CS230

Deep Learning for Partial Differential Equations (PDEs)

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Abstract

Partial differential equations (PDEs) have been widely used. However, solving PDEs using traditional methods in high dimensions suffers from the curse of dimensionality. The newly emerging deep learning technqiues are promising in resolving this problem because of its success in many high dimensional problems. In this project we derived and proposed a coupled deep learning neural network for solving the Laplace problem in two and higher dimensions. Numerical results showed that the model is efficient for modest dimension problems. We also showed the current limitation of the algorithm for high dimension problems and proposed an explaination.

1 Introduction & Related Work

Solving PDEs (partial differential equations) numerically is the most computation-intensive aspect of engineering and scientific applications. Recently, deep learning emerges as a powerful technique in many applications. The success inspires us to apply such a technique to solving PDEs. One of the main feature is that it can represent complex-shaped functions effectively compared to traditional finite basis function representations, which may require large number of parameters or sophisticated basis. It can also be treated as a black-box approach for solving PDEs, which may serve as a first-to-try method. The biggest challenge is that this topic is rather new and there are few literature (for some examples on this topic, see [2]-[7] that we can refer to. Whether it can work reasonably well remains to be explored.

$$L(\theta) = (\mathcal{L}\hat{u}(x,t|\theta) - f)^2 \tag{1}$$

reads to a very accurate solution (up to 7 digits) to

$$\mathcal{L}u = f \tag{2}$$

where $\mathcal{L}$ is some certain differential operator.
Since 2017, many authors begin to apply deep learning neural network to solve PDE. Raissi, et al[3] considers,

$$u_t = N(t, x, u_x, u_{xx}, ...), \quad f := u_t - N(t, x, u_x, u_{xx}, ...) \tag{3}$$

where $u(x,t)$ is also represented by a neural network. Parameters of the neural network can be learnt by minimizing

$$\sum_{i=1}^{N} (|u(t^2, x^i) - u^i|^2 + |f(t^i, x^i)|^2) \tag{4}$$

where the term $|u(t^2, x^i) - u^i|^2$ tries to fit the data on the boundary and $|f(t^i, x^i)|^2$ tries to minimize the error on the collocation points.

I.E. Lagaris et al has already applied artificial neural network to solve PDEs. Limited by computational resources they only used a single hidden layer and model the solution $u(x,t)$ by a neural network $\hat{u}(x, t(\theta))$.

2 Dataset and Features

The data set is generated randomly both on the boundaries and in the innerdomain. For every update, we randomly generate $\{(x_i, y_i)\}_{i=1}^{M}, (x_i, y_i) \in \partial\Omega$ and compute $g_i = g_D(x_i, y_i)$. The data are then fed to (2) for computing loss and derivatives.

For every update, we randomly generate $\{(x_i, y_i)\}_{i=1}^{N}, (x_i, y_i) \in \Omega$ and compute $f_i = f(x_i, y_i)$. The data are then fed to (1) for computing loss and derivatives.

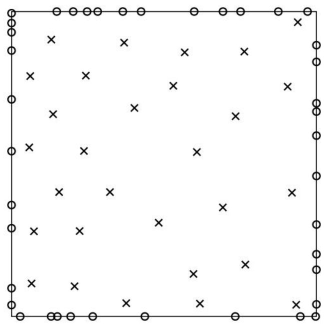


Figure 1: Data Generation for Training the Neural Network. We sample randomly from the inner domain Ω and its boundary $\partial\Omega$. Here $\times$ represents the sampling points within the domain and $\circ$ represents the sampling points on the boundary.

3 Approach

Our main focus is elliptic PDEs, which is generally presented as:

$$\begin{aligned} -\frac{\partial}{\partial x}\big(p(x,y)\frac{\partial u}{\partial x}\big) - -\frac{\partial}{\partial y}\big(q(x,y)\frac{\partial u}{\partial y}\big) + r(x,y)u = f(x,y), &\quad \text{in } \Omega \\ u = g_D(x,y), &\quad \text{on } \Omega_D \\ p(x,y)\frac{\partial u}{\partial x}\frac{\partial y}{\partial s} - q(x,y)\frac{\partial u}{\partial y}\frac{\partial x}{\partial s} + c(x,y)u = g_N(x,y), &\quad \text{on } \Omega_N \end{aligned} \tag{5}$$

In the case $p = q \equiv -1, r \equiv 0, \partial\Omega_D = \partial\Omega$, we obtain the Poisson equation:

$$\begin{cases} \triangle u = f, & \text{in } \Omega \\ u = g_D & \text{on } \partial\Omega \end{cases} \tag{6}$$

