STRUCTURE-GUIDED GAUSS-NEWTON METHOD: LSNN FOR LINEAR ADVECTION-REACTION EQUATION

César Herrera

Joint work with Zhiqiang Cai

41st Colorado Conference On Iterative and Multigrid Methods

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Approximation of Functions

How can we approximate a function?

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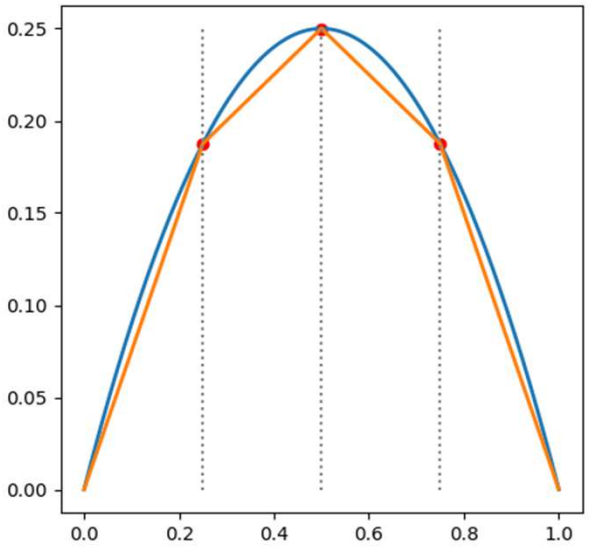
Simple and effective idea: **continuous piecewise linear functions.**



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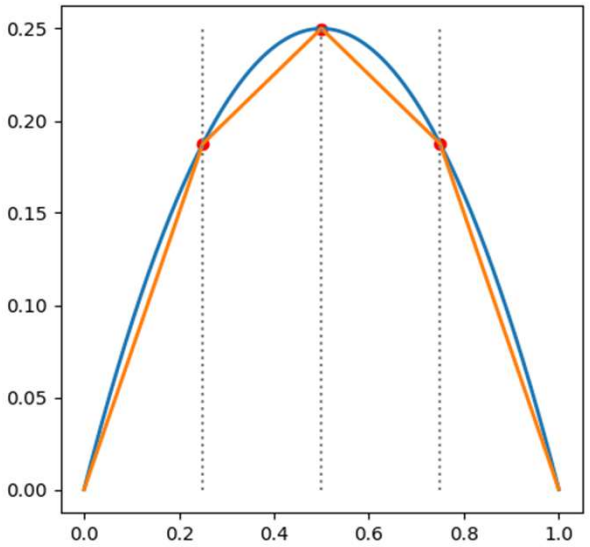
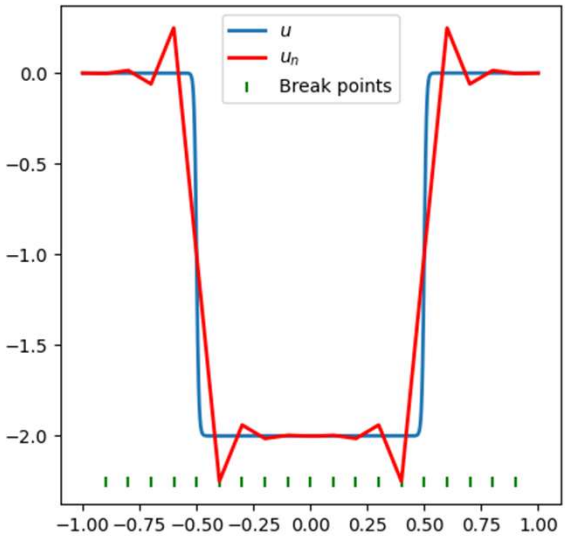


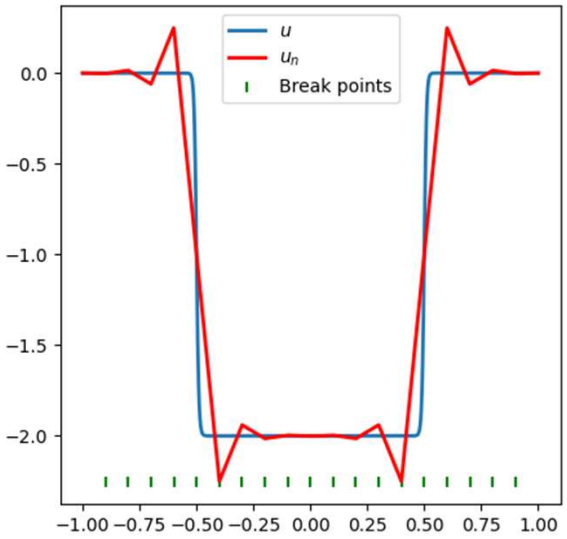
- **Finite Element Methods:** continuous piecewise linear approximation on a **fixed uniform mesh.**

Moving the Mesh



Fixed uniform mesh

Moving the Mesh



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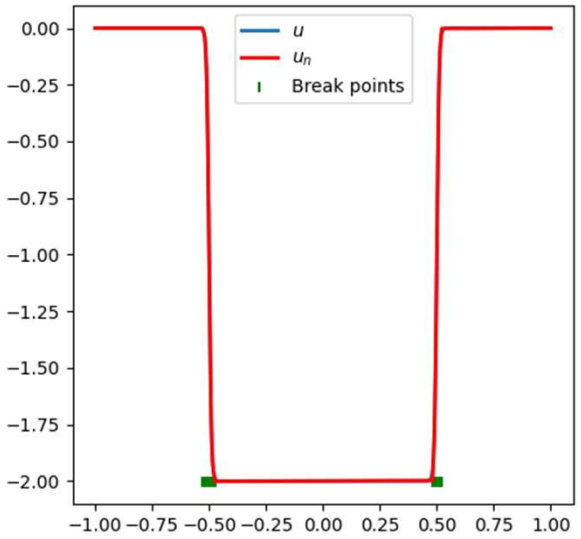

Moving mesh

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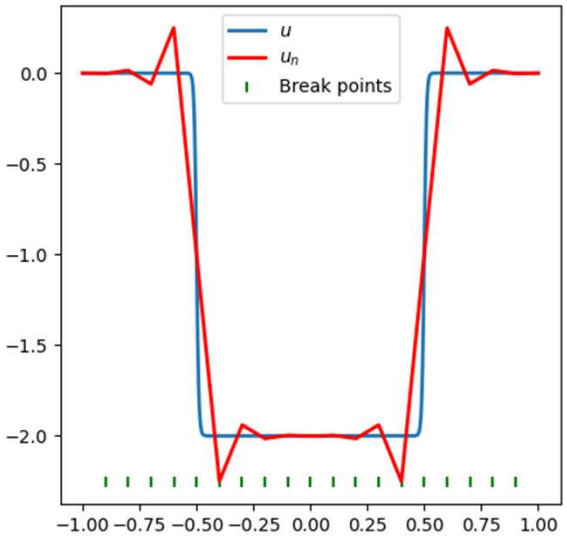

