in (x_{i-1}, x_i), \\ \dfrac{x_{i+1} - x}{x_{i+1} - x_i}, & x \in (x_i, x_{i+1}), \\ 0, & \text{otherwise} \end{cases}$$

$$u(x) = x^{0.01}, \ x \in [0,1]$$

- C^0 Linear **free knot** spline in [a,b] (1960s)

$$\begin{aligned} \mathcal{S}_1^0(n) &= \left\{\sum_{i=0}^n c_i\phi_i(x; x_{i-1}, x_i, x_{i+1}) : c_i \in \mathcal{R}, \ x_i \in [a,b]\right\} \\ &= \left\{c_0 + c_1(x-a) + \sum_{i=2}^n c_i\sigma(x - x_i) : c_i \in \mathcal{R}, \ x_i \in (a,b)\right\} \end{aligned}$$

Shallow ReLU NN in R^d

- **Shallow ReLU NN** (C^0 piecewise linear function)

$$\mathcal{M}_n(d) = \left\{ c_0 + \sum_{i=1}^{n} c_i \sigma(\boldsymbol{\omega}_i \mathbf{x} + b_i) : c_i, b_i \in \mathcal{R},\ \boldsymbol{\omega}_i \in \mathcal{S}^{d-1} \right\}$$

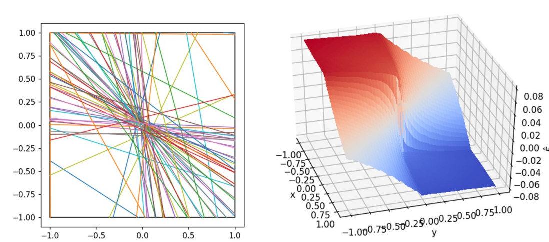
- **Linear Independence**

$\{\sigma(\boldsymbol{\omega}_i \mathbf{x} + b_i)\}_{i=1}^{n}$ are linearly independent if $\{\mathcal{P}_i\}_{i=1}^{n}$ are distinct.

- **Breaking Hyper-Planes**

$$\mathcal{P}_i : \boldsymbol{\omega}_i \mathbf{x} + b_i = 0 \quad \text{for } i = 1, \ldots, n$$

- **Physical Partition of NN approximation to Kellogg function**



(h) Optimum break lines (69 neurons, 1286 elements)

(i) Optimum NN model of 69 neurons, $\xi = 0.008476$

How to Design NN Methods from Numerical Analysis Perspective?

- **For a given PDE, start with a proper equivalent formulation**

  natural energy minimization

  various artificial least-squares minimizations

- **Choose a proper NN architecture -- a difficult task (adaptive NN, Liu-C. 22)**
- **Numerical Issues**
  - Numerical Integration (important): adaptive numerical integration (L-C-R 23)
  - Numerical Differentiation (critical): proper discrete differential operator
  - Algebraic solver (training NN) (critical): iterative solvers ???

Physics-Informed Neural Network (PINN)

Dissanayake-Phan-Tien (94), Lagaris-Likas-Ftiadis (98), Rasissi-Perdikaris-Karniadakis (19), …

PDE: $\mathcal{L}(u(x)) = 0$ at $x \in \Omega \in \mathcal{R}^d$ and $\mathcal{B}(u(x)) = 0$ at $x \in \partial\Omega$

training data: $\{x_i^u\}_{i=1}^{N_u} \subset \Omega$ and $\{x_i^b\}_{i=1}^{N_b} \subset \partial\Omega$

l^2 **residual:** $$L(u) = \frac{1}{N_u}\sum_{i=1}^{N_u}\left(\mathcal{L}(u(x_i^u))\right)^2 + \frac{1}{N_b}\sum_{i=1}^{N_b}\left(\mathcal{B}(u(x_i^b))\right)^2$$

PINN: $$u_{\mathcal{N}} = \arg\min_{v\in\mathcal{N}} L(v)$$

PDE at points: $\mathcal{L}(u(x_i^u)) = 0$ and $\mathcal{B}(u(x_i^b)) = 0$ for $i = 1, \ldots, N_u(N_b)$

(continuous LS) $G(u) = \int_\Omega \left[\mathcal{L}(u(x))\right]^2 dx + \int_{\partial\Omega} \left[\mathcal{B}(u(x))\right]^2 ds$

PINN is a discrete least-squares neural network (LSNN) method and produces unreasonable approximation!

Scalar Hyperbolic Conservation Laws

- **Scalar Nonlinear Hyperbolic Conservation Laws**

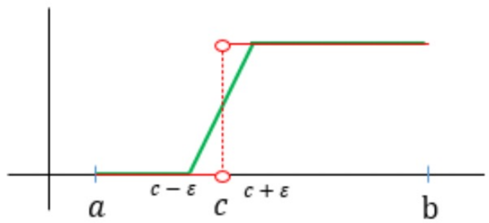
$$\begin{cases} \dfrac{\partial}{\partial t} u(\mathbf{x},t) + \displaystyle\sum_{i=1}^{d} \dfrac{\partial}{\partial x_i} f_i(u(\mathbf{x},t)) & = & 0, & \text{in} \quad \mathcal{R}^d \times (0,T), \\ u(\mathbf{x},0) & = & u_0(\mathbf{x}), & \text{in} \quad \mathcal{R}^d \end{cases}$$

- **Numerical Difficulties**
  - PDE theory
  - Discontinuous solution with unknown interfaces

Approximation to Unit Step Function with Unknown Interface

- **Unit step function and its CPWL approximation**

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



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

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

- **How to compute or approximate $p_c(x)$ when c is unknown?**

(1) On fixed quasi-uniform mesh

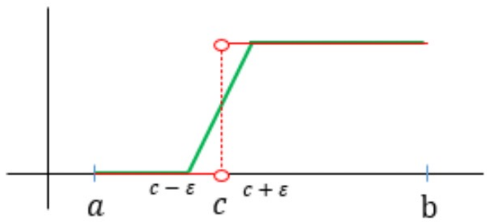
- very fine mesh-size: $h = \varepsilon$
- overshooting, oscillation, etc.

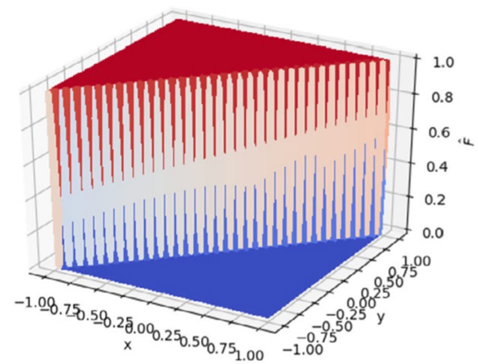
(2) On moving mesh (neural network)

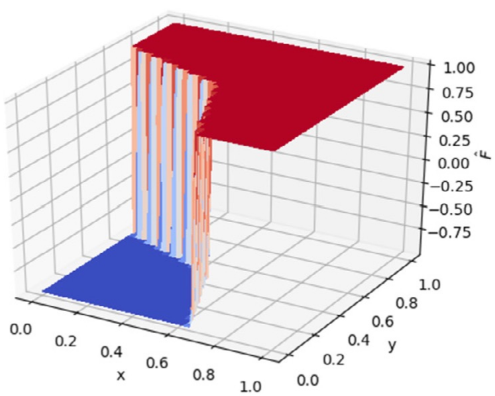
- two neurons
- no overshooting or oscillation

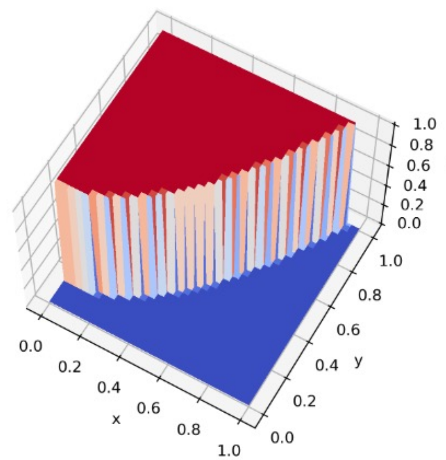
$$p_c(x) = \frac{1}{b_2 - b_1}\left[\sigma(x - b_1) - \sigma(x - b_2)\right], \quad b_1 = c - \varepsilon, \; b_2 = c + \varepsilon$$

Interface of Unit Step Function in R^d









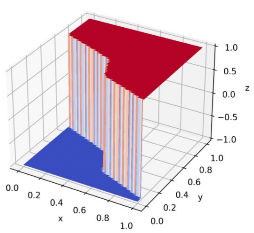
Approximation to Unit Step Function with Unknown Interface in R^d

- **Piecewise Constant function with unknow interface**

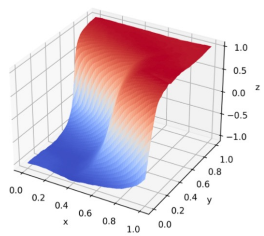
C., J. Choi, and M. Liu (2022) (d=2, 3, l=2; d=4,...,8, l=3)

Let χ(x) be a piecewise constant function with C^0 piecewise smooth interface I, then there exists a CPWL function p(x) generated by a NN with L=$\lceil \log_2(d+1) \rceil$ hidden layers such that for any given $\varepsilon > 0$, we have

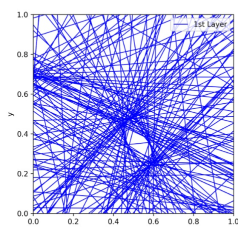
$$\left|\!\left|\!\left| \chi - p \right|\!\right|\!\right|_{\boldsymbol{\beta}} \le \sqrt{2|I|}\,\left|\alpha_1 - \alpha_2\right|\sqrt{\varepsilon},$$



(b) Exact solution

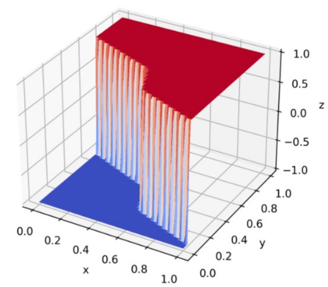


(c) 2 layer NN approximation



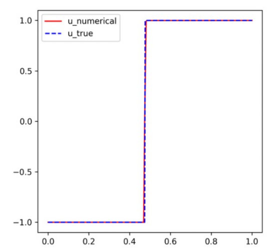
(g) 2 layer NN breaking lines

2-300-1

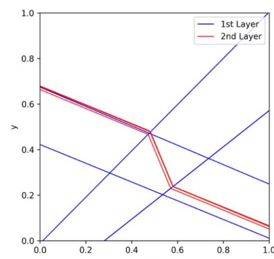


(d) 3 layer NN approximation

2-5-5-1



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



(h) 3 layer NN breaking lines

Linear Advection-Reaction Problem and its Least-squares Formulation

- **Linear advection-reaction problem**

$$u_{\boldsymbol\beta} + \gamma\, u = f \text{ in } \Omega, \qquad u\big|_{\Gamma_-} = g$$

- **Least-squares formulation** Find $u \in V_{\boldsymbol\beta}(\Omega) = \{v \in L^2(\Omega) : v_{\boldsymbol\beta} \in L^2(\Omega)\}$ such that

$$\mathcal{L}(u; \mathbf{f}) = \min_{v \in V_{\boldsymbol\beta}} \mathcal{L}(v; \mathbf{f})$$

where $\mathcal{L}(v; \mathbf{f}) = \|v_{\boldsymbol\beta} + \gamma\, v - f\|^2_{0,\Omega} + \|v - g\|^2_{-\boldsymbol\beta}$

- **Coercivity and continuity** there exists positive constants α and M such that

$$\alpha\, |||v|||^2_{\boldsymbol\beta} \le \mathcal{L}(v; \mathbf{0}) \le M\, |||v|||^2_{\boldsymbol\beta}$$

De Sterck-Manteuffel-McCormick-Olson, 2004

Numerical Issues

- **Numerical integration**

$$\int_{\Omega} (v_{\boldsymbol{\beta}} + \gamma\, v - f)^2\, (\mathbf{x})\, d\mathbf{x}$$

Adaptive numerical integration (Liu-Ramani-C 2023)

- **Numerical differentiation**

$$u_{\boldsymbol{\beta}}(\mathbf{x}) = \sum_{i=1}^{d} \beta_i(\mathbf{x}) \frac{\partial u(\mathbf{x})}{\partial x_i}.$$

Is invalid at where the solution is discontinuous.

