Fast Iterative Solver for Neural Network Method: I. 1D Diffusion Problems

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FIG. 1 — Organization of a biological brain. (Red areas indicate active cells, responding to the letter X.)

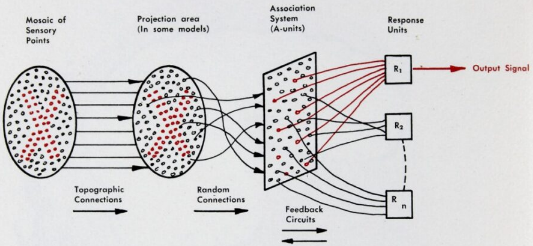


FIG. 2 — Organization of a perceptron.

[1] F. Rosenblatt. "The perceptron: A probabilistic model for information storage and organization in the brain.". In: *Psychological Review* 65.6 (1958), pp. 386–408. ISSN: 0033-295X. DOI: 10.1037/h0042519. URL: http://dx.doi.org/10.1037/h0042519.

Introduction: Neural Networks (Fully-Connected Feed-Forward NN)

Let $\mathbf{x}^{(0)} = \mathbf{x}$ and $\mathbf{x}^{(i)} = \sigma\left(W^{(i)}_{n_i\times(n_{i-1}+1)}\begin{bmatrix}1\\ \mathbf{x}^{(i-1)}\end{bmatrix}\right)$ for $i = 1, \ldots, L-1$.

Output: $u(\mathbf{x}) = W^{(L)}_{c\times(n_{L-1}+1)}\begin{bmatrix}1\\ \mathbf{x}^{(L-1)}\end{bmatrix}$

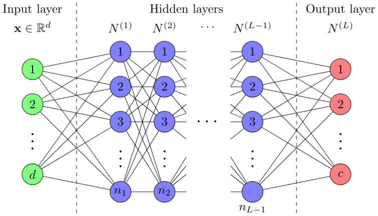


Figure: The neural network function structure[2]

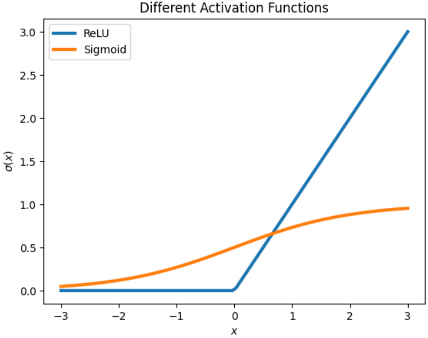
[2] Z. Cai, J. Choi, and M. Liu. *Least-Squares Neural Network (LSNN) Method For Linear Advection-Reaction Equation: Discontinuity Interface*. 2024. arXiv: 2301.06156 [math.NA].

Activation Functions and Shallow Neural Network

- **Shallow neural network (one hidden layer):**

$$\mathcal{M}_n(\sigma, d) = \left\{ c_{-1} + \sum_{i=0}^{n} c_i \sigma(\omega_i \cdot \mathbf{x} - b_i) : c_i, b_i \in \mathbb{R}, \omega_i \in \mathcal{S}^{d-1} \right\}$$

- **Some activation functions:**
  1. ReLU: $\sigma(x) = \max\{0, x\}$
  2. Sigmoid: $\sigma(x) = \frac{1}{1+e^x}$



A New Class of Approximating Functions

Universal Aproximation Theorem (Cybenko 1989, Hornik-Stinchcombe-White 1990)

$\mathcal{M}(\sigma, d) = \{v(\mathbf{x}) \in \mathcal{M}_n(\sigma, d) : n \in \mathbb{Z}_+\}$ is dense in $C(K)$ for any compact set $K \subset \mathbb{R}^d$, provided that $\sigma \in C(\mathbb{R})$ is not a polynomial.

A Priori Error Estimate

See, e.g., Daubechies-DeVore-Foucart-Hanin-Petrova 2021, Yarotsky 2017, DeVore-Hanin-Petrova 2021.