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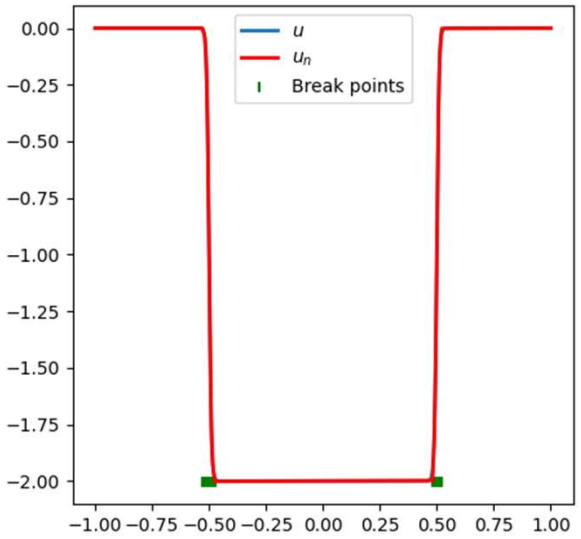


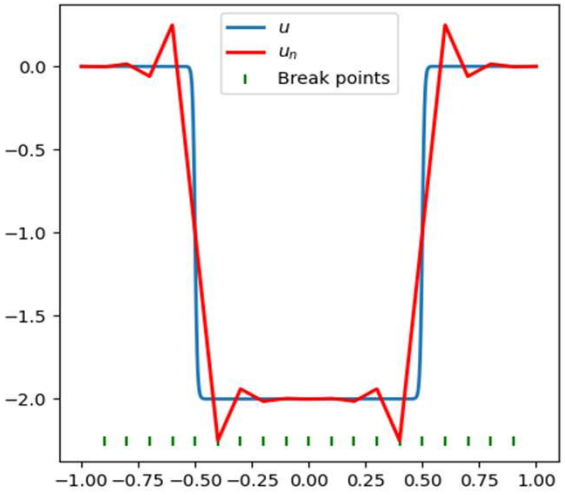
Moving mesh

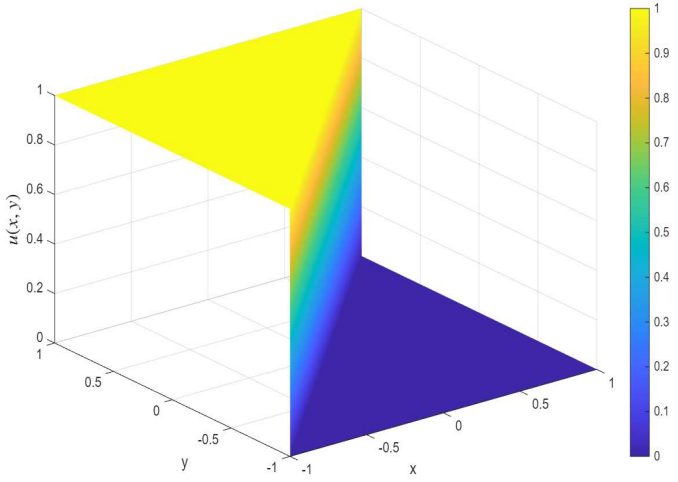
- **Neural networks: continuous piecewise linear approximations.**
- **Feature: moving the mesh.**

Broader Goals

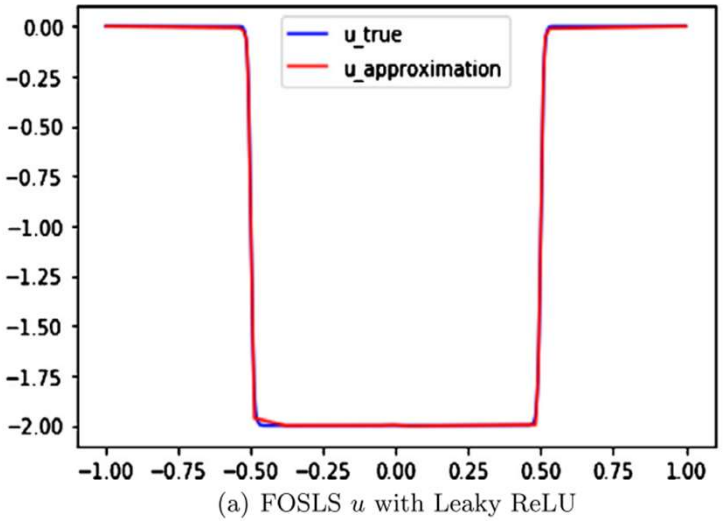
We aim to solve numerical PDEs with challenges such as

- **Boundary/interior layers:** e.g., singularly perturbed elliptic problems.
- **Shocks/discontinuidades and unknown interface**: e.g., hyperbolic conservation laws.





Efficient Neural Network Methods



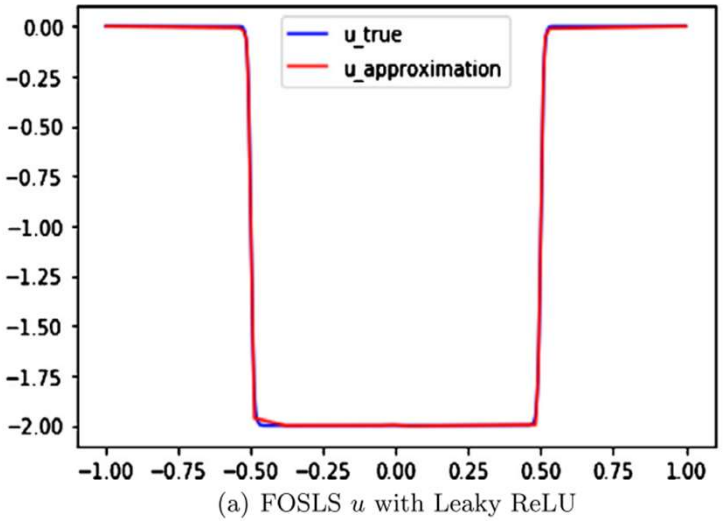
(a) FOSLS u with Leaky ReLU

2962 parameters, 20 hours[1]

- **Important: efficient optimization methods.**

1. Zhiqiang Cai et al. "Deep least-squares methods: An unsupervised learning-based numericalmethod for solving elliptic PDEs". J. Comput. Phys.(2020)

