Multi-level Neural Networks for Accurate Solutions of Boundary-Value Problems

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Deep Neural Networks

Let us consider a feedforward neural network consisting of n hidden layers, each layer being of width N_i. The DNN with input $\boldsymbol{z}_0$ and output $\boldsymbol{z}_{n+1}$ is defined as

$$\boxed{\begin{array}{ll} \text{Input layer:} & \boldsymbol{z}_0, \\ \text{Hidden layers:} & \boldsymbol{z}_i = \sigma(W_i \boldsymbol{z}_{i-1} + \boldsymbol{b}_i), \quad i = 1, \cdots, n, \\ \text{Output layer:} & \boldsymbol{z}_{n+1} = W_{n+1} \boldsymbol{z}_n + \boldsymbol{b}_{n+1}, \end{array}}$$

where

$$\begin{aligned} \sigma &= \text{given activation function}, \\ \boldsymbol{W}_i &= \text{weights matrix with size } N_i \times N_{i-1}, \\ \boldsymbol{b}_i &= \text{biases vector with size } N_i. \end{aligned}$$

PINNs [Raissi et al.(2019)]

Consider the linear PDE in its residual form:

$$R\big(\boldsymbol{x}, u(\boldsymbol{x})\big) := f(\boldsymbol{x}) - Au(\boldsymbol{x}) = 0, \quad \forall \boldsymbol{x} \in \Omega,$$

with the zero Dirichlet boundary conditions

$$B\big(\boldsymbol{x}, u(\boldsymbol{x})\big) := u(\boldsymbol{x}) = 0, \quad \forall \boldsymbol{x} \in \partial\Omega.$$

Defining a function $g(\boldsymbol{x})$ that vanishes on the boundary, we approximate u with

$$\tilde{u} = \tilde{u}_\theta = g(\boldsymbol{x}) z_{n+1},$$

by minimizing the **loss function**

$$\boxed{\mathcal{L}(\theta) := \int_\Omega R\big(\boldsymbol{x}, \tilde{u}(\boldsymbol{x})\big)^2 dx.}$$

Model Problem

We will use the one dimensional Poisson problem to back our findings. Our goal is to find $u(x)$ that satisfies

$$\boxed{\begin{aligned} -\partial_{xx} u(x) &= f(x), \qquad \forall x \in (0,1), \\ u(0) &= 0, \\ u(1) &= 0. \end{aligned}}$$

The source term f is chosen such that the exact solution is

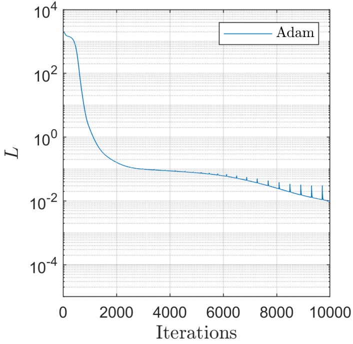
$$u(x) = e^{\sin(k\pi x)} + x^3 - x - 1,$$

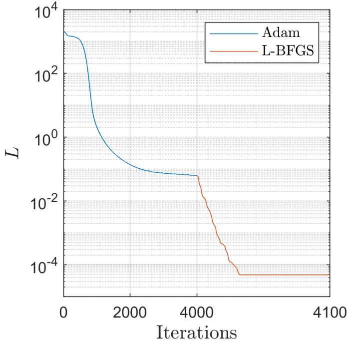
where k is a given integer.

Optimization Algorithm

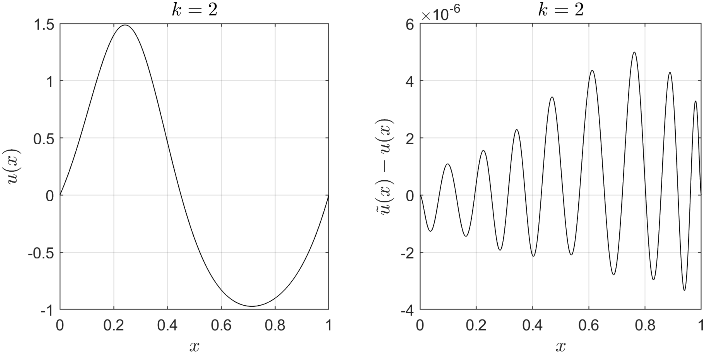
Solving Poisson problem for $k = 2$ using:

- ▷ Adam
- ▷ Adam followed by L-BFGS





Error Analysis



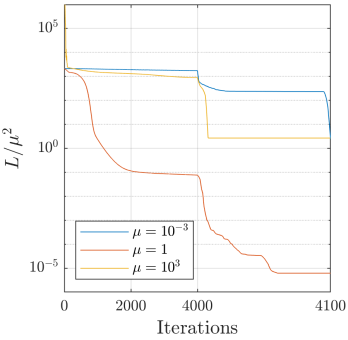
If we want to approximate the remaining error with a new neural network, two issues arise:

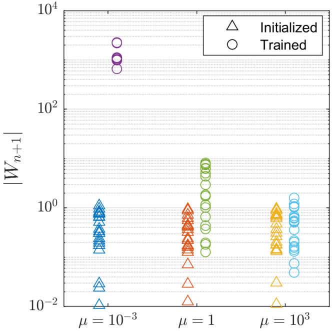
- the error is **not normalized**
- the error exhibits **higher frequencies**

Normalization

Poisson problem with the exact solution:

$$u(x) = \frac{1}{\mu}\left(e^{\sin(2\pi x)} + x^3 - x - 1\right)$$





High Frequencies

We consider again the Poisson problem on $\Omega = (0,1)$, with $k = 10$.

To approximate high frequencies we present the Fourier feature mapping:

$$\gamma(x) = [\cos(\boldsymbol{\omega}_M x), \sin(\boldsymbol{\omega}_M x)], \qquad \gamma_g(x) = [\sin(\boldsymbol{\omega}_M x)].$$

with

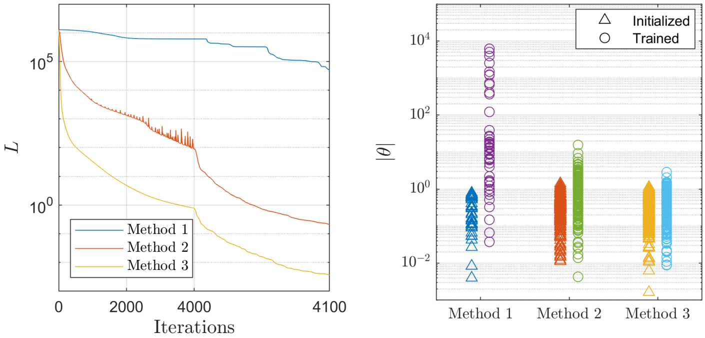
$$\boldsymbol{\omega}_M = [2^0\pi, \dots, 2^{M-1}\pi]$$

	Method 1	**Method 2**	**Method 3**
$\boldsymbol{z}_0$	x	$\gamma(x)$	$\gamma(x)$
$\tilde{u}$	$z_{n+1}x(1-x)$	$z_{n+1}x(1-x)$	$M^{-1}\gamma_g(x) \cdot \boldsymbol{z}_{n+1}$

High Frequencies

Poisson problem with the exact solution:

$$u(x) = e^{\sin(10\pi x)} + x^3 - x - 1$$



Correction Neural Network

Consider an initial solution $\tilde{u}_0$ to the boundary value problem.

We define the error in $\tilde{u}_0$ as $e(\boldsymbol{x}) = u(\boldsymbol{x}) - \tilde{u}_0(\boldsymbol{x})$ and satisfies:

$$\begin{aligned} R(\boldsymbol{x}, \tilde{u}_0(\boldsymbol{x})) - Ae(\boldsymbol{x}) &= 0, \quad \forall \boldsymbol{x} \in \Omega, \\ B(\boldsymbol{x}, e(\boldsymbol{x})) &= 0, \quad \forall \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

In order to normalize the solution we will modify the problem to:

$$\begin{aligned} \tilde{R}(\boldsymbol{x}, \tilde{e}(\boldsymbol{x})) = \mu R(\boldsymbol{x}, \tilde{u}_0(\boldsymbol{x})) - A\tilde{e}(\boldsymbol{x}) &= 0, \quad \forall \boldsymbol{x} \in \Omega, \\ B(\boldsymbol{x}, \tilde{e}(\boldsymbol{x})) &= 0, \quad \forall \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