Physics-preserved numerical differentiation

$$D_{\boldsymbol{\beta}} v(\mathbf{x}) := \frac{v(\mathbf{x}) - v\big(\mathbf{x} - \rho\bar{\boldsymbol{\beta}}(\mathbf{x})\big)}{\rho/|\boldsymbol{\beta}(\mathbf{x})|} \approx v_{\boldsymbol{\beta}}(\mathbf{x}),$$

- **Algebraic solver (training algorithm)** ???

Least-squares neural network (LSNN) method

- **Discrete LS functional**

$$\mathcal{L}_{\mathcal{T}}\left(v;\mathbf{f}\right) = \sum_{K\in\mathcal{T}} \mathcal{Q}_K\left((D_{\boldsymbol{\beta}}v + \gamma v - f)^2\right).$$

- **LSNN method** find $u_{\mathcal{T}}^N \in \mathcal{M}(L,n)$ such that

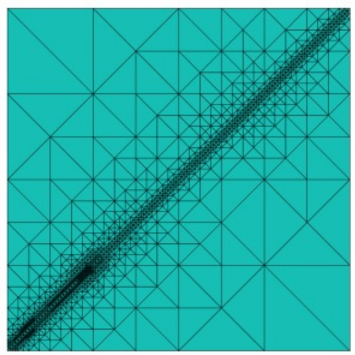
$$\mathcal{L}_{\mathcal{T}}\left(u_{\mathcal{T}}^N;\mathbf{f}\right) = \min_{v\in\mathcal{M}(L,n)} \mathcal{L}_{\mathcal{T}}\left(v;\mathbf{f}\right)$$

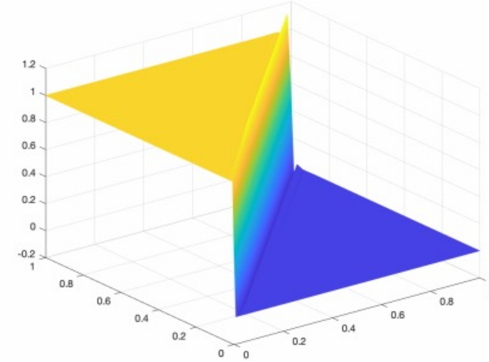
- **A priori error estimate**

$$|||u - u_N|||_{\boldsymbol{\beta}} \le C\left(\left|\alpha_1 - \alpha_2\right|\sqrt{\varepsilon} + \inf_{v\in\mathcal{M}(d,n)} |||\hat{u} + p - v|||_{\boldsymbol{\beta}}\right)$$

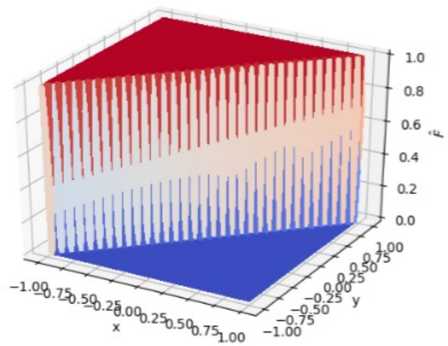
C.-Chen-Liu, JCP, 443 (2021), 110514; C.-Choi-Liu (2022)

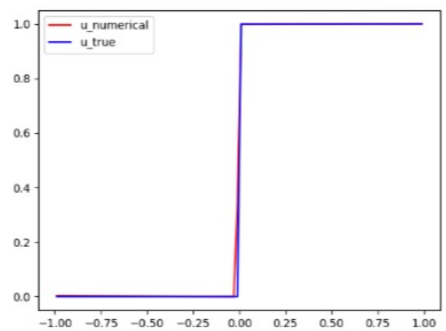
Famous Transport Equation $u_t+u_x=0$

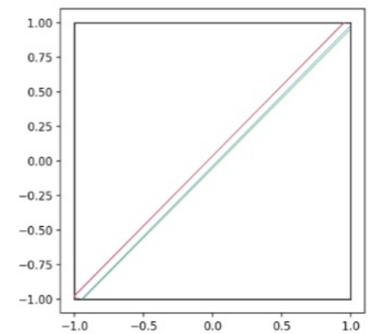




Liu-Zhang, CMAME, 2020

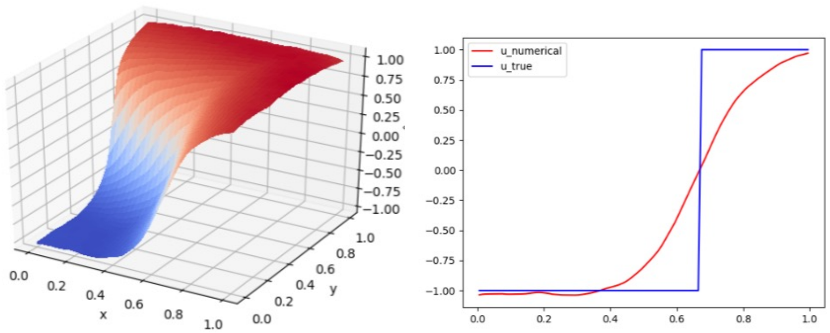






(2-6-1)

C.-Chen-Liu, JCP, 2021



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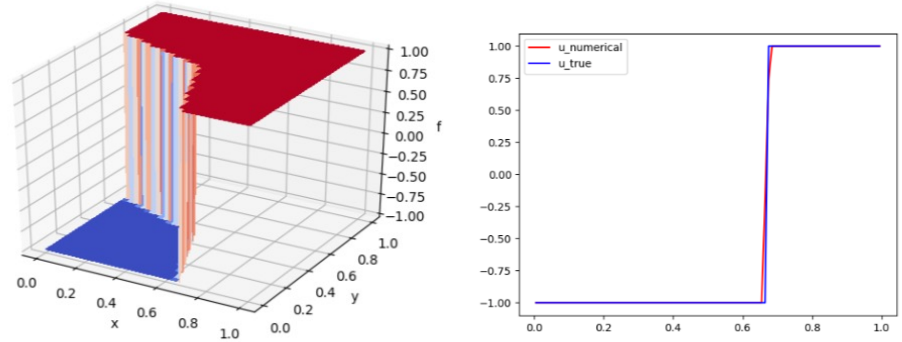
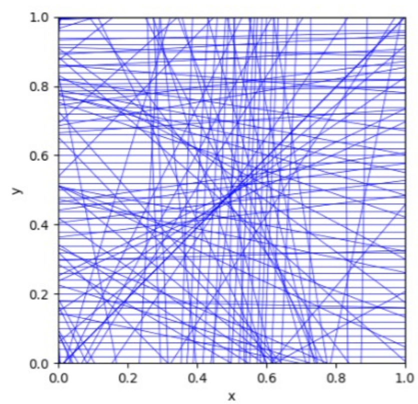
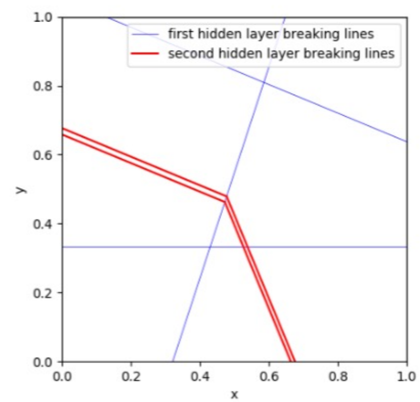


(2-5-5-1)



(e) 2-layer NN breaking lines



(f) 3-layer NN breaking lines

C.-Chen-Liu, LSNN method for linear advection-reaction equation, JCP, 443(2021), 110514.

Least-Squares Neural Network (LSNN) method

- **Scalar nonlinear hyperbolic conservation laws**

$$\frac{\partial}{\partial t}u(\mathbf{x},t)+\sum_{i=1}^{d}\frac{\partial}{\partial x_i}f_i(u(\mathbf{x},t))=0,\ \text{ in } \mathcal{R}^d\times(0,T),\qquad u(\mathbf{x},0)=u_0(\mathbf{x}),\ \text{ in } \mathcal{R}^d$$

- **Least-squares formulation**

Find $u \in V_{\mathbf{f}} = \{v \in L^2(\Omega)\times I \,|\, (\mathbf{f}(v), v) \in H(\text{div};\, \Omega \times I)\}$ such that

$$u = \operatorname*{arg\,min}_{v\in V_{\mathbf{f}}} \mathcal{L}(v;\mathbf{f}),\qquad \text{where } \mathcal{L}(v;\mathbf{f}) = \|v_t+\nabla_{\mathbf{x}}\cdot\mathbf{f}(v)\|^2_{0,\Omega\times I}+\|v(\cdot,0)-u_0\|^2_{0,\Omega}$$

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

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

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

Discrete Divergence Operator

- Divergence operator

$$0 = u_t + \nabla \cdot \mathbf{f}(u) = \textbf{div}\,(\mathbf{f}(u), u) = \textbf{div}\,\mathbf{F}(u)$$

- Discrete divergence operator
  + based on conservative numerical schemes (C.-Chen-Liu, ANM(2022))
  + new 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.