Efficient Neural Network Methods



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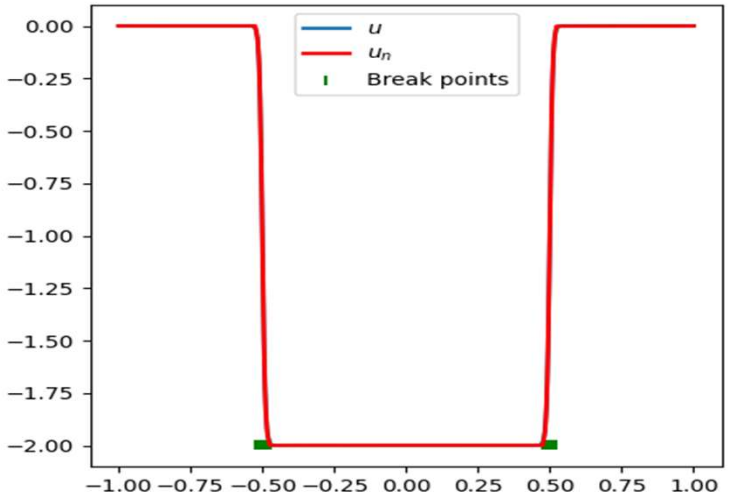

41 parameters, 30 seconds

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OUTLINE

I. Neural networks for numerical PDEs

II. One-dimensional problems

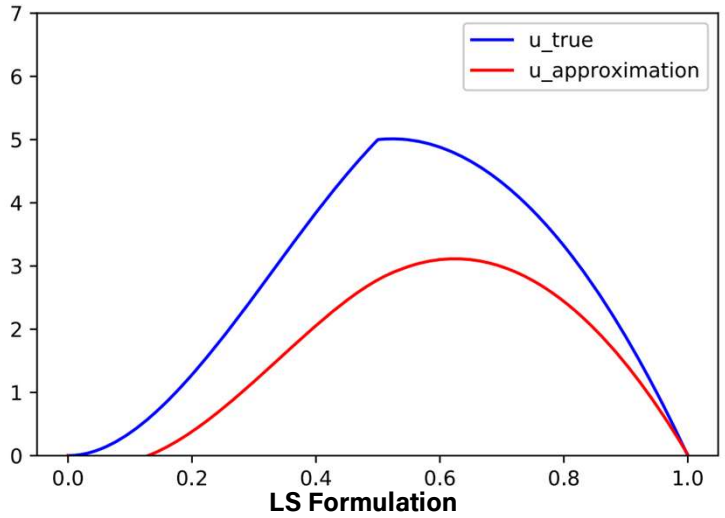
III. Two-dimensional linear advection-reaction equation

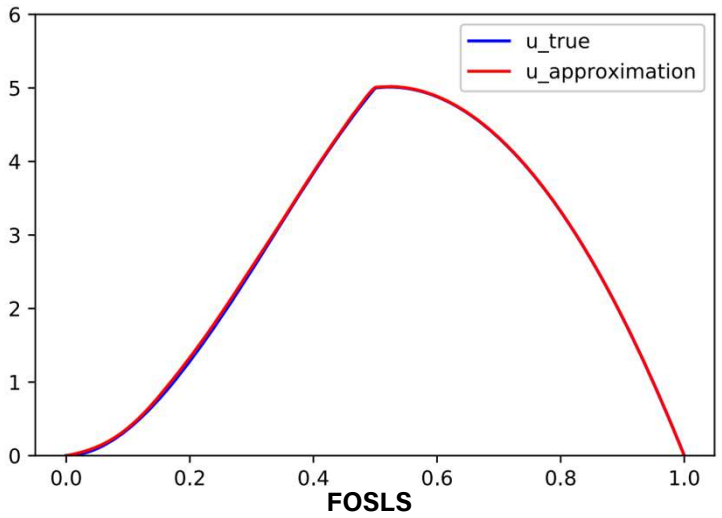
I. NEURAL NETWORKS FOR NUMERICAL PDES

Neural Networks for Numerical PDEs

What do we need to solve numerical PDEs using neural networks?

Neural Networks for Numerical PDEs





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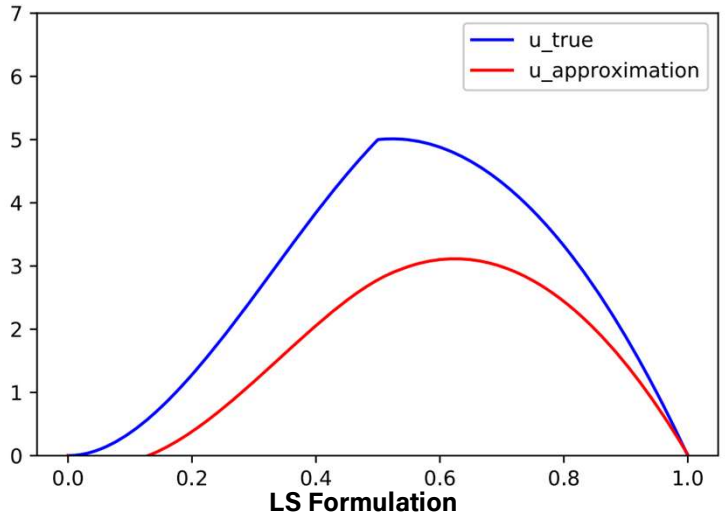

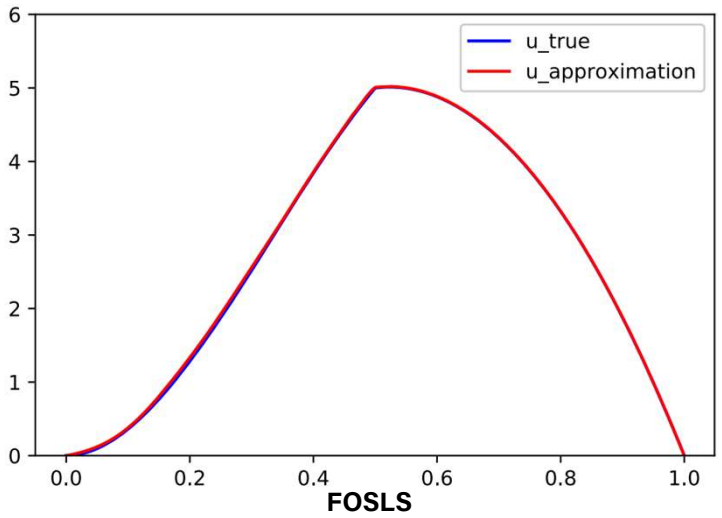

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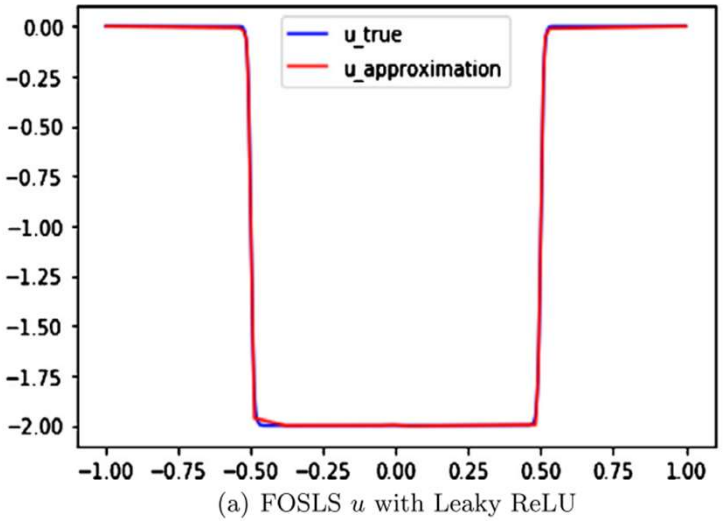