The corrected solution is given as:

$$\boxed{\tilde{u}(\boldsymbol{x}) = \tilde{u}_0(\boldsymbol{x}) + \frac{1}{\mu}\tilde{e}(\boldsymbol{x}).}$$

Multi-level Neural Networks

Considering the first normalized approximation verifying:

$$\begin{aligned} R_0(\boldsymbol{x}, u_0(\boldsymbol{x})) = \mu_0 f(\boldsymbol{x}) - A u_0(\boldsymbol{x}) &= 0, \quad \forall \boldsymbol{x} \in \Omega, \\ B(\boldsymbol{x}, u_0(\boldsymbol{x})) &= 0, \quad \forall \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

Each new correction u_i then satisfies the boundary-value problem:

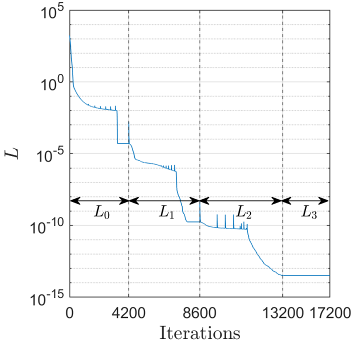
$$\begin{aligned} R_i(\boldsymbol{x}, u_i(\boldsymbol{x})) = \mu_i R_{i-1}(\boldsymbol{x}, \tilde{u}_{i-1}(\boldsymbol{x})) - A u_i(\boldsymbol{x}) &= 0, \quad \forall \boldsymbol{x} \in \Omega, \\ B(\boldsymbol{x}, u_i(\boldsymbol{x})) &= 0, \quad \forall \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

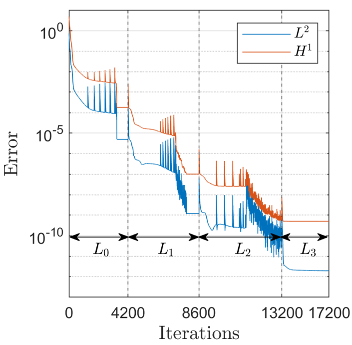
The final approximation $\tilde{u}$ of u is given as:

$$\boxed{\tilde{u}(\boldsymbol{x}) = \frac{1}{\mu_0}\tilde{u}_0(\boldsymbol{x}) + \frac{1}{\mu_0\mu_1}\tilde{u}_1(\boldsymbol{x}) + \ldots + \frac{1}{\mu_0\mu_1\ldots\mu_L}\tilde{u}_L(\boldsymbol{x}).}$$

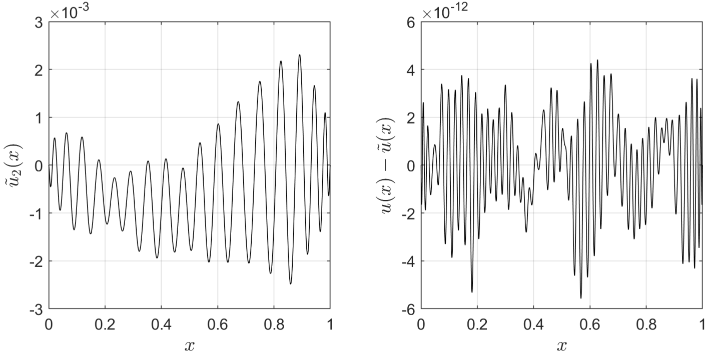
MLNNs Example

	$\tilde{u}_0$	$\tilde{u}_1$	$\tilde{u}_2$	$\tilde{u}_3$
Wave numbers M	1	3	5	1
Normalization μ_i	1	10^3	10^3	10^2





MLNNs Example



- The error is reduced to the order of 10^{-12} after three corrections
- Even after normalizing the amplitude of $\tilde{u}_2(x)$ is small

Extreme Learning Method

To suitably choose the normalizing factors μ_i we will:

- Calculate a coarse prediction of the remaining error using the **Extreme Learning Method**
- Choose μ_i using the amplitude of the estimated error