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

Discrete Divergence Operator in 1D

- **Primitive form over K_{ij}**

$$\frac{1}{|K_{ij}|}\int_{\partial K_{ij}} \mathbf{F}(u)\cdot\mathbf{n}ds = \frac{1}{\delta}\int_{t_j}^{t_{j+1}} \sigma(x_i, x_{i+1}; t)\, dt + \frac{1}{h}\int_{x_i}^{x_{i+1}} u(x; t_j, t_{j+1})dx$$

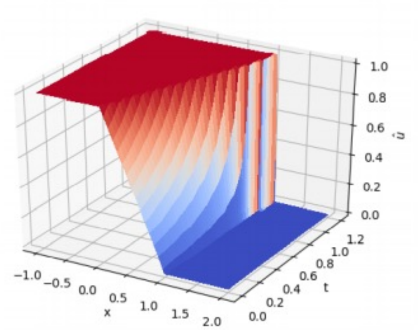
$$\approx \frac{1}{\delta}Q(\sigma(x_i, x_{i+1}; t); t_j, t_{j+1}, \hat{n}) + \frac{1}{h}Q(u(x; t_j, t_{j+1}); x_i, x_{i+1}, \hat{m}) = \mathsf{div}_{\mathcal{T}}\mathbf{F}\big(u_{ij}\big)$$

- **Error estimate**

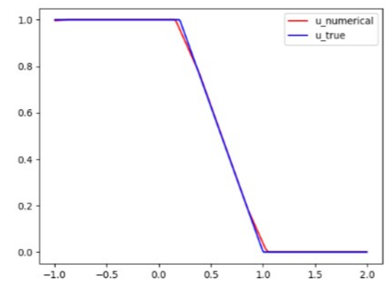
Lemma 4.3. *Assume that u is a C^2 function of t and a piece-wise C^2 function of x on two vertical and two horizontal edges of K_{ij}, respectively. Moreover, u has only one discontinuous point on each horizontal edge. Then there exists a constant $C > 0$ such that*

$$\|\mathbf{div}_{\mathcal{T}}\mathbf{f}(u) - \mathrm{avg}_{\mathcal{T}}\mathbf{div}\,\mathbf{f}(u)\|_{L^p(K_{ij})}$$

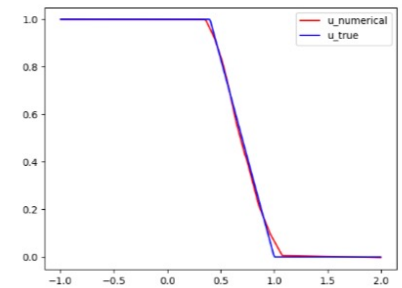
$$\leq C\left(\frac{h^{1/p}\delta^2}{\hat{n}^2} + \frac{h^2\delta^{1/p}}{\hat{m}^2} + \frac{h\delta^{1/p}}{\hat{m}^{1+1/q}}\right) + \frac{(h\delta)^{1/p}}{\hat{m}}\sum_{l=j}^{j+1}[\![u_{ij}]\!]_{t_l}. \tag{4.7}$$



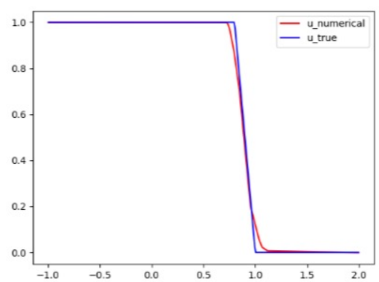
(a) Exact solution u on $\Omega \times I$



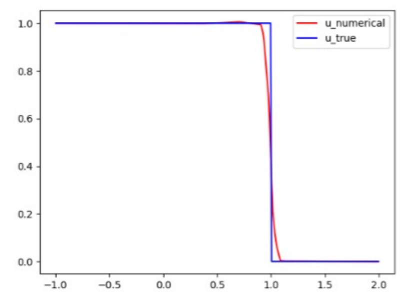
(a) Traces of exact solution and approximation $u_{1,\mathcal{T}}$ on the plane $t = 0.2$



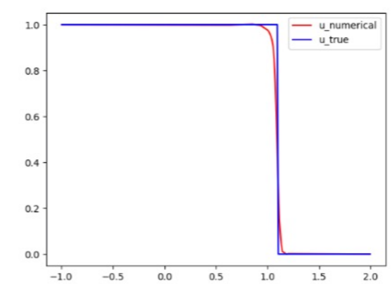
(c) Traces of exact and numerical solutions $u_{2,\mathcal{T}}$ on the plane $t = 0.4$



(d) Traces of exact solution and approximation $u_{4,\mathcal{T}}$ on the plane $t = 0.8$



(e) Traces of exact solution and approximation $u_{5,\mathcal{T}}$ on the plane $t = 1.0$

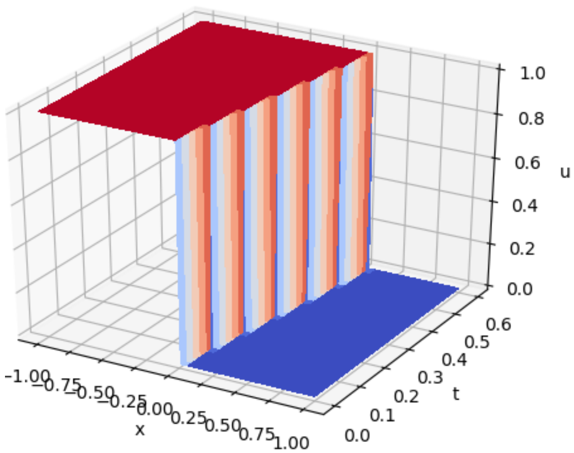


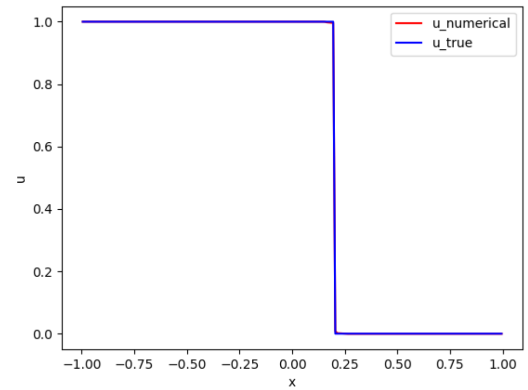
(f) Traces of exact solution and approximation $u_{6,\mathcal{T}}$ on the plane $t = 1.2$

C.-Chen-Liu, Applied Numer. Math., 174 (2022), 163-176

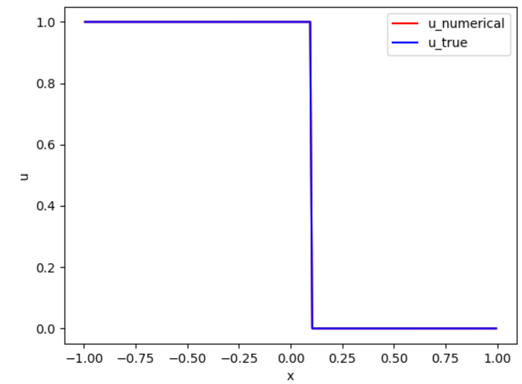
Inviscid Burger Equation $f(u) = \frac{1}{2}u^2$

Riemann Problem Shock formation: exact solution

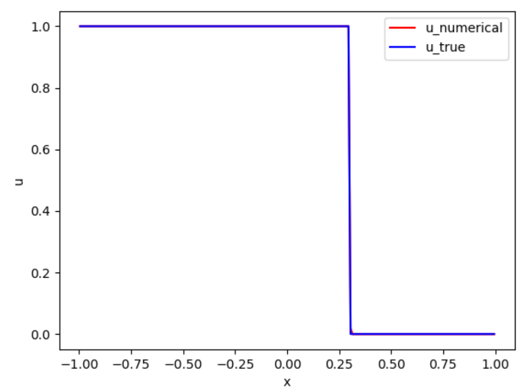




t=0.2



t=0.4

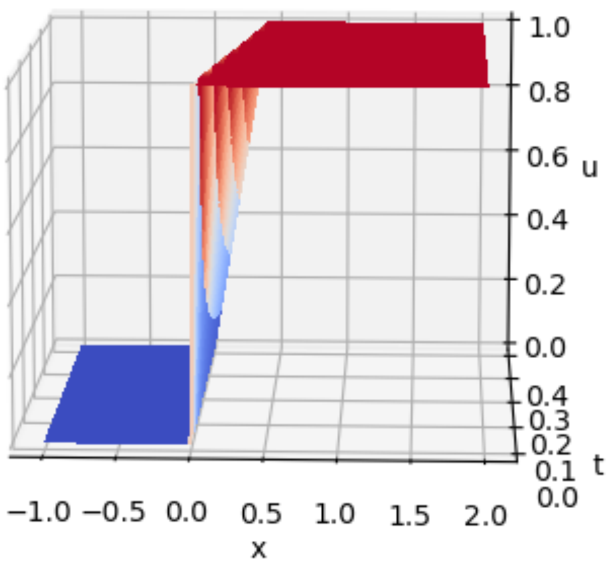


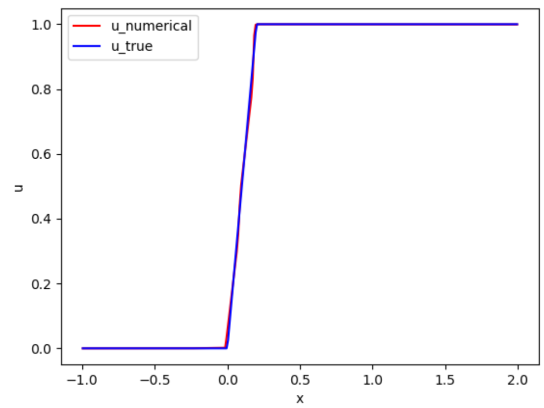
t=0.6

(2-10-10-1)

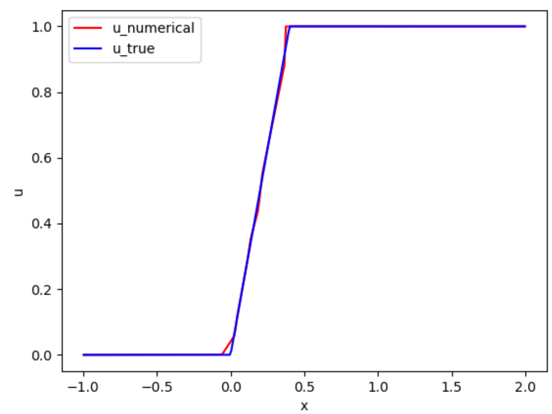
C.-Chen-Liu, arXiv: 2110.10895 [math.NA]

Riemann Problem
Rarefaction wave: exact solution





t=0.2

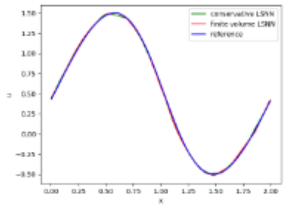


t=0.4

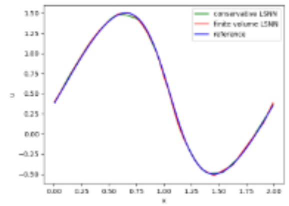
(2-10-10-1)