In the case $f = 0$, we obtain the Laplace equation.
Our algorithm for solving Poisson equation (12) is as follows: we approximate u with

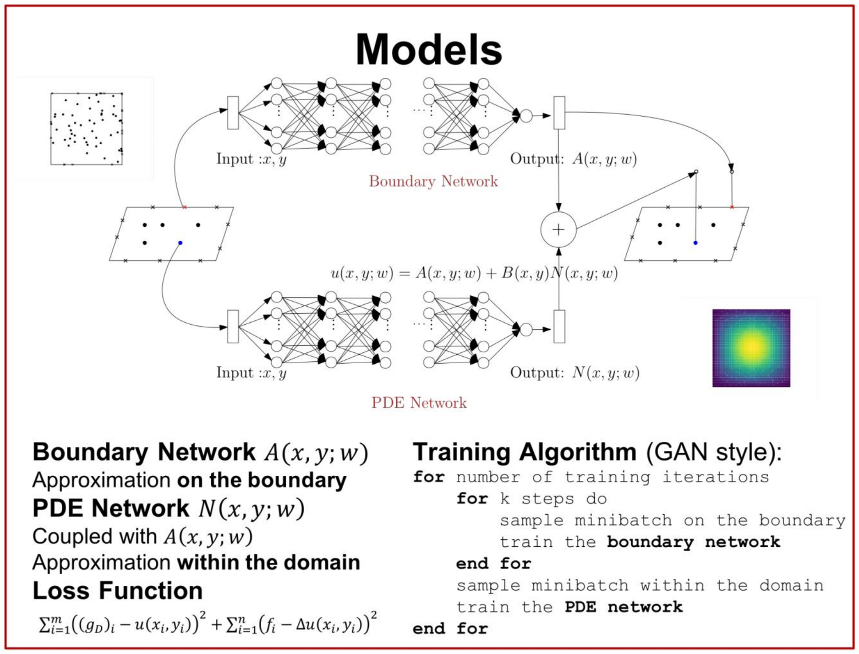
$$u(x, y; w_1, w_2) = A(x, y; w_1) + B(x, y) \cdot N(x, y; w_2)$$

where $A(x, y; w_1)$ is a neural network that approximates the boundary condition

$$A(x, y; w_1)|_{\partial\Omega} \approx g_D \tag{7}$$

and where $B(x, y)$ satisfies $B(x, y)|_{\partial\Omega} \equiv 0$. Our network looks like this fig. 2. To evaluate the effectiveness of our method, we will report three error metrics, which can be used as indicators for different purposes.

$$\begin{aligned} \text{Bounding loss} \quad & L_b = \textstyle\sum_{i=1}^{n_b} \Big(A(x_i, y_i; w_i) - u_i\Big)^2 \\ \text{PDE loss} \quad & L_p = \textstyle\sum_{i=1}^{n_p} \Big(\triangle u_h(x_i, y_i; w_1, w_2) - f_i\Big)^2 \\ L_2 \text{ error} \quad & L_2 = \sqrt{\tfrac{1}{m} \textstyle\sum_{i=1}^{m} |u_h(x_i, y_i; w_1, w_2) - u(x_i, y_i)|^2} \end{aligned}$$



Models

Boundary Network $A(x, y; w)$
Approximation **on the boundary**
PDE Network $N(x, y; w)$
Coupled with $A(x, y; w)$
Approximation **within the domain**
Loss Function
$\sum_{i=1}^{m}\left((g_D)_i - u(x_i, y_i)\right)^2 + \sum_{i=1}^{n}\left(f_i - \Delta u(x_i, y_i)\right)^2$

Training Algorithm (GAN style):

```
for number of training iterations
    for k steps do
        sample minibatch on the boundary
        train the boundary network
    end for
    sample minibatch within the domain
    train the PDE network
end for
```

Figure 2: The structure of our network. We proposed this idea at the inspiration of GAN, where we update the boundary network for several times before we update the PDE network once. Our loss function is made up of two components: boundary loss and interior loss.

4 Experiments/Results/Discussion

To demonstrate the effectiveness of our method, we applied method of manufactured solution (MMS), i.e. construct some equations with analytic solutions and then compare the numerical solution with the analytic solutions. We consider problems on the unit square $\Omega = [0, 1]^2$, and the reference solution is computed on a uniform 50×50 grid. The test is on well-behaved solutions, solutions with peaks and some other less regular solutions. All of them were manufactured.

4.1 Example 1: Well-behaved Solution

Consider the analytical solution

$$u(x, y) = \sin \pi x \sin \pi y, \quad (x, y) \in [0, 1]^2 \tag{8}$$

then we have

$$f(x, y) = \Delta u(x, y) = -2\pi^2 \sin \pi x \sin \pi y \tag{9}$$

and the boundary condition is zero boundary condition.