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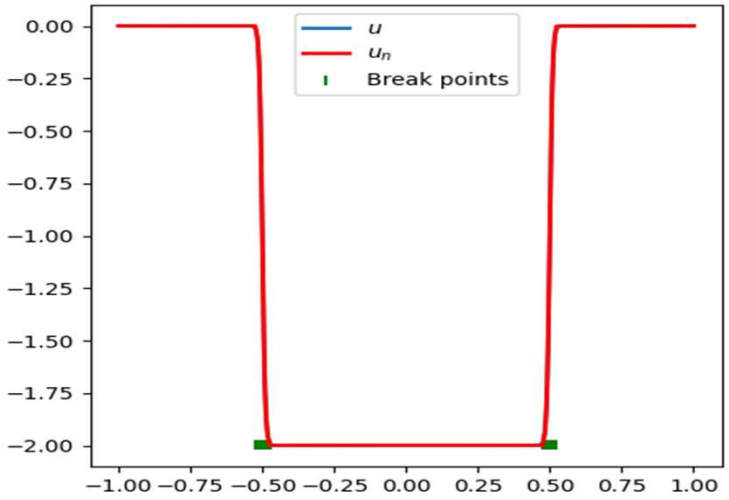

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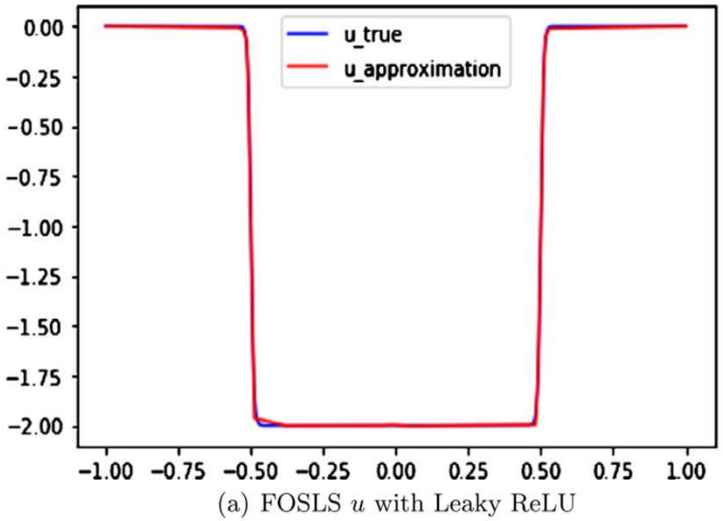

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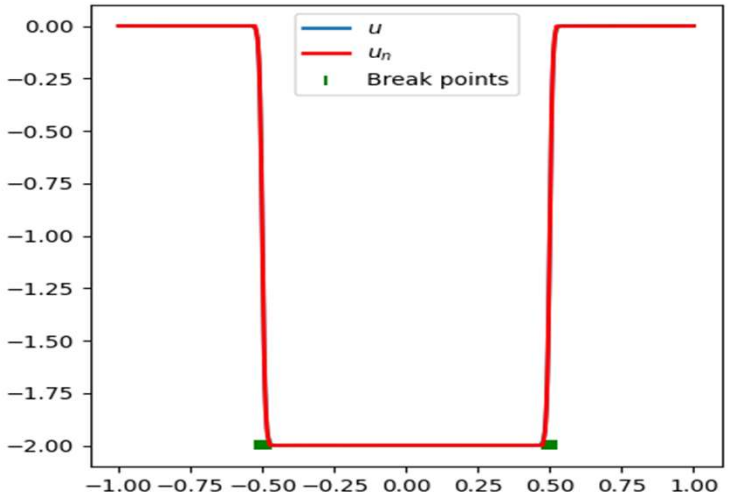

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- **Important:** 2. NN architecture.

  3. Efficient optimization methods.

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Neural Networks for Numerical PDEs

What do we need to solve numerical PDEs using neural networks?

1. **Formulation:** finding a physics preserving formulation.
2. **Architecture:** number of layers and neurons.
3. **Optimization:** designing efficient optimization methods.

II. ONE-DIMENSIONAL PROBLEMS

One-dimensional Elliptic Problems

One-dimensional diffusion-reaction equation

$$\begin{cases} -\big(a(x)u'(x)\big)' + r(x)u(x) = f(x), & x \in (0,\ 1), \\ u(0) = u(1) = 0. \end{cases}$$

1. Formulation

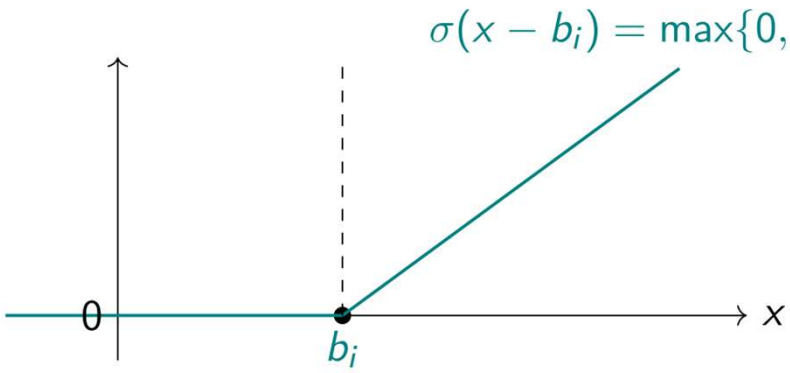
- **Ritz formulation:** find $u \in V$ such that

$$J(u) = \min_{v \in V} J(v), \qquad J(v) = \frac{1}{2}\int_0^1 [(av')^2 + rv^2]\, dx - \int_0^1 fv\, dx.$$

Architecture: One Hidden Layer

One-dimensional shallow (ReLU) neural network

$$\mathcal{M}_n(0,1) = \left\{ c_0 + \sum_{i=1}^{n} c_i \sigma(x - b_i) : c_i \in \mathbb{R}, b_i \in [0,1] \right\}$$



- Continuos piecewise linear function.
- Parameters:
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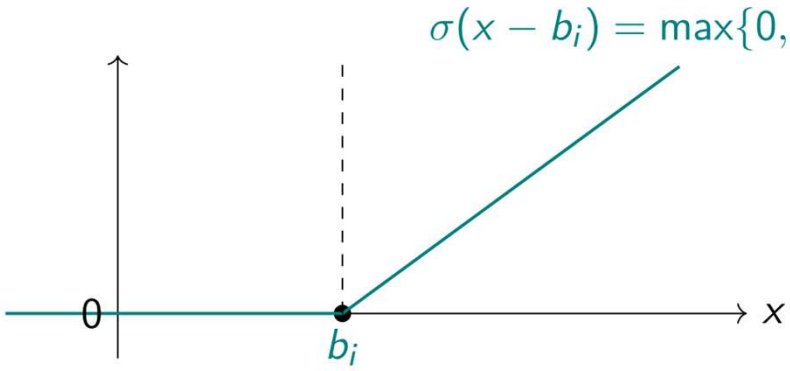

- Continuos piecewise linear function.
- Parameters:
  - c_i: **linear** parameters.
  - b_i: **non-linear** parameters (breaking points).
- Capable of approximating non-smooth functions.