Inviscid Burgers equation with smooth initial

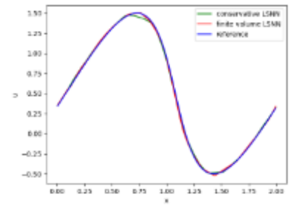
$$u_0(x) = 0.5 + \sin(\pi x).$$



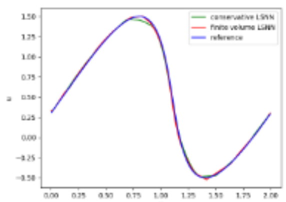
(a) Traces of reference and numerical solutions $u_{1,\mathcal{T}}$ on the plane $t = 0.05$



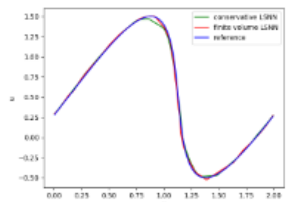
(b) Traces of reference and numerical solutions $u_{2,\mathcal{T}}$ on the plane $t = 0.1$



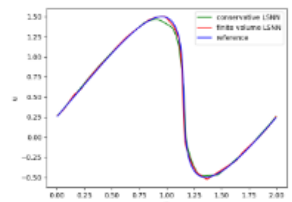
(c) Traces of reference and numerical solutions $u_{3,\mathcal{T}}$ on the plane $t = 0.15$



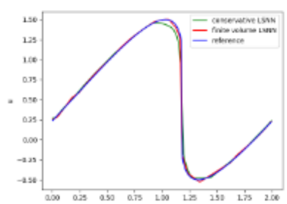
(d) Traces of reference and numerical solutions $u_{4,\mathcal{T}}$ on the plane $t = 0.2$



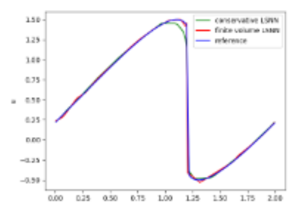
(e) Traces of reference and numerical solutions $u_{5,\mathcal{T}}$ on the plane $t = 0.25$



(f) Traces of reference and numerical solutions $u_{6,\mathcal{T}}$ on the plane $t = 0.3$



(g) Traces of reference and numerical solutions $u_{7,\mathcal{T}}$ on the plane $t = 0.35$

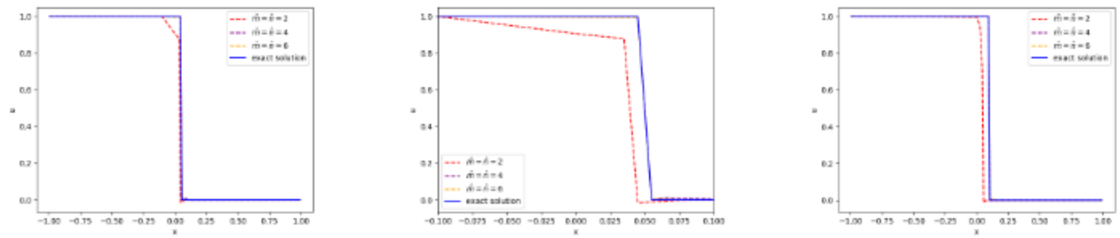


(h) Traces of reference and numerical solutions $u_{8,\mathcal{T}}$ on the plane $t = 0.4$

(2-30-30-1)

Fig. 3. *Approximation results of Burgers' equation with a sinusoidal initial condition*

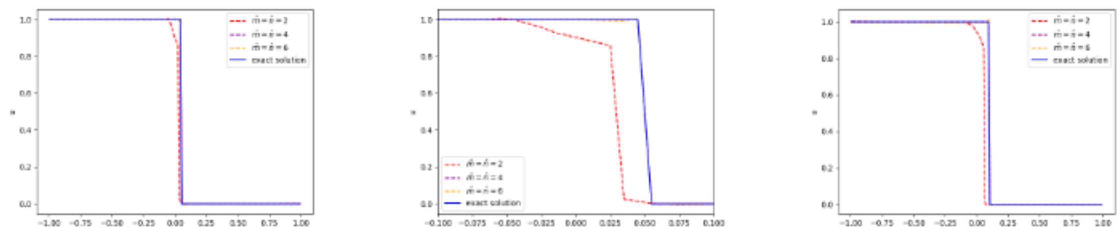
Riemann Problem with Higher order flux $f(u) = \frac{1}{4}u^4$



(a) Traces of exact and numerical solutions $u_{1,\mathcal{T}}$ using the trapezoidal rule on the plane $t = 0.2$

(b) Zoom-in plot near the discontinuous interface of sub-figure (a)

(c) Traces of exact and numerical solutions $u_{2,\mathcal{T}}$ using the trapezoidal rule on the plane $t = 0.4$



(d) Traces of exact and numerical solutions $u_{1,\mathcal{T}}$ using the mid-point rule on the plane $t = 0.2$

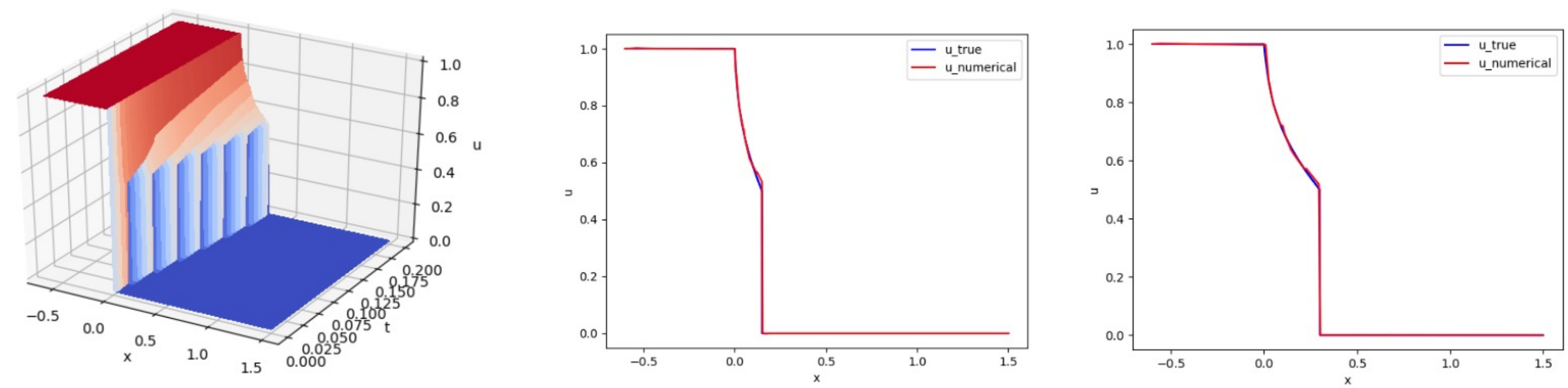
(e) Zoom-in plot near the discontinuous interface of sub-figure (d)

(f) Traces of exact and numerical solutions $u_{2,\mathcal{T}}$ using the mid-point rule on the plane $t = 0.4$

FIG. 5. *Numerical results of the problem with* $f(u) = \frac{1}{4}u^4$ *using the composite trapezoidal and mid-point rules*

(2-10-10-1)

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

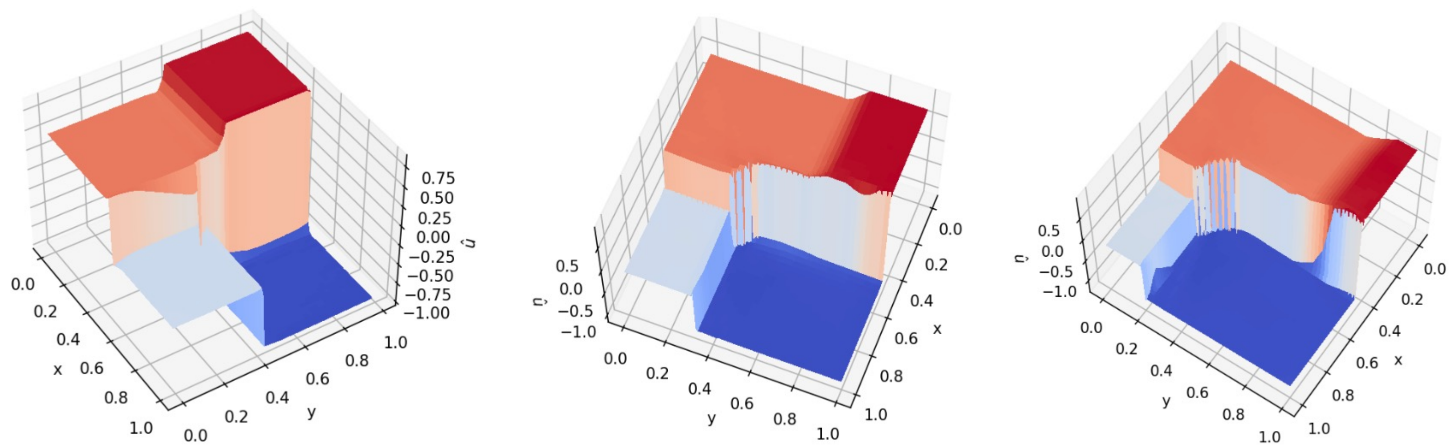


(a) Numerical solution u_N on Ω (b) Traces at $t = 0.1$ (c) Traces at $t = 0.2$

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**

$$
\left\{
\begin{array}{rcll}
\dfrac{\partial}{\partial t}u(x,t) + \dfrac{\partial}{\partial x} f\big(u(x,t)\big) & = & 0, & \text{in } \ \Omega \times (0,T), \\[2ex]
u(x,t) & = & g(t), & \text{on } \ \Gamma_-, \\[2ex]
u(x,0) & = & u_0(x), & \text{in } \ \Omega
\end{array}
\right.
$$

- **Characteristic Line**

$$
\left\{
\begin{array}{rcl}
\dfrac{d}{dt}x(t) & = & f'\big(u(x(t),t)\big) \\[2ex]
x(t_0) & = & x_0
\end{array}
\right.
$$

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

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

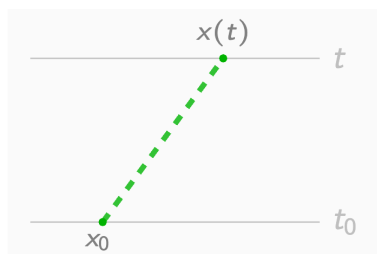
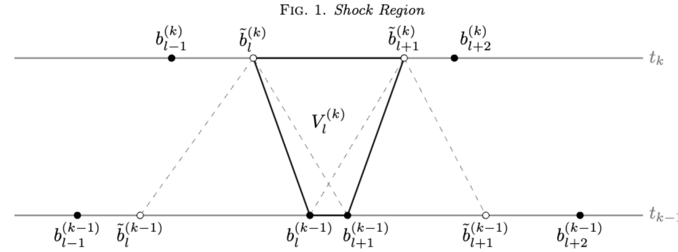