- **C^0 piecewise linear functions on a fixed mesh in $[0, 1]$:**

$$S_1^0(\Delta) = \left\{ \sum_{i=1}^{n} c_i \phi_i(x) : c_i \in \mathbb{R} \right\},$$

where

$$\phi_i(x) = \begin{cases} (x - x_{i-1})/(x_i - x_{i-1}), & x \in (x_{i-1}, x_i), \\ (x_{i+1} - x)/(x_{i+1} - x_i), & x \in (x_i, x_{i+1}), \\ 0, & \text{otherwise.} \end{cases}$$

- **C^0 piecewise linear functions on a moving mesh in $[0, 1]$:**

$$S_1^0(n) = \left\{ \sum_{i=1}^{n} c_i \phi_i(x; x_{i-1}, x_i, x_{i+1}) : c_i \in \mathbb{R}, , x_i \in [0, 1] \right\}$$

- **One-dimensional shallow neural network:**

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

- **Important inclusion[3]:**

$$S_1^0(n) \subset \mathcal{M}_n(I) \subset S_1^0(n+1)$$

[3] I. Daubechies et al. "Nonlinear Approximation and (Deep) ReLU Networks". English (US). in: *Constructive Approximation* 55.1 (Feb. 2022), pp. 127–172. ISSN: 0176-4276. DOI: 10.1007/s00365-021-09548-z.

Broader Goals

1. Solve PDEs using NNs
2. Design Competitive NN Methods that utilize
   - Physical information from the PDE
   - Geometric interpretation of the NN

Why Neural Networks?

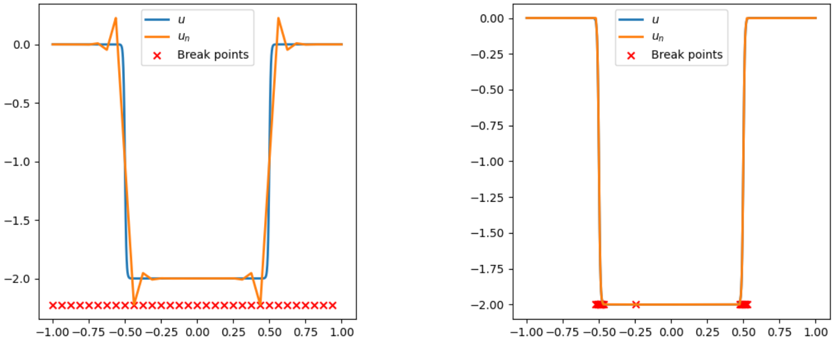


Figure: Solution $u(x)$ of a singularly perturbed reaction-diffusion equation approximated by NN. Left: 32 uniform breakpoints. Right: optimized NN model with 32 breakpoints, 500 iterations of the dBN method.

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1D Diffusion Problem

Consider the one-dimensional Poisson equation

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

Ritz formulation: find $u \in H^1(I)$ such that

$$u = \underset{\substack{v \in H^1(I) \\ v(0)=\alpha, v(1)=\beta}}{\arg\min} \left\{ \frac{1}{2} \int_0^1 a(x)(v'(x))^2 dx - \int_0^1 f(x)v(x)dx \right\}$$

Modified Ritz Formulation

Given $\gamma > 0$, let $J : H^1(I) \to \mathbb{R}$ be the modified energy functional given by

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

Let

$$\mathcal{M}_n(I) = \left\{ c_{-1} + \sum_{i=0}^{n} c_i \sigma(x - b_i) \, : \, c_i \in \mathbb{R}, 0 \le b_i \le 1, b_i < b_{i+1} \right\}$$

Ritz neural network approximation: find $u_n(x) \in \mathcal{M}_n(I)$ such that

$$J(u_n) = \min_{\substack{v \in \mathcal{M}_n(I) \\ v(0) = \alpha}} J(v)$$

Error Estimate

Proposition

Let u be the exact solution of the diffusion problem and $u_n \in \mathcal{M}_n(I)$ be the Ritz neural network approximation. Assume that $a \in L^\infty(I)$, then there exists a constant C depending on u such that

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

where $\|v\|_a^2 = \int_0^1 a(x)(v'(x))^2 dx + \gamma(v(1))^2$.