One-dimensional Elliptic Problems

1. Formulation

- **Ritz formulation:** find $u \in V$ such that

$$J(u) = \min_{\substack{v \in V \\ v(0) = v(1) = 0}} J(v).$$

2. Architecture

- **One hidden layer**

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Discretization: find $u_n \in \mathcal{M}_n(0,1)$ that minimizes J:

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3. Optimization?

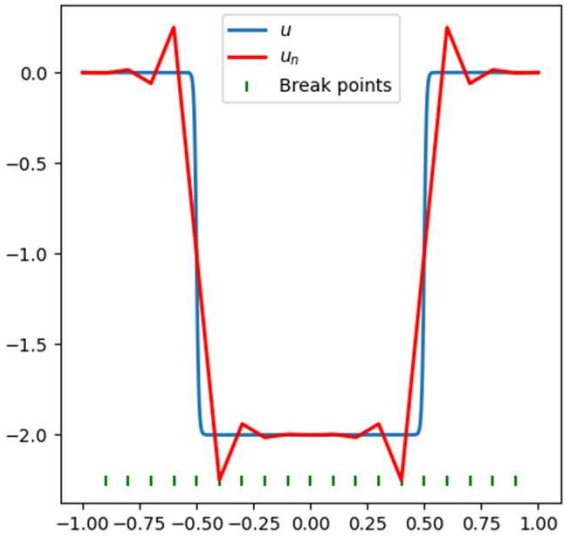
Efficient Iterative Method

3. Optimization

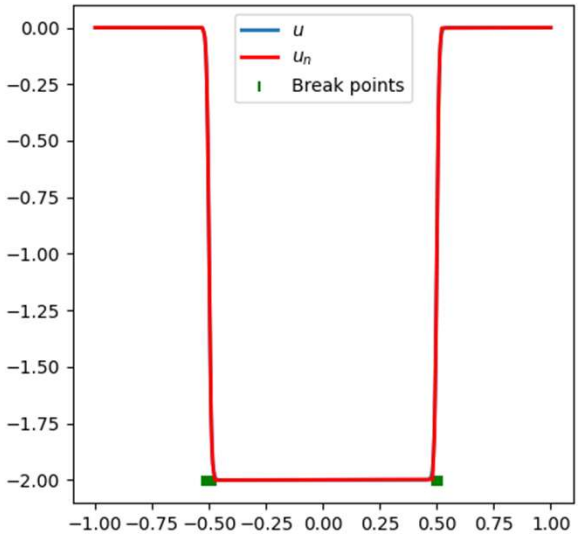
- Block Newton methods:
  - Z. Cai, A. Doktorova, R. D. Falgout, and C.Herrera. *Efficient Shallow Ritz Method for 1D Diffusion Problems.* Comput. Math. Appl, 2025
  - Z. Cai, A. Doktorova, R. D. Falgout, and C.Herrera. *Efficient Shallow Ritz Method for 1D Diffusion-Reaction Problems.* SISC, 2025
  - **Efficient methods ($\mathcal{O}(n)$ per iteration).**
  - Capable of **moving** the mesh.

Numerical Experiment

Solving $-\varepsilon^2 u''(x) + u(x) = f(x),\ \varepsilon^2 = 10^{-4}$.



Initial NN Approximation



Optimized NN Approximation-200 itr.

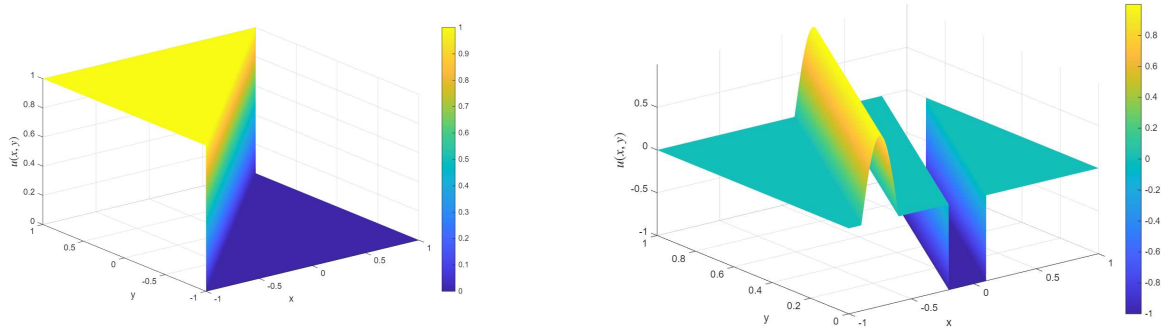
III. TWO-DIMENSIONAL LINEAR ADVECTION-REACTION EQUATION

Linear Advection-Reaction Equation

Two-dimensional advection-reaction equation

$$\begin{cases} u_{\boldsymbol{\beta}} + \gamma u = f & \text{in } \Omega, \\ u = \mathrm{g} & \text{on } \Gamma_{-}, \end{cases}$$

where $u_{\boldsymbol{\beta}}$ denotes the **directional derivative** along the velocity field $\boldsymbol{\beta}$.



Goal: approximating **discontinuous** solutions without using the **known** interface.

Linear Advection-Reaction Equation

Two-dimensional advection-reaction equation

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1. Formulation

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

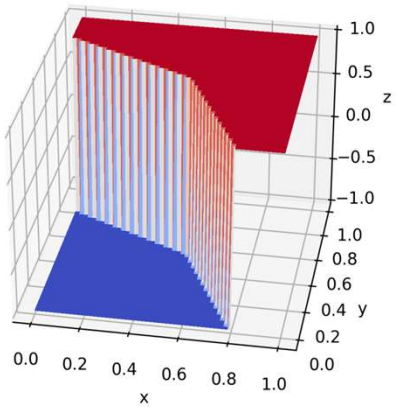
$$\mathcal{L}(u;\, \boldsymbol{f}) = \min_{v \in V_{\boldsymbol{\beta}}} \mathcal{L}\,(v;\, \boldsymbol{f}) \qquad \mathcal{L}(v;\, \boldsymbol{f}) = \int_{\Omega} (v_{\boldsymbol{\beta}} + \gamma u - f)^2\, d\boldsymbol{x} + \int_{\Gamma_{-}} |\boldsymbol{\beta} \cdot \boldsymbol{n}| (v - g)^2 ds\,.$$

- **Coercivity and continuity (De Sterck, Manteuffel, McCormick, Olson, 2004):** there exists positive constants α and M such that