Fig. 1. *Shock Region*



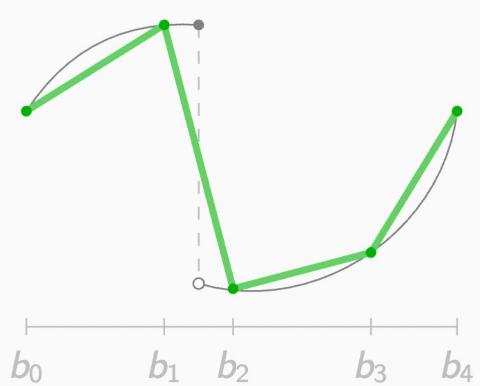
Representation of Initial Data

Set of Neural Network Functions:

$$M_n = \left\{ N(x) = c_{-1} + \sum_{i=0}^{n} c_i \sigma(\omega_i x - b_i) \,:\, b_i,\ c_i,\ \omega_i \in \mathbb{R} \right\}$$

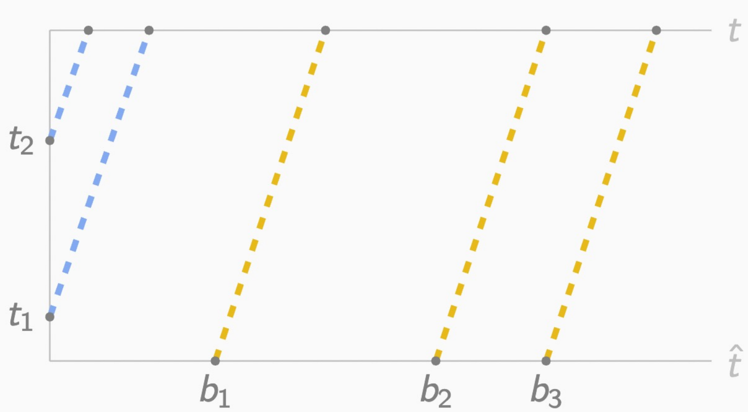
Least-Squares Approximation: Find $u_N^{(0)} \in M_n$ such that

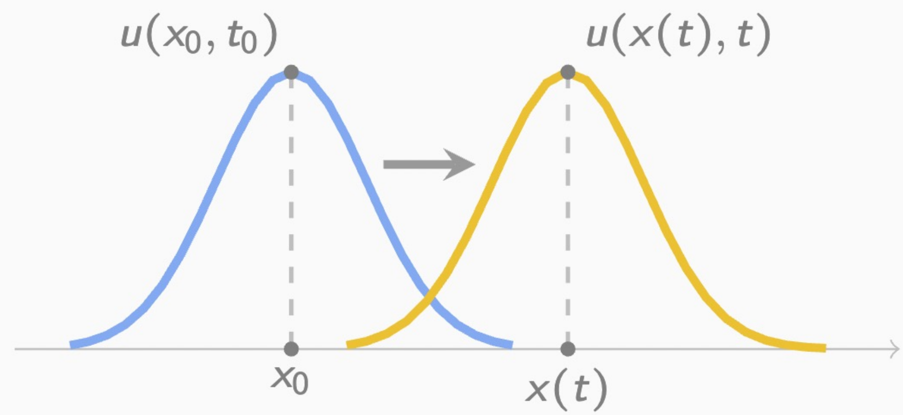
$$\| u_N^{(0)} - u_0 \|_{L^2(\Omega)} = \min_{v \in M_n} \| v - u_0 \|_{L^2(\Omega)}$$



Characteristic Scheme

- Propagate breaking points of the initial and boundary data

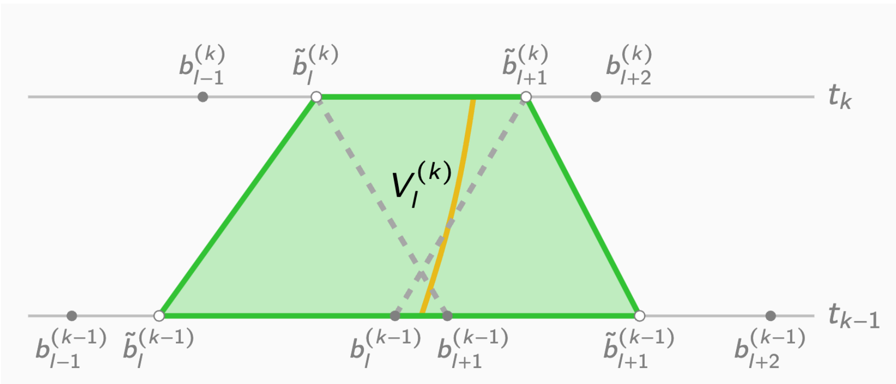




- Error Estimate

$$\left\| u(\cdot, t_k) - u_N^{(k)} \right\|_{L^p(\Omega)} \leq \left(\left\| u_0 - u_N^{(0)} \right\|_{L^p(\Omega)}^p + \| g - g_N \|_{L^p(I)}^p \right)^{1/p}$$

Finite Volume Characteristic Scheme



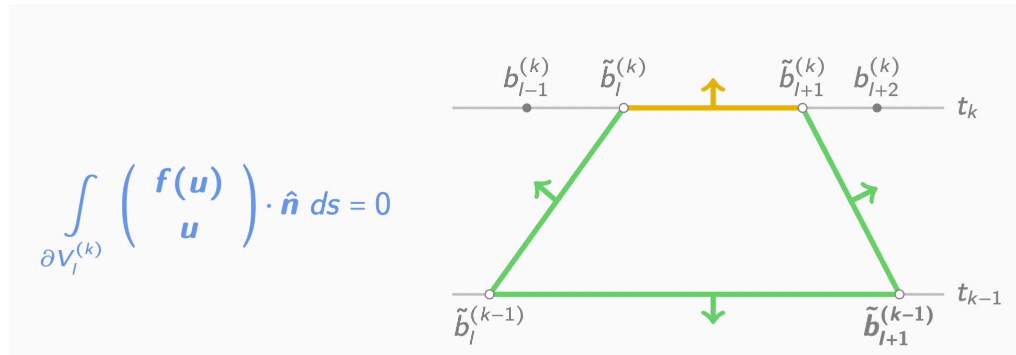
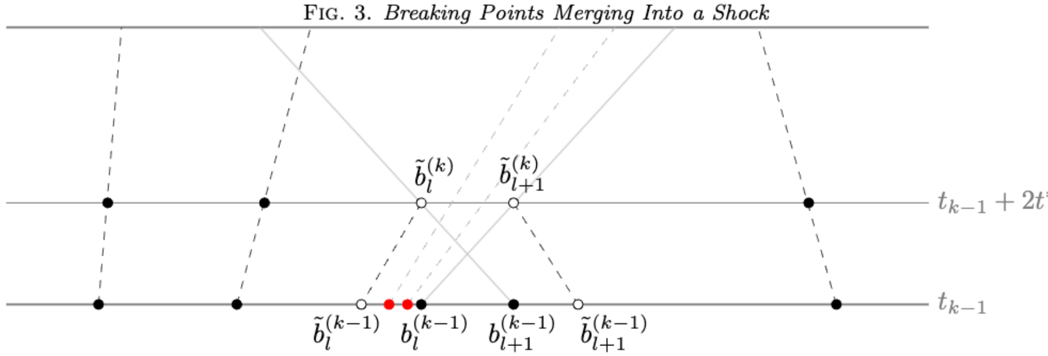
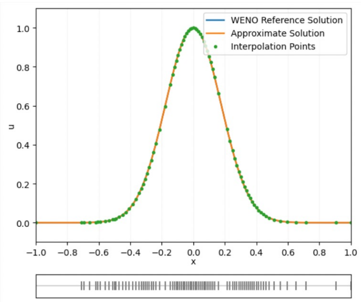


FIG. 3. *Breaking Points Merging Into a Shock*

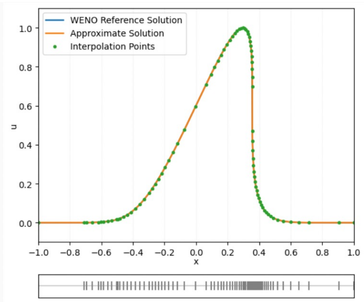


Shock Formation (exponential initial profile)

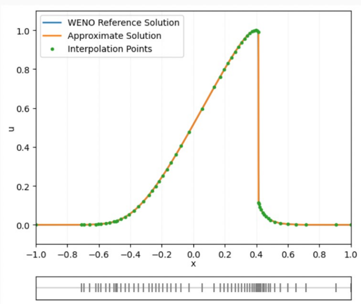
Inviscid Burgers' Equation



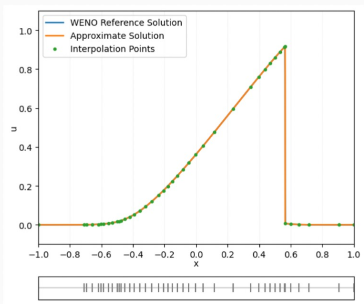
Initial data



$t = 0.3$



$t = 0.4$



$t = 0.7$

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

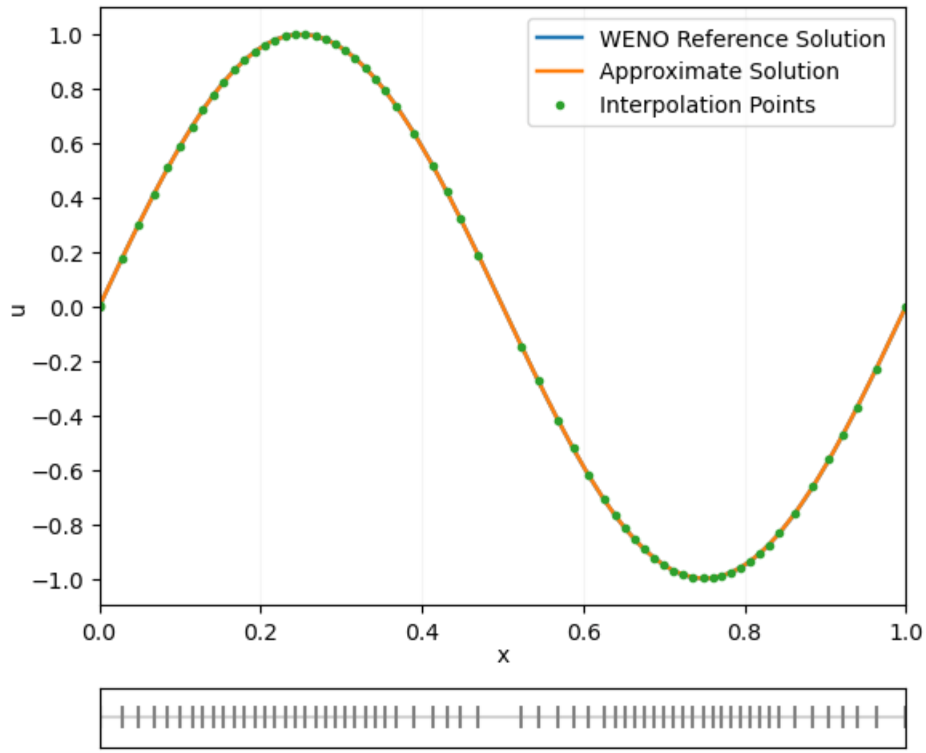
Time	$\frac{\|\tilde{u}(\cdot,t_k)-u_N^{(k)}\|_{L^2(\Omega)}}{\|\tilde{u}(\cdot,t_k)\|_{L^2(\Omega)}}$	n_k
0.0	6.6923×10^{-4}	78
0.1	7.8352×10^{-4}	78
0.2	4.0166×10^{-2}	56
0.3	5.1491×10^{-2}	38
0.4	5.3515×10^{-2}	30
0.5	5.4162×10^{-2}	25