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Systems of Algebraic Equations

Let

$$u_n = u_n(x) = u_n(x; \mathbf{c}, \mathbf{b}) = \alpha + \sum_{i=0}^{n} c_i \sigma(x - b_i)$$

be a solution of the previous minimization problem. Then the linear and nonlinear parameters

$$\mathbf{c} = (c_0, \ldots, c_n)^T \quad \text{and} \quad \mathbf{b} = (b_0, \ldots, b_n)^T$$

satisfy the following system of algebraic equations

$$\nabla_{\mathbf{c}} J(u_n) = \mathbf{0} \quad \text{and} \quad \nabla_{\mathbf{b}} J(u_n) = \mathbf{0}.$$

Linear Parameters $\mathbf{c}$

The equation $\nabla_{\mathbf{c}} J(u_n) = 0$ has the form

$$\left(A(\mathbf{b}) + \gamma \mathbf{d}\mathbf{d}^T\right) \mathbf{c} = \mathbf{f}(\mathbf{b}) + \gamma(\beta - \alpha)\mathbf{d},$$

where

- $A(\mathbf{b}) = \int_0^1 a(x) \nabla_{\mathbf{c}} u_n'(x) \left(\nabla_{\mathbf{c}} u_n'(x)\right)^T dx$
  - i.e, $(A(\mathbf{b}))_{ij} = \int_0^1 a(x)\sigma'(x - b_{i-1})\sigma'(x - b_{j-1}) dx$
- $\mathbf{f}(\mathbf{b}) = \int_0^1 f(x) \nabla_{\mathbf{c}} u_n(x) dx$
- $\mathbf{d} = (b - b_0, \ldots, b - b_n)^T$

Coefficient Matrix

$$A(\mathbf{b}) \quad = \quad \begin{pmatrix} \int_{b_0}^{1} a(x)dx & \int_{b_1}^{1} a(x)dx & \int_{b_2}^{1} a(x)dx & \cdots & \int_{b_n}^{1} a(x)dx \\ \int_{b_1}^{1} a(x)dx & \int_{b_1}^{1} a(x)dx & \int_{b_2}^{1} a(x)dx & \cdots & \int_{b_n}^{1} a(x)dx \\ \int_{b_2}^{1} a(x)dx & \int_{b_2}^{1} a(x)dx & \int_{b_2}^{1} a(x)dx & \cdots & \int_{b_n}^{1} a(x)dx \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \int_{b_n}^{1} a(x)dx & \int_{b_n}^{1} a(x)dx & \int_{b_n}^{1} a(x)dx & \cdots & \int_{b_n}^{1} a(x)dx \end{pmatrix},$$

particularly, when $a(x) = 1$

$$A(\mathbf{b}) \quad = \quad \begin{pmatrix} 1-b_0 & 1-b_1 & 1-b_2 & \cdots & 1-b_n \\ 1-b_1 & 1-b_1 & 1-b_2 & \cdots & 1-b_n \\ 1-b_2 & 1-b_2 & 1-b_2 & \cdots & 1-b_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1-b_n & 1-b_n & 1-b_n & \cdots & 1-b_n \end{pmatrix}$$

Condition Number

Lemma

Let $a(x) = 1$, then the condition number of the coefficient matrix $A(\mathbf{b})$ is bounded above by $\mathcal{O}(n/h_{\min})$.

Inverse of the Coefficient Matrix (Uniform Partition)

For the uniform mesh and $a(x) = 1$, the inverse of the coefficient matrix is given by

$$A(\mathbf{b})^{-1} = \begin{pmatrix} \frac{1}{n+1} & -\frac{1}{n+1} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{n+1} & \frac{2}{n+1} & -\frac{1}{n+1} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{n+1} & \frac{2}{n+1} & -\frac{1}{n+1} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{n+1} & -\frac{1}{n+1} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{n+1} & \frac{2}{n+1} \end{pmatrix}$$

Inverse of the Coefficient Matrix

Lemma

The coefficient matrix is invertible and its inverse is given by

$$A(\mathbf{b})^{-1} = \begin{pmatrix} \frac{1}{s_1} & -\frac{1}{s_1} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{s_1} & \frac{1}{s_1}+\frac{1}{s_2} & -\frac{1}{s_2} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{s_2} & \frac{1}{s_2}+\frac{1}{s_3} & -\frac{1}{s_3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{1}{s_{n-1}}+\frac{1}{s_n} & -\frac{1}{s_n} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{s_n} & \frac{1}{s_n}+\frac{1}{s_{n+1}} \end{pmatrix},$$

where $s_i := \int_{b_{i-1}}^{b_i} a(x)dx$.