The hyper-parameters for the network include $\varepsilon = 10^{-5}$, $L = 3$, $n^{[1]} = n^{[2]} = n^{[3]} = 64$. In figures below, the red profile shows exact solutions while the green profile shows the neural network approximation. Figure 3 *(a)* shows the initial profiles of the neural network approximation, while fig. 3 *(c)* shows that after 300 iterations it is nearly impossible to distinguish the exact solution and the numerical approximation.

4.2 Example 2: Solutions with a Peak

Consider the manufactured solution

$$u(x, y) = \exp[-1000(x - 0.5)^2 - 1000(y - 0.5)^2] + v(x, y) \tag{10}$$

where $v(x, y)$ is a well-behaved solution, such as the one in section 4.1. Figure 5 shows the plot of $\exp[-1000(x - 0.5)^2 - 1000(y - 0.5)^2]$. Very large Laplacian at some point can be difficult for the approximation. As an illustration, let $v(x, y) = \sin(\pi x)$. If we do not do the singularity subtraction and run the neural network directly, we obtain fig. 5. We see that the numerical solution diverges.

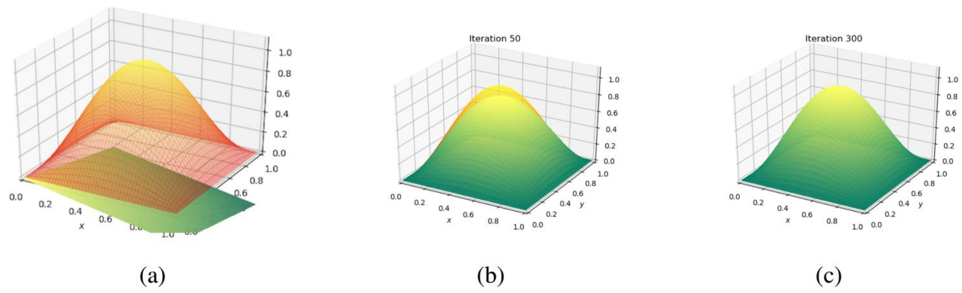


Figure 3: Evolution of the neural network approximation. At 300 iteration, it is hard to distinguish numerical solution and exact solution by eyes.

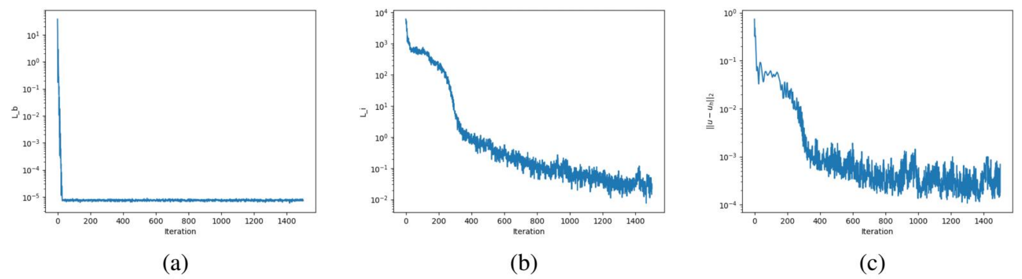


Figure 4: Loss and error of the neural network. For L_b, we have adopted an early termination strategy and therefore the error stays around 10^{-5} once it reaches the threshold. The PDE error L_i and L_2 error approximation keeps decreasing, indicating effectiveness of the algorithm.