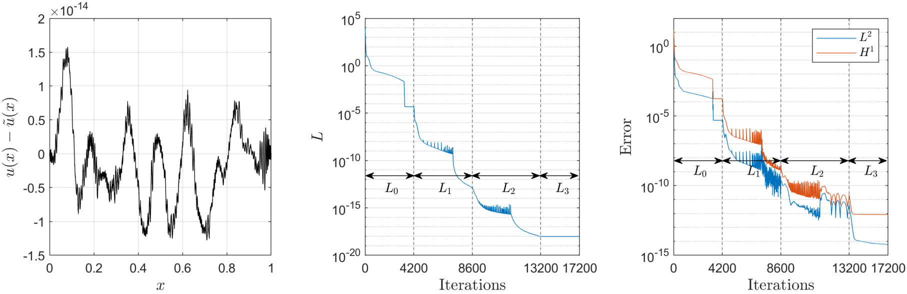
In the **Extreme Learning Method** the solution is approximated with a neural network by:

- Fixing the parameters of the hidden layers
- Minimizing the loss function with respect to the output layer parameters using a least square method

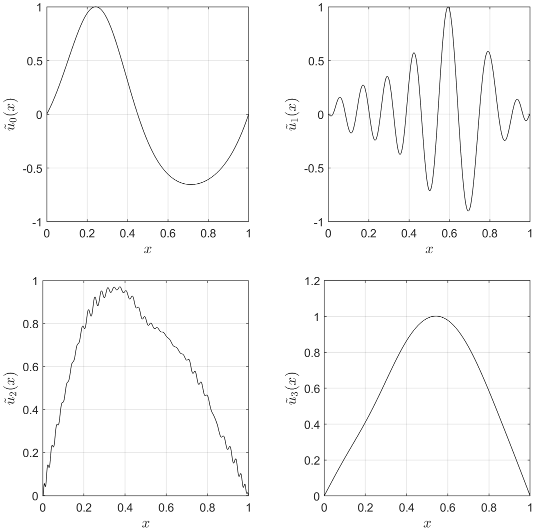
We choose the **Extreme Learning Method** because it is **fast** and **scale independent.**

MLNNs Example with ELM

	$\tilde{u}_0$	$\tilde{u}_1$	$\tilde{u}_2$	$\tilde{u}_3$
Wave numbers M	1	3	5	1



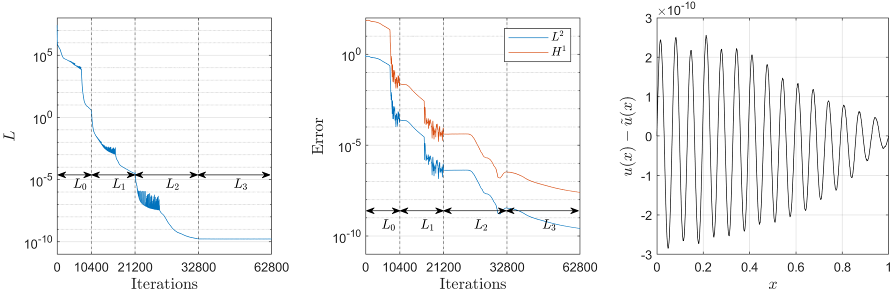
MLNNs Example with ELM



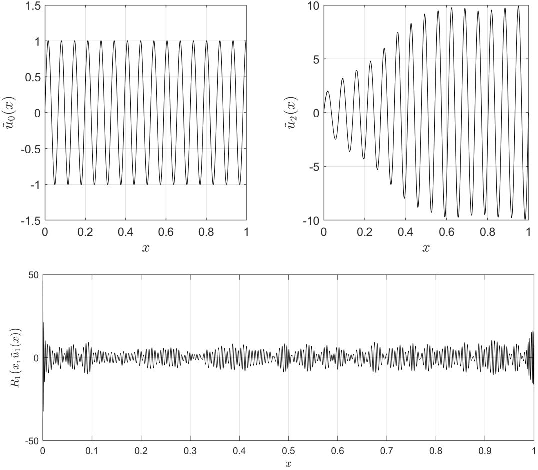
Helmholtz Equation

One dimensional Helmholtz equation

$$-\partial_{xx}u(x) - 9200u(x) = 0, \qquad \forall x \in (0,1),$$
$$u(0) = 0, \qquad u(1) = 1.$$