Nonlinear Parameters $\mathbf{b}$

Lemma

For $j = 0, 1, \ldots, n$, let

$$g(b_j) = f(c_j) + a'(b_j)\left(\sum_{i=0}^{j-1} c_i + \frac{c_j}{2}\right).$$

Then the Hessian matrix $\nabla^2_{\mathbf{b}} J(u_n)$ has the form

$$\mathcal{H}(\mathbf{c}, \mathbf{b}) = \mathbf{B}(\mathbf{c}, \mathbf{b}) + \gamma \mathbf{c}\mathbf{c}^T,$$

where $\mathbf{B}(\mathbf{c}, \mathbf{b}) := \text{diag}(-c_0 g(b_0), \ldots, -c_n g(b_n))$

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A Damped Block Newton (dBN) Method

We want to solve

$$\nabla_{\mathbf{c}} J\left(u_n\right) = \mathbf{0} \quad \text{and} \quad \nabla_{\mathbf{b}} J\left(u_n\right) = \mathbf{0}.$$

The equation $\nabla_{\mathbf{c}} J(u_n) = 0$ has the form

$$\left(A(\mathbf{b}) + \gamma \mathbf{d}\mathbf{d}^T\right)\mathbf{c} = \mathbf{f}(\mathbf{b}) + \gamma(\beta - \alpha)\mathbf{d},$$

The Hessian matrix $\nabla^2_{\mathbf{b}} J(u_n)$ has the form

$$\mathcal{H}(\mathbf{c}, \mathbf{b}) = \mathbf{B}(\mathbf{c}, \mathbf{b}) + \gamma \mathbf{c}\mathbf{c}^T,$$

where $\mathbf{B}(\mathbf{c}, \mathbf{b})$ is a diagonal matrix.

The Sherman-Morrison Formula

Let $\mathcal{A}(\mathbf{b}) = A(\mathbf{b}) + \gamma \mathbf{d}\mathbf{d}^T$, by the Sherman-Morrison formula, we have

$$\mathcal{A}(\mathbf{b})^{-1} = A(\mathbf{b})^{-1} - \frac{\gamma A(\mathbf{b})^{-1}\mathbf{d}\mathbf{d}^T A(\mathbf{b})^{-1}}{1 + \gamma \mathbf{d}^T A(\mathbf{b})^{-1}\mathbf{d}}.$$

Lemma

If $c_i g(b_i) \neq 0$ for all $i = 0, 1, \ldots, n$ and $1 - \gamma \mathbf{c}^T \mathbf{B}^{-1}(\mathbf{c}, \mathbf{b})\mathbf{c} \neq 0$, then the Hessian matrix $\mathcal{H}(\mathbf{c}, \mathbf{b})$ is invertible. Moreover, its inverse is given by

$$\mathcal{H}^{-1}(\mathbf{c}, \mathbf{b}) = -\left[\mathbf{B}^{-1}(\mathbf{c}, \mathbf{b}) + \frac{\gamma \mathbf{B}^{-1}(\mathbf{c}, \mathbf{b})\mathbf{c}\mathbf{c}^T \mathbf{B}^{-1}(\mathbf{c}, \mathbf{b})}{1 - \gamma \mathbf{c}^T \mathbf{B}^{-1}(\mathbf{c}, \mathbf{b})\mathbf{c}}\right].$$

A Damped Block Newton (dBN) Method

Let $\left(\mathbf{c}^{(k)}, \mathbf{b}^{(k)}\right)$ be the previous iterate. We then compute the current state $\left(\mathbf{c}^{(k+1)}, \mathbf{b}^{(k+1)}\right)$ by doing the following:

(i) Compute the linear parameters $\mathbf{c}^{(k+1)}$ by

$$\mathbf{c}^{(k+1)} = \mathcal{A}(\mathbf{b}^{(k)})^{-1} \left\{ \mathbf{f}(\mathbf{b}^{(k)}) + \gamma(\beta - \alpha)\mathbf{d}(\mathbf{b}^{(k)}) \right\}.$$