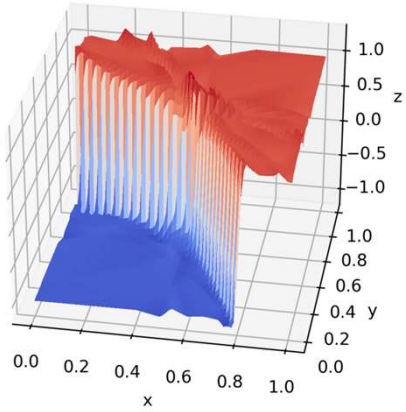
$$\alpha \|v\|_{\boldsymbol{\beta}} \leq \mathcal{L}(v;\, \mathbf{0}) \leq M \|v\|_{\boldsymbol{\beta}}$$

One vs Two Hidden Layers

2. Architecture



Solution [2]



1 hidden layer [2]
2-158-1

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2. Z. Cai, J. Choi, and M. Liu. "Least-Squares Neural Network (LSNN) Method for Linear Advection-Reaction Equation: Discontinuity Interface". SISC (2024)

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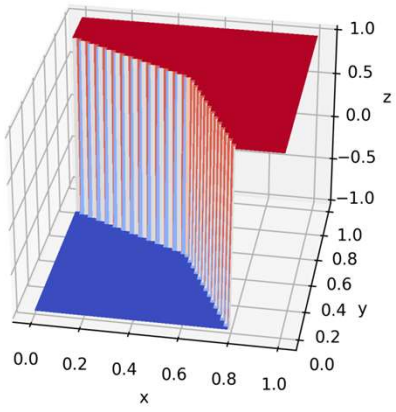

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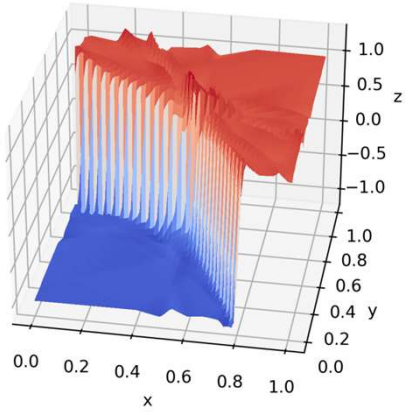

1 hidden layer [2]
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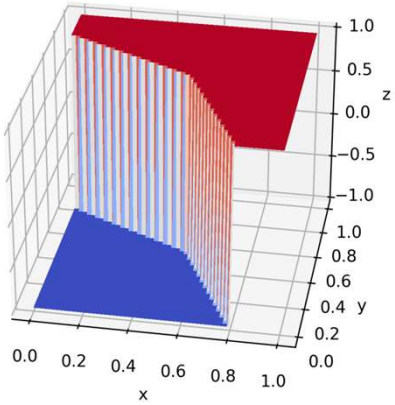

2 hidden layers [2]
2-4-4-1

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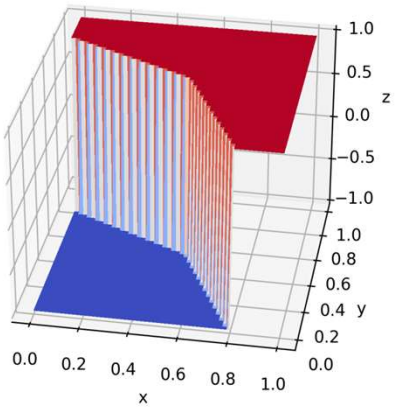
One vs Two Hidden Layers

2. Architecture

Z. Cai, J. Choi, M. Liu (2024): Two hidden layers are necessary and sufficient for two or more dimensions.



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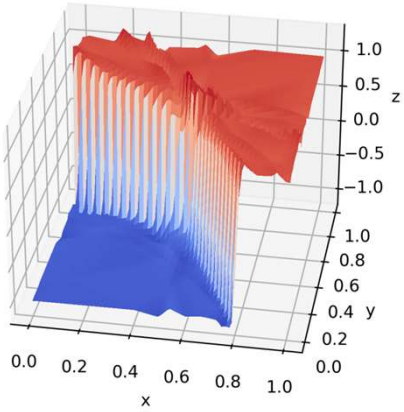

1 hidden layer [2]
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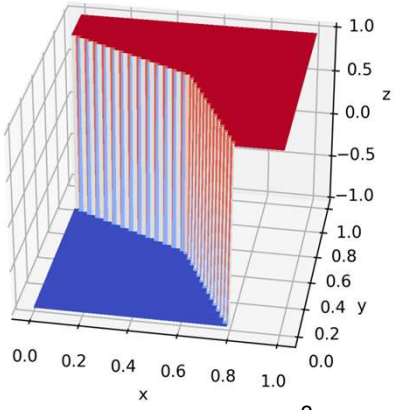

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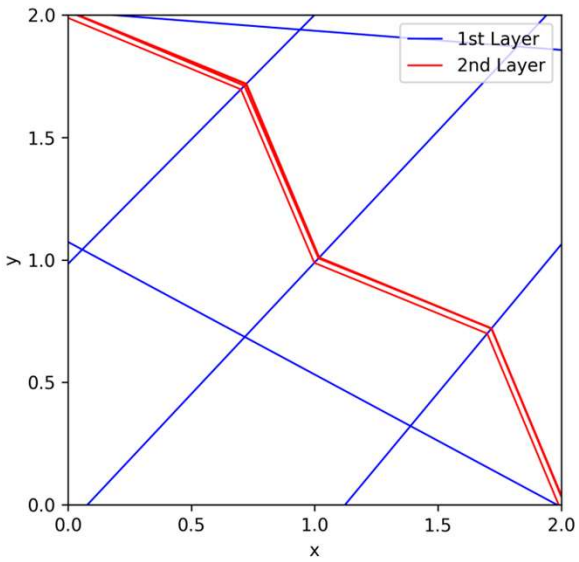
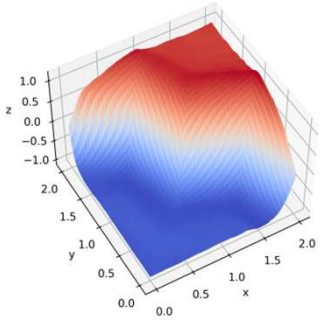
One vs Two Hidden Layers

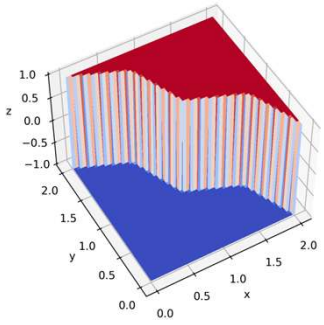
2. Architecture

- **1 hidden layer:** interface is a line segment
- **2 hidden layers:** interface is a curve





1 hidden layers[2]
2-300-1



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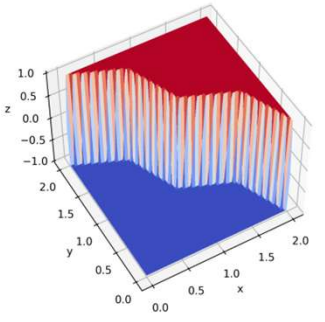