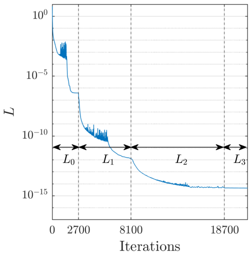
Helmholtz Equation

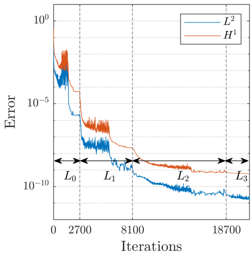


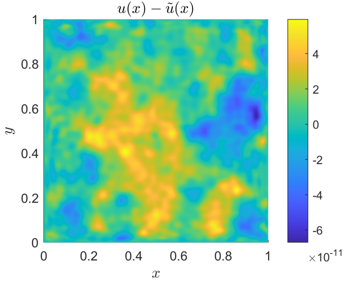
2D Poisson Equation

Two dimensional Poisson problem

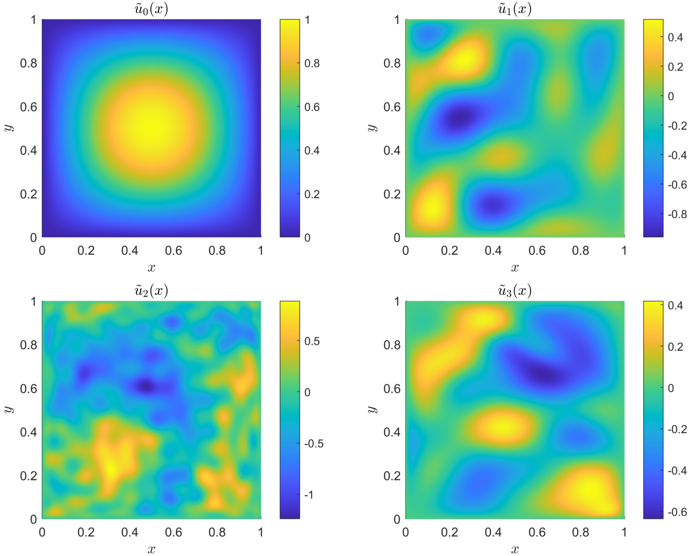
$$\begin{aligned} -\nabla^2 u(x,y) &= f(x,y), && \forall x \in \Omega, \\ u(x,y) &= 0, && \forall x \in \partial\Omega. \end{aligned}$$







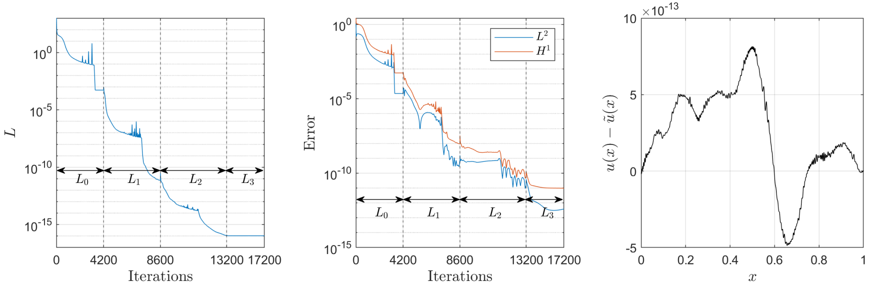
2D Poisson Equation



Non-linear problem

Non-linear boundary value problem

$$
\begin{aligned}
&-\partial_{xx}u(x) - 8u(x)\partial_x u(x) = 0, \qquad \forall x \in (0,1),\\
&u(0) = -1, \qquad u(1) = -1/5.
\end{aligned}
$$



Summary

- Introduced the multi-level neural networks to control and reduce the errors for linear BVPs when using deep learning approaches
- Addressed the issues of low amplitudes and high frequencies to correct the resulting errors
- Exhibited the potential of MLNNs to significantly reduce L^2 and H^1 errors for various BVPs, achieving machine precision in some cases
- For future work, we aim to extend MLNNs to other deep learning approaches and propose automated hyper-parameter selection for different levels

Thank you!

For further details:
Aldirany, Z., Cottereau, R., Laforest, M., Prudhomme, S. (2024). Multi-level Neural Networks for Accurate Solutions of Boundary-Value Problems. *Comp. Meth. Appl. Mech. Eng.* 419(116666).
arXiv:2308.11503.