(ii) Assume that the Hessian matrix $\mathcal{H}(\mathbf{c}^{(k+1)}, \mathbf{b}^{(k)})$ is invertible. Set the search direction

$$\mathbf{p}^{(k)} = -\mathcal{H}(\mathbf{c}^{(k+1)}, \mathbf{b}^{(k)})^{-1} \nabla_{\mathbf{b}} J(u_n(x; \mathbf{c}^{(k+1)}, \mathbf{b}^{(k)})).$$

(iii) Compute the stepsize η_k

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

Set the current nonlinear parameters by

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

Some Remarks

- If $\mathbf{c}_i^{(k+1)} g(\mathbf{b}_i^{(k)})$ vanishes for some $i \in \{0, \ldots, n\}$, then the corresponding nonlinear parameter will remain unchanged, i.e., $\mathbf{b}_i^{(k+1)} = \mathbf{b}_i^{(k)}$, and be removed at the step (ii) of the method.
- The computational cost per iteration is $\mathcal{O}(n)$. More specifically, the linear parameters $\mathbf{c}^{(k+1)}$ and the direction vector $\mathbf{p}^{(k)}$ are calculated in $8(n+1)$ and $4(n+1)$ operations, respectively.

Numerical Experiments

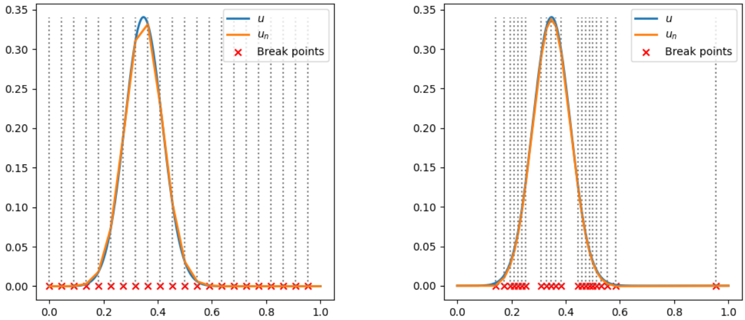
Example 1

$$u(x) = x\left(\exp\left(-\frac{(x-\frac{1}{3})^2}{0.01}\right) - \exp\left(-\frac{4}{9\times 0.01}\right)\right)$$

Consider the relative H^1 seminorm error given by

$$e_n = \frac{|u-u_n|_{H^1(I)}}{|u|_{H^1(I)}}$$

Numerical Experiments

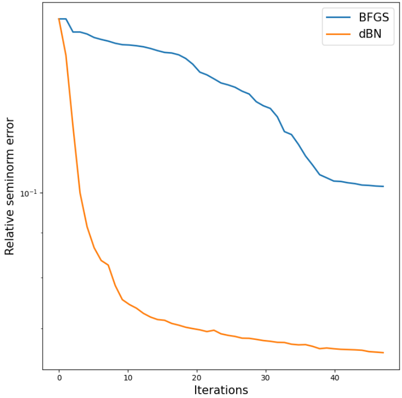


(a) Initial NN model with 22 uniform breakpoints, $e_n = 0.227$

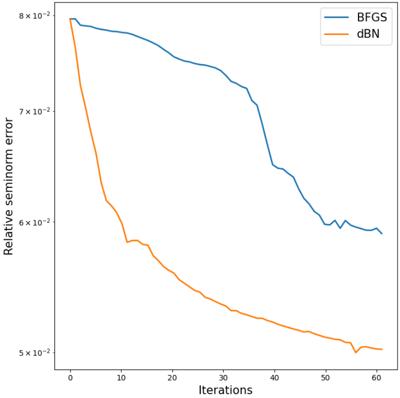
(b) Optimized NN model with 22 breakpoints, 500 iterations, $e_n = 0.100$

Figure: Using ReLU networks for approximating the function in Example 1

Numerical Experiments: dBN vs BFGS



(a) e_n vs number of iterations using 32 neurons, the ratio between the final errors is 0.673



(b) e_n vs number of iterations using 64 neurons, the ratio between the final errors is 0.783