2 hidden layers[2]
2-6-6-1

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Shallow Neural Network

Two-dimensional shallow (ReLU) neural network

$$\mathcal{M}_n(\Omega) = \left\{ c_0 + \sum_{i=1}^{n} c_i \sigma(\boldsymbol{\omega}_i \cdot \boldsymbol{x} + b_i) : c_i \in \mathbb{R}, b_i \in \mathbb{R}, \boldsymbol{\omega}_i \in \mathbb{R}^2 \right\}$$

- Continuos piecewise linear function.
- Parameters:
  - c_i: **linear** parameters.
  - $\boldsymbol{\omega}_i$, b_i: **non-linear** parameters
  - **Breaking lines**: $\{\boldsymbol{x} \in \Omega: \boldsymbol{\omega}_i \cdot \boldsymbol{x} + b_i = 0\}$

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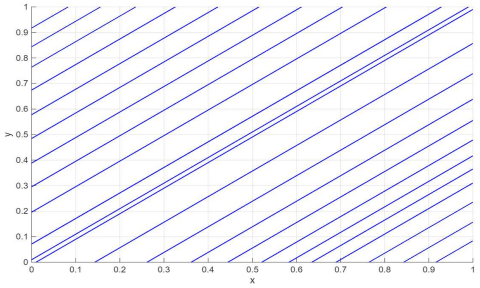

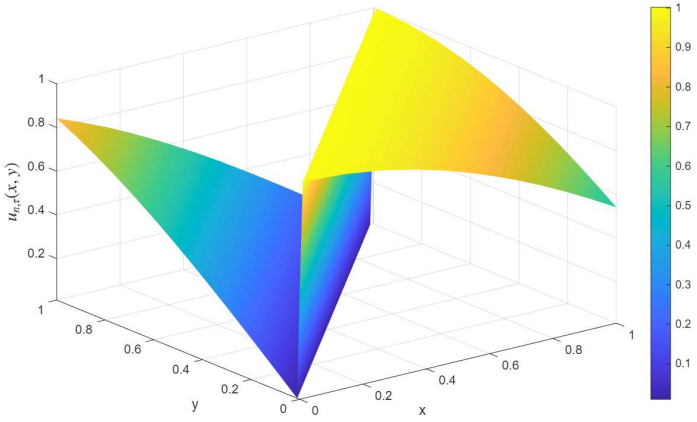

Linear Advection-Reaction Equation

1. Formulation

- **Least-squares formulation:** find $u \in V_{\boldsymbol{\beta}}$ that minimizes

$$\mathcal{L}(v) = \int_{\Omega} (v_{\boldsymbol{\beta}} + \gamma u - f)^2 \, d\boldsymbol{x} + \int_{\Gamma_-} |\boldsymbol{\beta} \cdot \boldsymbol{n}| (v - g)^2 ds \,.$$

2. Architecture

- **One hidden layer**

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Discretization: find a neural network $u_n \in \mathcal{M}_n(\Omega)$ that minimizes $\mathcal{L}$:

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

Optimality Conditions

3. Optimization

Non-convex optimization problem: find a neuronal network u_n that minimizes the functional $\mathcal{L}$.

Difficulties:

- Initialization.
- ReLU is not pointwise differentiable.
- Possible matrix singularities.

Optimality Conditions

3. Optimization

Non-convex optimization problem: find a neuronal network u_n that minimizes the functional $\mathcal{L}$.

Neural network representation:

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

where

$$\boldsymbol{c} = (c_0, c_1, \dots, c_n)^T, \qquad \boldsymbol{r} = (b_1, \boldsymbol{\omega}_1, \dots, b_n, \boldsymbol{\omega}_n)^T.$$

First-order optimality conditions:

$$\nabla_{\boldsymbol{c}} \mathcal{L}(\boldsymbol{c}, \boldsymbol{r}) = \mathbf{0}, \qquad \nabla_{\boldsymbol{r}} \mathcal{L}(\boldsymbol{c}, \boldsymbol{r}) = \mathbf{0}.$$

Mass and Gauss-Newton Matrices

- **Linear parameters**

$$\mathbf{0} = \nabla_c \mathcal{L}(c, r) = A(r)c - F(r)$$

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- **Non-linear parameters**

$$\mathbf{0} = \nabla_r \mathcal{L}(c, r) = (\boldsymbol{D}(c) \otimes \boldsymbol{I_3})\boldsymbol{G}(c, r)$$

  - Gauss-Newton matrix.

$$(\boldsymbol{D}(c) \otimes \boldsymbol{I_3})\mathcal{H}(c, r)(\boldsymbol{D}(c) \otimes \boldsymbol{I_3})$$

  - Layer Gauss-Newton $\mathcal{H}(c, r)$ matrix is spd.
  - If $c_i = 0$, we do not need to update $r_i = (b_i, \omega_i)$.

Structure Guided Gauss Newton Method (SgGN)

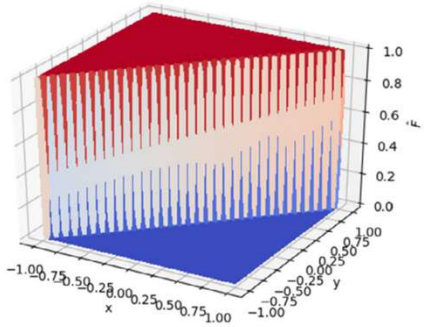
Iterative method:

1. **Inicialization:** $r^{(0)}$-> **uniform** partition.

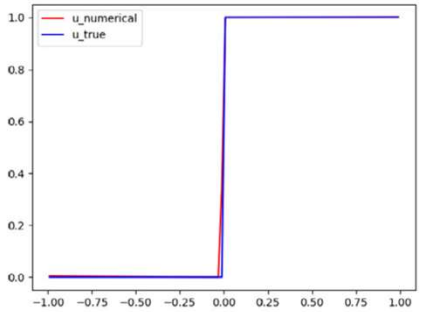
2. **Iterate:** given $\left(c^{(k)}, r^{(k)}\right)$**,** we compute $\left(c^{(k+1)}, r^{(k+1)}\right)$

   - **Linear parameters:** compute $c^{(k+1)}$ by solving the **system of linear equations** $\nabla_c \mathcal{L}\left(c, r^{(k)}\right) = \mathbf{0}$.
   - **Non-linear parameters:** compute $r^{(k+1)}$ using one **Gauss-Newton iteration.**