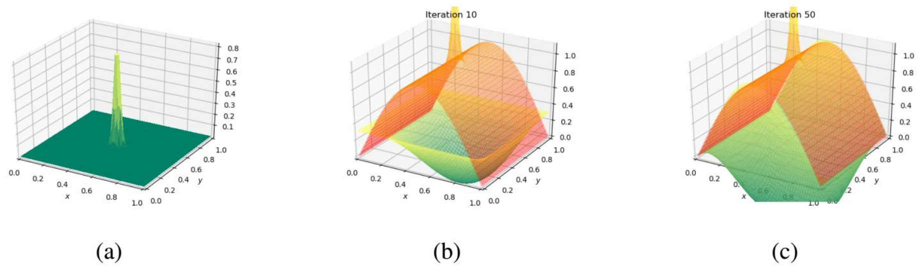


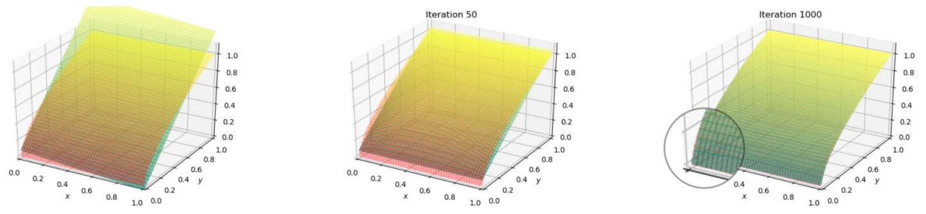
Figure 5: Plot of $\exp[-1000(x-0.5)^2-1000(y-0.5)^2]$, which has a peak at $(0.5, 0.5)$, and the evolution across iterations. This extreme behavior proposes difficulty for neural network approximation, since the Laplacian around $(0.5, 0.5)$ changes dramatically and can be very large. Solution converges on the boundary after several iterations but because of the peak, it diverges within the domain.

4.3 Example 3: Less Regular Solutions

Consider the following manufactured solution

$$u(x, y) = y^{0.6} \tag{11}$$

the derivative of the solution goes to infinity as $y \to \infty$, which makes the loss function hard to optimize. In the meanwhile, we notice that for any interval $[\delta, 1], \delta > 0$, the derivatives of $u(x, y)$ on $[0, 1] \times [\delta, 1]$ is bounded, that is to say, only the derivatives near $y = 0$ bring trouble to the optimization. Figure fig. 6 shows the initial profile of the neural network approximation. See Section 4.1 for detailed description of the surface and notation. Even at 1000 iteration, we can still observe obvious mismatch between the exact solution and the numerical solution (fig. 6).



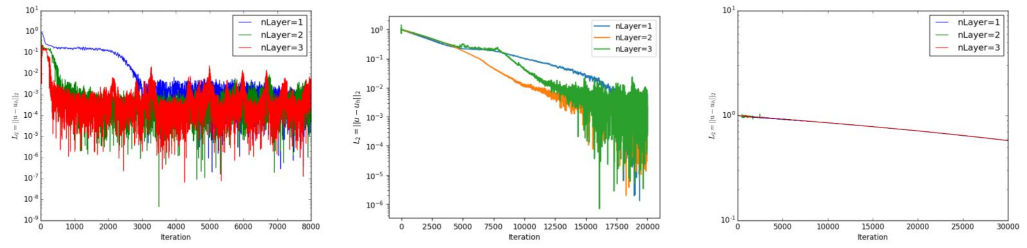
(a) (b) (c)

Figure 6: Numerical solution at iteration 1000. Near $y = 0$, there is data mismatch between numerical solution, exact solution and network approximation. At $y \approx 0$, the derivative $\frac{\partial u}{\partial y} \to \infty$. We can see the distortion between approximation solution and exact solution near $y = 0$.

4.4 Higher dimensions

In the plots presented, we observe that, when dimension is small, increasing the number of layers does not help with the ultimate performance of our approximation. The convergence speed, however, increased when there are more layers in the network. As we see, this holds true for *(a)* and *(b)*, where dimensions are 2 and 5 (in fig. 7).

Our approximation for high dimensions is constrained by computation power. In 7D approximation, all settings show promises, as the L_2 loss is dropping. But we do not witness the convergence because 30K iterations is not enough. For 10D domain approximation, it is even worse, because the loss seems not to reduce at all. However, this result is reasonable, since high dimensional curve itself is complex and difficult to approximate, and our network may simply do not have enough parameters to finish this task. We are happy to share our results of higher dimension explorations upon request.



(a) (b) (c)

Figure 7: Performance of approximation for domains in different dimensions. In low dimensional problems, it converges fast, and the more layers we have, the faster convergence we observe; the number of layers do not affect the ultimate performance. The higher the dimensions are, the longer it takes to train to converge. Notice in *(c)*, for 7D domain approximation, we cannot see the convergence in 30K iterations, but in general the loss is being reduced. For even higher dimensions, the converge will be much slower.

5 Conclusion/Future Work

In this project, we proposed novel deep learning approaches to solve the Laplace equation,

$$\begin{cases} \triangle u = f, & \text{in } \Omega \\ u = g_D & \text{on } \partial\Omega \end{cases} \tag{12}$$

We also showed results for different kinds of solutions, and discussed the high dimension cases as well. In the future, we will generalize results to other types of PDEs, and also investigate algorithms for ill-behaved solutions, such as peaks, exploding gradients, oscillations, etc.

6 Contributions

Kailai worked on mathematical formulation of the methods, while Bella and Shuyi worked on the model tuning and realization. The source code was developed from scratch by us and can be found at https://github.com/kailaix/nnpde.

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