Order of Convergence

n	e_n	r
60	4.65×10^{-2}	0.749
90	3.41×10^{-2}	0.751
120	2.49×10^{-2}	0.771
150	1.97×10^{-2}	0.783
180	1.78×10^{-2}	0.775
210	1.59×10^{-2}	0.775
240	1.27×10^{-2}	0.796
270	1.22×10^{-2}	0.787
300	1.09×10^{-2}	0.792
330	1.01×10^{-2}	0.792
360	9.94×10^{-3}	0.783
390	9.54×10^{-3}	0.780
420	8.07×10^{-3}	0.798

Table: Relative errors e_n and powers r for n neurons after 1000 iterations.

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Adaptivity

The true error $\|u_n - u\|_{a,K}$ on some interval $K \subseteq I$ is estimated by the ZZ-estimator:

$$\xi_K = \|a^{-1/2}\left(G(au_n') - au_n'\right)\|_{L^2(K)},$$

where $G(au_n')$ is the projection of au_n'. For a given $u_n \in \mathcal{M}_n(I)$ with the breakpoints

$$0 = b_{-1} < b_0 < \ldots < b_n < b_{n+1} = 1,$$

let $\mathcal{K}^i = [b_{i-1}, b_i]$, then $\mathcal{K}_n = \left\{\mathcal{K}^i\right\}_{i=0}^{n+1}$ is a partition of the interval $[0, 1]$.

Adaptivity

Then, we define a subset $\widehat{\mathcal{K}_n} \subset \mathcal{K}_n$ using the average marking strategy[4,5]:

$$\widehat{\mathcal{K}_n} = \left\{ K \in \mathcal{K}_n : \xi_{\mathcal{K}} \geq \frac{1}{\#\mathcal{K}_n} \sum_{K \in \mathcal{K}_n} \xi_{\mathcal{K}} \right\}$$

where $\#\mathcal{K}_n$ is the number of elements in $\mathcal{K}_n$. For a refinement step, a meshpoint gets added at the midpoint within each element of $\widehat{\mathcal{K}_n}$.

[4] M. Liu, Z. Cai, and J. Chen. "Adaptive two-layer ReLU neural network: I. Best least-squares approximation". In: *Computers & Mathematics with Applications* 113 (May 2022), pp. 34–44. ISSN: 0898-1221. DOI: 10.1016/j.camwa.2022.03.005.

[5] M. Liu and Z. Cai. "Adaptive two-layer ReLU neural network: II. Ritz approximation to elliptic PDEs". In: *Computers & Mathematics with Applications* 113 (2022), pp. 103–116. ISSN: 0898-1221. DOI: https://doi.org/10.1016/j.camwa.2022.03.010.

Adaptive Damped Block Newton (AdBN) method

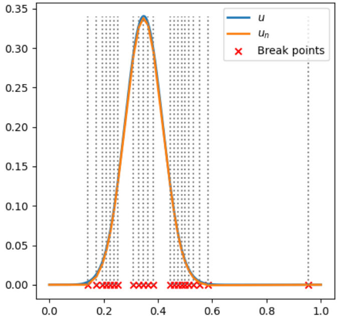
Given a tolerance ϵ, start with a small number of neurons n_0, then

(i) Compute the solution u_n using dBN

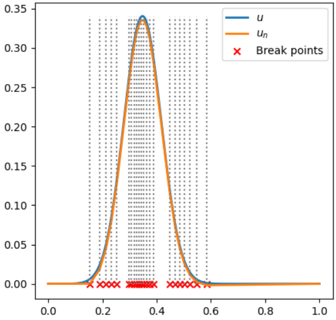
(ii) Estimate the total error by computing $\xi = \left(\sum_{K \in \mathcal{K}} \xi_K^2 \right)^{1/2} / |u_n|_{H^1(I)}$

(iii) If $\xi \leq \epsilon$, then stop; otherwise go to step (iv)

(iv) Add new neurons to the network by using the network enhancement strategy, then go to step (i)



(a) Optimized NN model with 22 breakpoints, 500 iterations, $e_n = 0.100$



(b) Adaptive NN model with 22 breakpoints: 10 initial breakpoints, 2 refinements (13, 22 neurons), $e_n = 0.083$