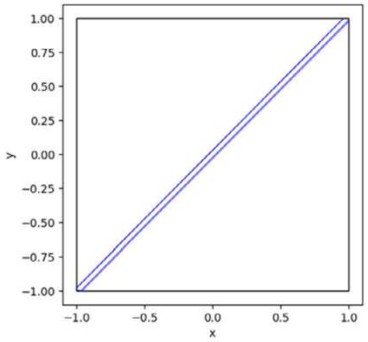
Transport equation $u_x + u_t = 0$



(a) Network approximation $\bar{u}_T^N$

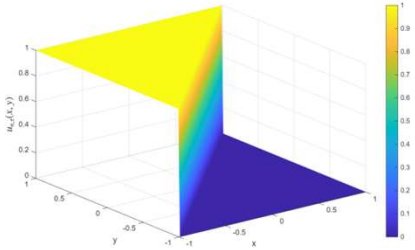


(b) Vertical cross section along $y = -x$

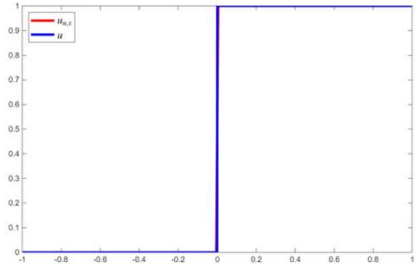


(c) Network breaking lines

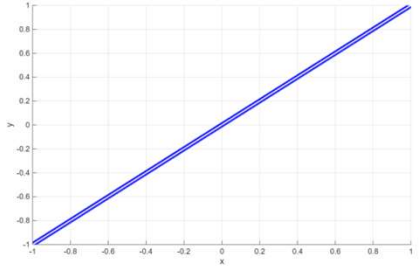
20000 ADAM iterations; the relative L^2 error is 5.8×10^{-2}



(a) NN approximation $u_{n,\tau}$



(b) Traces on $y = -x$



(c) NN breaking lines

100 SgGN iterations; the relative L^2 error is 5.3×10^{-11}

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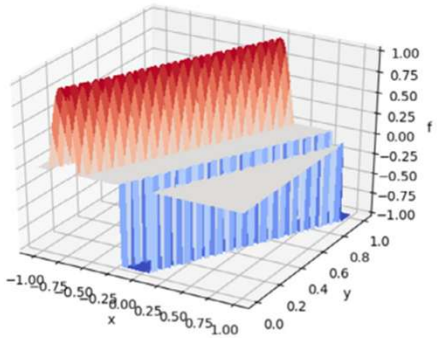
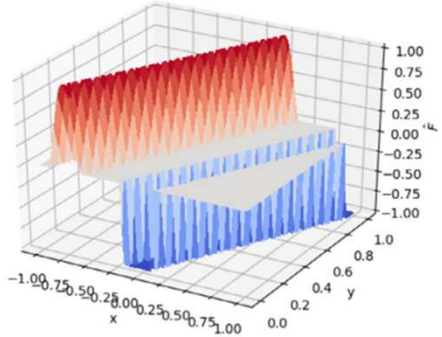
5. Z. Cai, J. Chen, and M. Liu. "Least-squares ReLU neural network (LSNN) method for linear advection-reaction equation". J. Comput. Phys (2021)

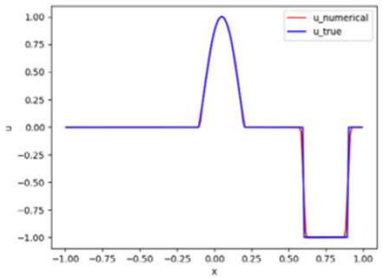
Two Discontinuous Interfaces



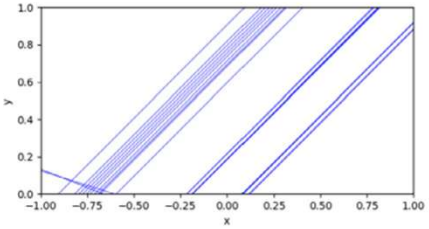
(a) Exact solution u



(b) Network approximation $\bar{u}_\tau^N$



(c) Traces of the exact solution and approximation $\bar{u}_\tau^N$ on the plane $y = 0.8$



(d) Network breaking lines

80000 ADAM iterations[5]; the relative L^2 error is 1.17×10^{-1}

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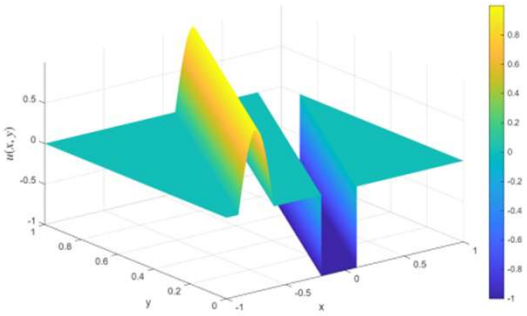
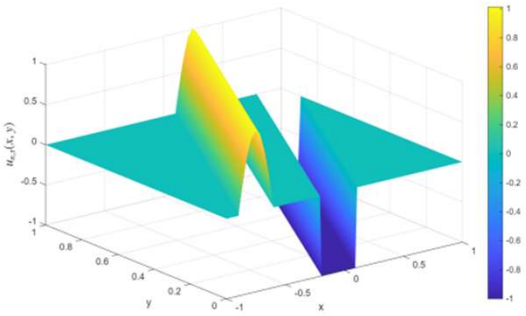
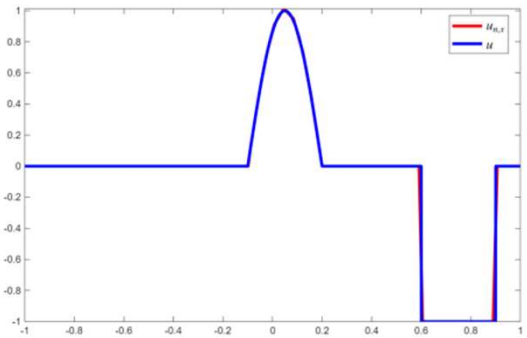


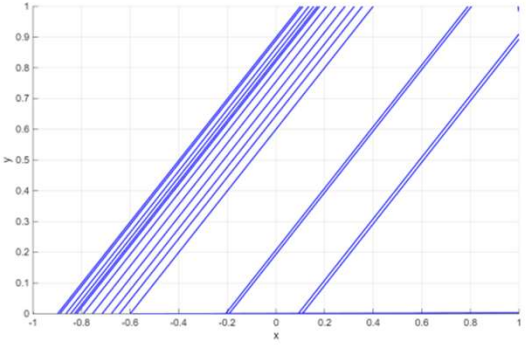
(a) Exact Solution



(b) NN Approximation



(c) Traces on $y = 0.8$



(d) NN breaking lines

100 SgGN iterations; the relative L^2 error is 2.80×10^{-3}

Conclusions and Final Remarks

- We can **accurately approximate discontinuos solutions** using neural networks.
- SgGN method **significantly reduces the number of iterations** compared to standard first order methods.
- Mass and Gauss-Newton matrices are **ill-conditioned**. **Efficient linear solvers?**
- Actual and future work:
  - Scalar hyperbolic conservation laws.
  - Iterative methods for 2 hidden layers NN.

THANKS

website

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