ENN

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

WENO

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

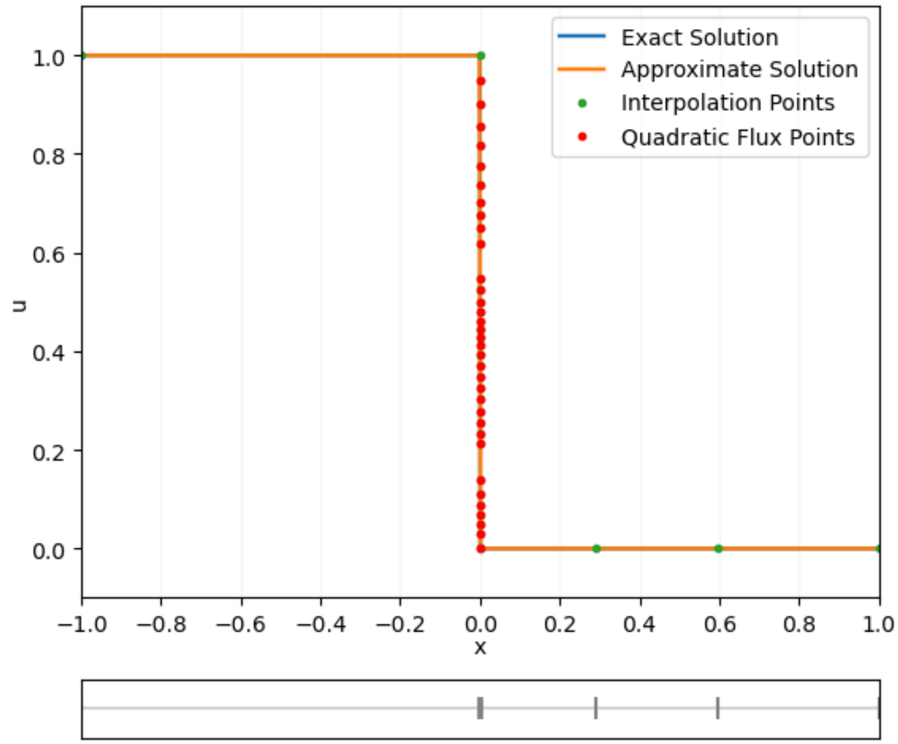


Compound Wave

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



Summary

- **NN provides a new class of approximating functions**

  "Moving" mesh vs uniform mesh and adaptive mesh

- **Scalar hyperbolic conservation laws**

  LSNN (a space-time approach)

  No numerical artifacts such as overshooting, oscillation, or smearing
  Complicated and expensive iterative solvers

  ENN (a time-marching approach)

  Super accurate and efficient for 1D scalar HCLs comparing with existing methods
  Extension to multi-dimension?

18th Copper Mountain Conference on
Iterative Methods
April 14-19, 2024

A Structure-Guided Gauss-Newton Method for Shallow ReLU Neural Network

Z. Cai

Collaborators: Tong Ding, Min Liu, Xinyu Liu, and Jianlin Xia

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

PURDUE UNIVERSITY

Department of Mathematics [1]
School of Mechanical Engineering [2]

Non-Convex Optimization in Machine Learning

Supervised Machine Learning (Least-squares Data Fitting)

For a given data set $\{(\mathbf{x}^i, u^i)\}_{i=1}^m$ with $\mathbf{x}^i \in \Omega \subset \mathcal{R}^d$ and $u^i \in \mathcal{R}$, let

- $\mathcal{J}(v) = \frac{1}{2}\sum_{i=1}^{m} \mu^i \left(v(\mathbf{x}^i;\boldsymbol{\theta}) - u^i\right)^2$ be a discrete LS loss function
- $\mathcal{M}_n(\Omega;\boldsymbol{\theta})$ be a set of neural network functions

finding $u_n(\mathbf{x}) \in \mathcal{M}_n(\Omega)$ such that

$$u_n(\mathbf{x}) = \arg\min_{v\in\mathcal{M}_n(\Omega)} \mathcal{J}(v) \qquad \text{or } u_n(\mathbf{x};\boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \mathcal{J}(v(\cdot;\boldsymbol{\theta})) = \arg\min_{\boldsymbol{\theta}\in R^N} f(\boldsymbol{\theta})$$

Iterative/Optimization/Training Algorithms

methods of gradient descent (Adam, SGD, ...),
Newton's methods (BFGS, ...),

Gauss-Newton's Methods

"Iterative Solution of Nonlinear Equations in Several Variables" by Ortega and Rheinboldt (1970)

268 8. MINIMIZATION METHODS

where we assume, of course, that the indicated inverse exists. In the special case that $f(x) = \frac{1}{2}x^{\mathrm{T}}x$, (4) reduces to the *Gauss–Newton method*

$$x^{k+1} = x^k - [F'(x^k)^{\mathrm{T}} F'(x^k)]^{-1} F'(x^k)^{\mathrm{T}} Fx^k, \qquad k = 0, 1, \ldots, \tag{5}$$

and, therefore, we shall call (4) a *generalized Gauss–Newton method*. Note that the iterate x^{k+1} of (5) is simply the unique global minimizer of the quadratic functional

$$[Fx^k + F'(x^k)(x - x^k)]^{\mathrm{T}} [Fx^k + F'(x^k)(x - x^k)],$$

and, hence, (5) is a paraboloid method for (2) in the sense of **8.1**.

In place of (5), we may also consider the modified Gauss–Newton iteration with parameters ω_k and λ_k :

$$x^{k+1} = x^k - \omega_k[F'(x^k)^{\mathrm{T}} F'(x^k) + \lambda_k I]^{-1} F'(x^k)^{\mathrm{T}} Fx^k. \tag{6}$$

Since $F'(x^k)^{\mathrm{T}} F'(x^k)$ is symmetric, positive semidefinite, the inverse in (6) will always exist provided only that $\lambda_k > 0$. As in **8.2**, the parameter ω_k may be chosen to ensure that $g(x^{k+1}) \leqslant g(x^k)$. Alternatively, this decrease may also be achieved by a suitable selection of λ_k (see **E 8.3-4**).

$$g(x) = \tfrac{1}{2}(Fx)^{\mathrm{T}} Fx$$

Levenberg-Marquardt's method

PURDUE UNIVERSITY

Non-Convex Optimization in Machine Learning

Supervised Machine Learning (Least-squares Data Fitting)

For a given data set $\left\{\left(\mathbf{x}^i, u^i\right)\right\}_{i=1}^m$ with $\mathbf{x}^i \in \Omega \subset \mathcal{R}^d$ and $u^i \in \mathcal{R}$, let

- $\mathcal{J}(v) = \frac{1}{2}\sum_{i=1}^m \mu^i \left(v(\mathbf{x}^i;\boldsymbol{\theta}) - u^i\right)^2$ be a discrete LS loss function
- $\mathcal{M}_n(\Omega;\boldsymbol{\theta})$ be a set of neural network functions

finding $u_n(\mathbf{x}) \in \mathcal{M}_n(\Omega)$ such that

$$u_n(\mathbf{x}) = \underset{v\in\mathcal{M}_n(\Omega)}{\arg\min}\ \mathcal{J}(v) \qquad \text{or} \quad u_n(\mathbf{x};\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\arg\min}\, \mathcal{J}(v(\cdot;\boldsymbol{\theta})) = \underset{\boldsymbol{\theta}\in R^N}{\arg\min} f(\boldsymbol{\theta})$$

Iterative/Optimization/Training Algorithms

methods of gradient descent (Adam, SGD, ...),
Newton's methods (BFGS, ...),
Gauss-Newton's methods

Algebraic Systems for Critical Points

- **neural network approximation**

$$u_n(\mathbf{x}) = c_0 + \sum_{i=1}^{n} c_i \sigma(\boldsymbol{\omega}_i \cdot \mathbf{x} + b_i) = c_0 + \sum_{i=1}^{n} c_i \sigma(\mathbf{r}_i \cdot \mathbf{y})$$

- **linear and nonlinear parameters**

$$\hat{\mathbf{c}} = (c_0, \mathbf{c}) \qquad \text{with } \mathbf{c} = (c_1, \ldots, c_n)$$

$$\text{and } \mathbf{r} = (\mathbf{r}_1, \ldots, \mathbf{r}_n) \qquad \text{with } \mathbf{r}_i = (\boldsymbol{\omega}_i, b_i)$$

- **Algebraic Systems for Critical Points**

$$\nabla_{\hat{\mathbf{c}}} \mathcal{J}\left(u_n(\cdot; \hat{\mathbf{c}}, \mathbf{r})\right) = \mathbf{0} \quad \text{and} \quad \nabla_{\mathbf{r}} \mathcal{J}\left(u_n(\cdot; \hat{\mathbf{c}}, \mathbf{r})\right) = \mathbf{0}$$

Mass and Layer Gauss-Newton Matrices

- **Mass Matrix A(r) for linear parameters**

$$\mathbf{0} = \nabla_{\hat{\mathbf{c}}} \mathcal{J}\left(u_n(\cdot; \hat{\mathbf{c}}, \mathbf{r})\right) = \mathbf{A}(\mathbf{r})\, \hat{\mathbf{c}} - \mathbf{f}(\mathbf{r})$$

where $\mathbf{A}(\mathbf{r}) = \sum_{i=1}^{m} \mu^i \left[\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T\right](\mathbf{x}^i)$ is SPD

- **Gradient with respect to r**

$$\mathbf{0} = \nabla_{\mathbf{r}} \mathcal{J}\left(u_n(\cdot; \hat{\mathbf{c}}, \mathbf{r})\right) = (D(\mathbf{c}) \otimes I_{d+1})\, \mathbf{G}(\hat{\mathbf{c}}, \mathbf{r})$$

- **Layer Gauss-Newton's matrix for nonlinear parameters**

$$GN = \big(D(\mathbf{c}) \otimes I_{d+1}\big)\mathcal{H}(\mathbf{r})\big(D(\mathbf{c}) \otimes I_{d+1}\big)$$

where $\mathcal{H}(\mathbf{r}) = \sum_{i=1}^{m} \mu^i \left[\mathbf{H}\mathbf{H}^T\right] \otimes \left[\mathbf{y}\mathbf{y}^T\right](\mathbf{x}^i)$ is SPD

The Structure-guided Gauss-Newton (SgGN) Method

Given $\left(\hat{\mathbf{c}}^{(k)}, \mathbf{r}^{(k)}\right) = \left(\mathbf{c}^{(k)}, c_0^{(k)}, \mathbf{r}^{(k)}\right)$, compute $\left(\hat{\mathbf{c}}^{(k+1)}, \mathbf{r}^{(k+1)}\right)$:

(i) Compute $\hat{\mathbf{c}}^{(k+1)}$ by solving the system of linear equations

$$\mathcal{A}\left(\mathbf{r}^{(k)}\right)\hat{\mathbf{c}}^{(k+1)} = \mathbf{f}\left(\mathbf{r}^{(k)}\right)$$

(ii) If $c_i^{(k+1)} \neq 0$ for all i, compute the search direction

$$\mathbf{p}^{(k+1)} = \left(D^{-1}\left(\mathbf{c}^{(k+1)}\right) \otimes I_{d+1}\right)\mathbf{s}^{(k+1)},$$

where $\mathbf{s}^{(k+1)} = -\mathcal{H}\left(\mathbf{r}^{(k)}\right)^{-1}\mathbf{G}\left(\mathbf{c}^{(k+1)}, c_0^{(k+1)}, \mathbf{r}^{(k)}\right)$.