Figure: Using ReLU networks for approximating the function in Example 1

Numerical Experiments: dBN vs AdBN

NN (n neurons)	e_n	ξ_n	r
Adaptive (19)	1.04×10^{-1}	0.149	0.768
Adaptive (27)	6.55×10^{-2}	0.089	0.827
Adaptive (32)	5.71×10^{-2}	0.075	0.826
Adaptive (45)	4.21×10^{-2}	0.054	0.832
Adaptive (68)	2.76×10^{-2}	0.032	0.851
Adaptive (94)	2.01×10^{-2}	0.023	0.860
Adaptive (137)	1.39×10^{-2}	0.015	0.869
Adaptive (187)	1.04×10^{-2}	0.011	0.873
Adaptive (280)	6.93×10^{-3}	0.007	0.882
Fixed (187)	1.87×10^{-2}	0.020	0.761
Fixed (280)	1.12×10^{-2}	0.013	0.781

Table: Comparison of an adaptive network with fixed networks for relative error e_n, relative error estimators ξ_n, and rates r

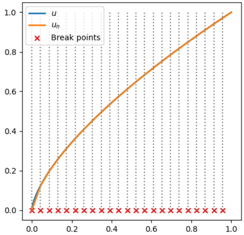
Numerical Experiments: Non-smooth Solution

Example 2

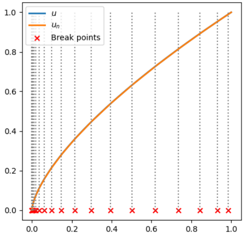
$$u(x) = x^{2/3}$$

This function belongs to $H^{1+\frac{1}{6}-\epsilon}(I)$ for any $\epsilon > 0$. We highlight that the order of convergence for approximating this solution with n uniform breakpoints is at most $\mathcal{O}\left(n^{-1/6}\right)$.

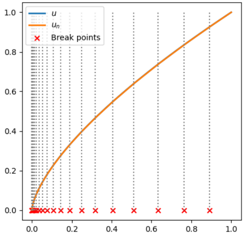
Figure: Results of using ReLU networks for approximating $u(x) = x^{2/3}$



(a) Initial NN model with 23 uniform breakpoints, $e_n = 0.284$



(b) Optimized NN model with 23 breakpoints, 500 iterations, $e_n = 0.056$



(c) Adaptive NN model with 23 breakpoints: 9 initial break points, 2 refinements (14, 23 neurons), $e_n = 0.042$

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Summary

- Approximating solutions to PDEs with NNs
  - Good initialization.
    - non-linear parameters $\longleftrightarrow$ uniform mesh.
    - linear parameters corresponding to uniform mesh are directly solved for.
  - Coefficient matrix has a sparse, tridiagonal inverse.
  - Hessian (from the non linear system) is diagonal.

Fast Iterative Solver for Neural Network Method: II. 1D General Elliptic Problems and Data Fitting

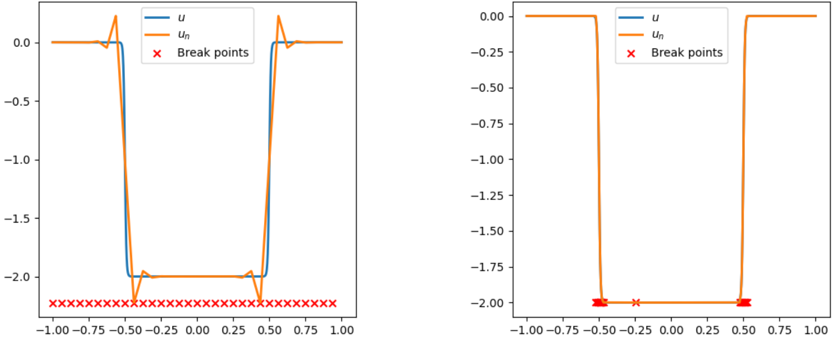

Figure: Solution $u(x)$ of a singularly perturbed reaction-diffusion equation approximated by NN. Left: 32 uniform breakpoints. Right: optimized NN model with 32 breakpoints, 500 iterations of the dBN method.

Thanks!