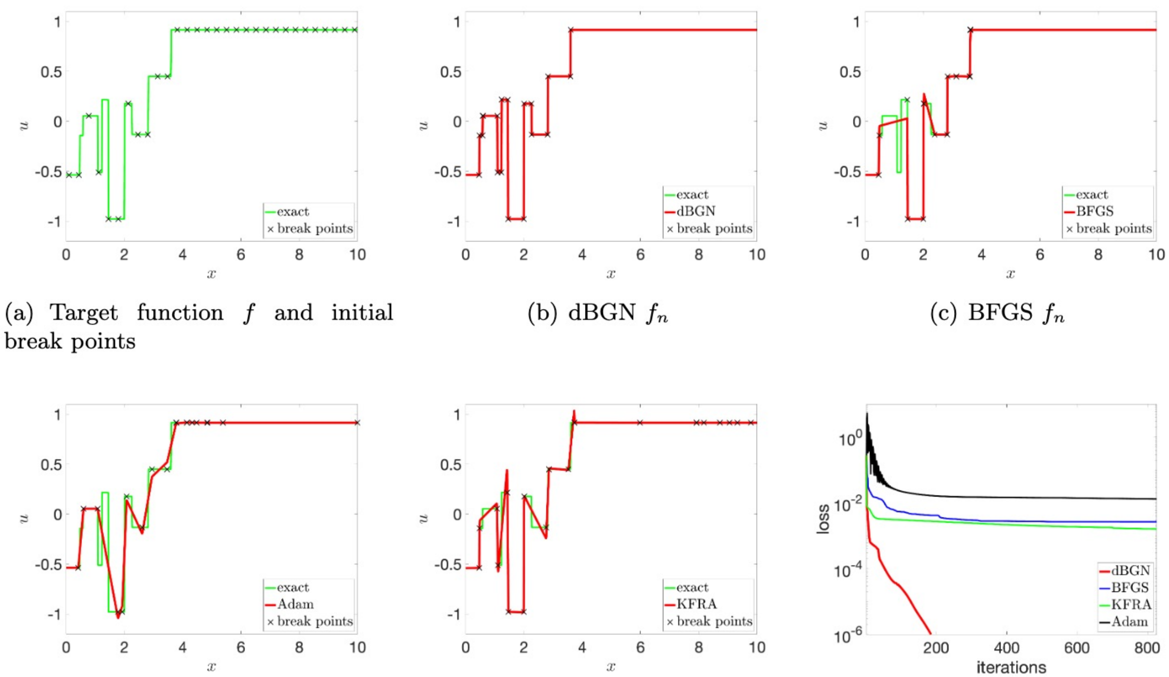
(iii) Compute the nonlinear parameter

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} + \gamma_{k+1}\mathbf{p}^{(k+1)},$$

where the damping parameter γ_{k+1} is computed by

$$\gamma_{k+1} = \underset{\gamma \in \mathcal{R}}{\arg\min}\, \mathcal{J}_\mu\left(u_n\left(\cdot; \mathbf{c}^{(k+1)}, \mathbf{r}^{(k)} + \gamma\mathbf{p}^{(k+1)}\right)\right).$$

Step Function



(a) Target function f and initial break points

(b) dBGN f_n

(c) BFGS f_n

(d) Adam f_n

(e) KFRA f_n

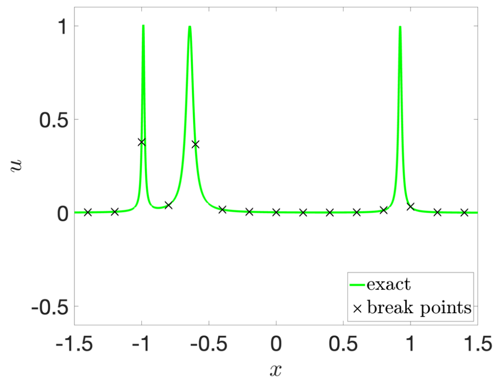
(f) Loss curves

Figure 2: One-dimensional piece-wise constant function approximation results

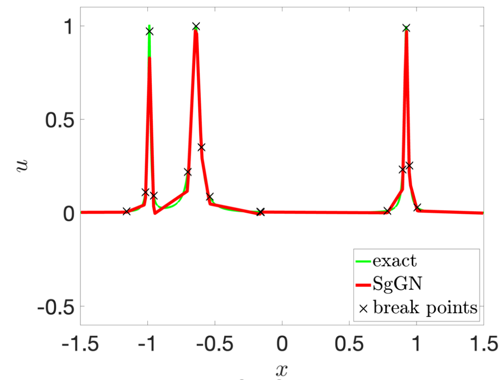
Table 1: Comparison for one-dimensional piece-wise constant function.

Method	dBGN		BFGS		KFRA	Adam
Iteration	9	825	207	825	825	$10,000$
$J(f_n)$	8.76E-4	6.56E-9	4.03E-3	2.65E-3	1.61E-3	8.14E-3

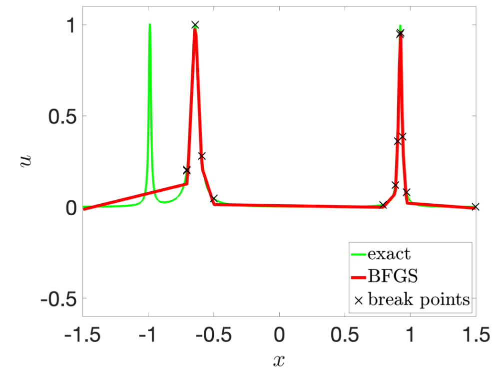
Delta-like Function



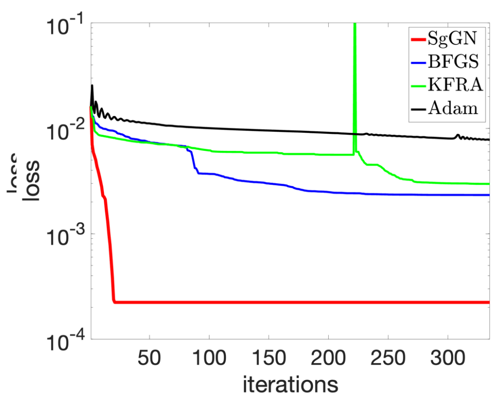
Function u and initial break points



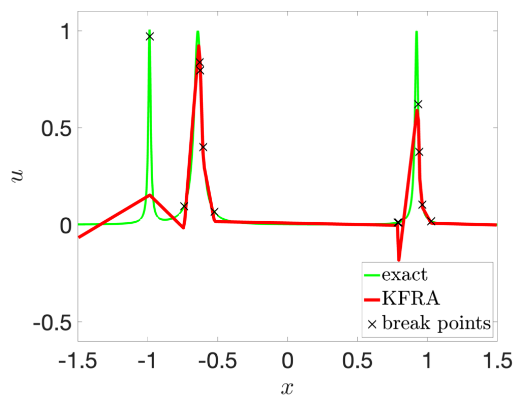
SgGN u_N



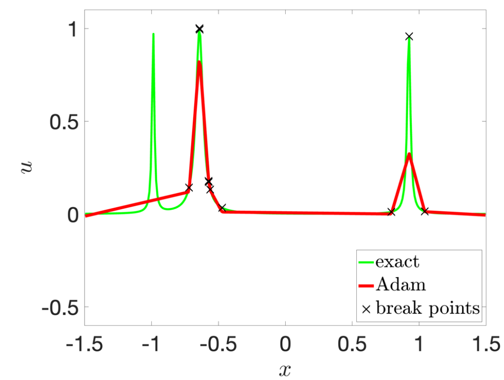
BFGS u_N



Loss curves

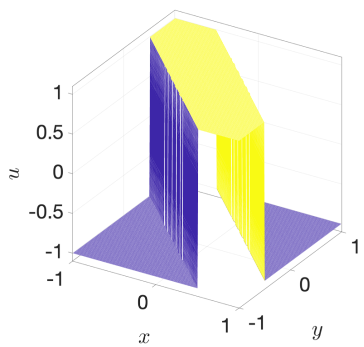


KFRA u_N

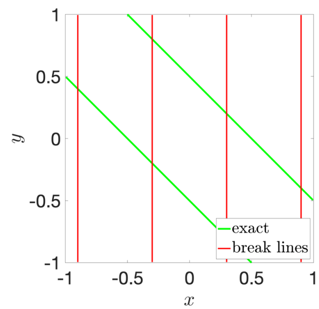


Adam u_N

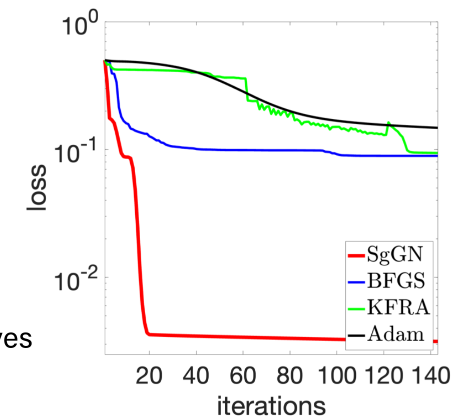
Piece-wise Constant Function



Function u

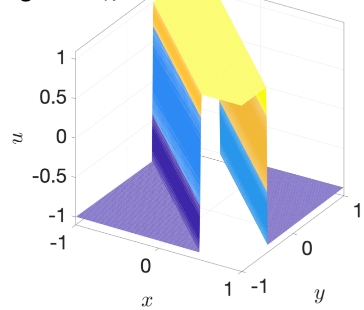


initial break lines

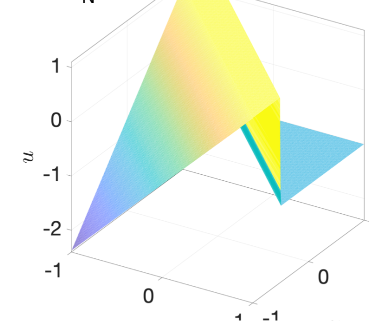


Loss curves

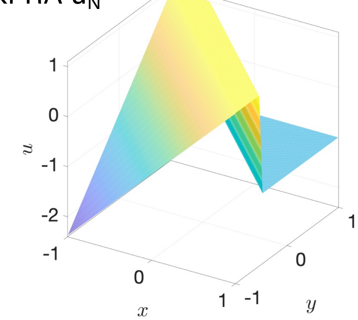
SgGN u_N



BFGS u_N



KFRA u_N



Adam u_N

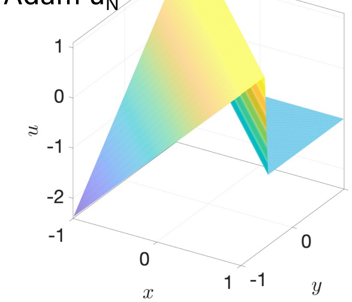
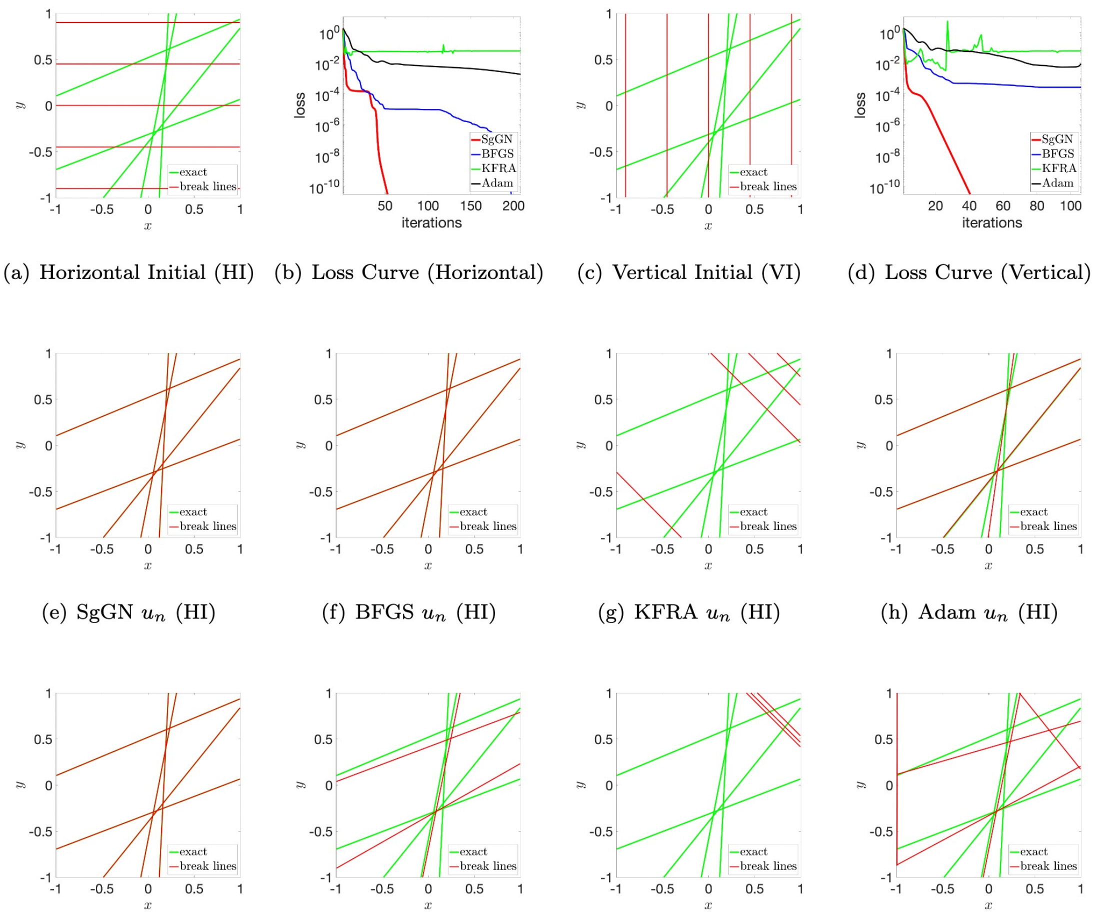


Table 6.4: Comparison for a two-dimensional piece-wise constant function.

Method	SgGN		BFGS		KFRA	Adam
Iteration	**9**	142	100	142	142	10,000
$\mathcal{J}_{m,\mu}$	8.82E-2	**3.16E-3**	9.20E-2	8.92E-2	9.40E-2	9.23E-2

Two-dimensional function in $\hat{\mathcal{M}}_n(\Omega)$



(a) Horizontal Initial (HI) (b) Loss Curve (Horizontal) (c) Vertical Initial (VI) (d) Loss Curve (Vertical)

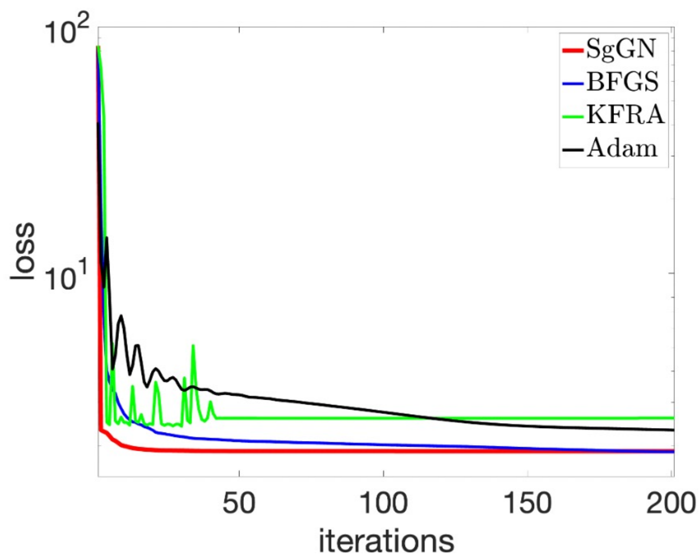
(e) SgGN u_n (HI) (f) BFGS u_n (HI) (g) KFRA u_n (HI) (h) Adam u_n (HI)

(i) SgGN u_n (VI) (j) BFGS u_n (VI) (k) KFRA u_n (VI) (l) Adam u_n (VI)

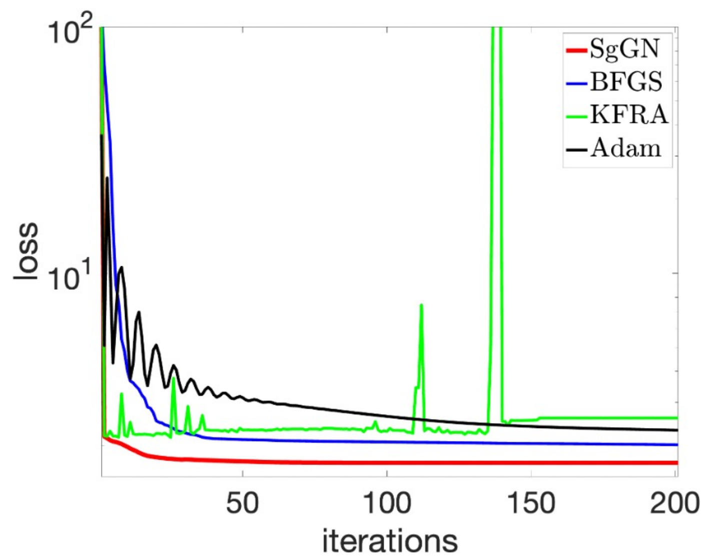
Table 6.5: Comparison for a two-dimensional piece-wise linear function with horizontal initial breaking lines (VI) and vertical initial breaking lines (VI).

Method	SgGN		BFGS		KFRA	Adam
Iteration	**99**	207	204	207	207	$10,000$
$\mathcal{J}_{m,\mu}$ (HI)	6.28E-22	**6.68E-27**	7.50E-22	7.50E-22	6.12E-2	1.17E-5
Iteration	**4**	105	30	105	105	$10,000$
$\mathcal{J}_{m,\mu}$ (VI)	2.35E-4	**4.34E-26**	5.21E-4	2.71E-4	5.56E-2	2.15E-4

A Data Science Application



(a) 40 neurons



(b) 80 neurons

Summary: the Structure-guided Gauss-Newton (SgGN) Method

- SgGN uses both the quadratic and NN structures
- more accurate approximation than other training algorithms
- mass and layer Gauss-Newton matrices

positive definite: no need of shifting

ill-conditioned: ??? fast linear solvers???

THANK YOU

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Tong Ding[1], Xinyu Liu[1], and Jianlin Xia[1]

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

Approximation to Unit Step Function with Unknown Interface in R^d

- **Piecewise Constant function with unknow interface**

C., J. Choi, and M. Liu (2022) (d=2, 3, L=2; d=4,...,8, L=3)

Let χ(x) be a piecewise constant function with C^0 piecewise smooth interface I, then there exists a CPWL function p(x) generated by a DNN with L= $\lceil \log_2(d+1) \rceil$ hidden layers such that for any given $\varepsilon > 0$, we have

$$|||\chi - p|||_{\boldsymbol{\beta}} \leq \sqrt{2|I|}\, \big|\alpha_1 - \alpha_2\big|\, \sqrt{\varepsilon},$$

P. Petersen and F. Voigtlaender (2018) (For C^1 and d=2, L=36)

Theorem 3.5. *For $r \in \mathbb{N}$, $d \in \mathbb{N}_{\geq 2}$, and $p, \beta, B > 0$, there are constants $c = c(d, r, p, \beta, B) > 0$ and $s = s(d, r, p, \beta, B) \in \mathbb{N}$, such that for any $K \in \mathcal{K}_{r,\beta,d,B}$ and any $\varepsilon \in (0, 1/2)$, there is a neural network Φ_ε^K with at most $(3 + \lceil \log_2 \beta \rceil) \cdot (11 + 2\beta/d)$ layers, and at most $c \cdot \varepsilon^{-p(d-1)/\beta}$ nonzero, (s, ε)-quantized weights such that*

$$\|\mathrm{R}_\varrho(\Phi_\varepsilon^K) - \chi_K\|_{L^p([-1/2,1/2]^d)} < \varepsilon \quad \textit{and} \quad \|\mathrm{R}_\varrho(\Phi_\varepsilon^K)\|_{\sup} \leq 1.$$

Remark 3.6. *Theorem 3.5 establishes approximation rates for piecewise constant functions. It should be noted that the number of required layers is fixed and only depends on the dimension d and the regularity parameter β; in particular, it does* not *depend on the approximation accuracy ε.*