CSE 6730 - Spring 2022
Project Proposal

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Project Title: Simulating Physical Systems with Modern Techniques
GitHub: https://github.gatech.edu/clee685/CSE-6730-Project

1 Checkpoint 1

1.1 Physical Problem and Math Formulation

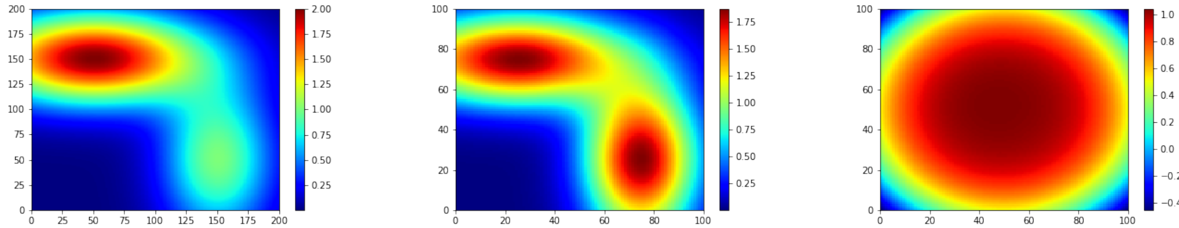
In this project, we consider physics problems such as the electrical impedance tomography(EIT) problem and solve them with some machine learning techniques. We will compare results from different type of methods.
Let γ be the electrical conductivity and u be the potential, there is a unique solution u for each given γ with suitable boundary condition $u|_\Omega$ or $\gamma\frac{\partial u}{\partial \mathbf{n}}$. The system is described by the following equations:

$$\nabla \cdot (\gamma \nabla u) = f \tag{1}$$
$$u|\partial\Omega = a(x) \tag{2}$$
$$\gamma|\partial\Omega = b(x) \tag{3}$$

We are only given the data f and the boundary conditions of u and γ without the expression of γ inside the region. We need to solve the value of γ and u for the whole space. That's the so called inverse problem. Notice that it is not a well-posed problem unless we specify some regularity constraints on the functions.

1.2 Modeling of the problem

There are many traditional methods applied to this problem. In [1], the authors suggested that neural network based approaches are more suitable for this type of problems. They applied WAN method to EIT problem and also implemented PINN. In the experiment, the strategy the authors used was updating the PDE solution u and the space dependent coefficient γ alternatively to better fit the data f and the boundary conditions a, b. In figure 1, we show the implemented result of one experiment from [1], where the predicted γ is very close to the ground truth γ^*.



(a) (b) (c)

Figure 1: (a) Ground truth γ^*, (b) predicted γ, (c) predicted u.

In our project, we will apply their strategy, run the programs with different neural network architectures. We will also try the Deep Ritz method on this problem. Deep Ritz method is a machine learning approach which is very effective to the elliptic PDEs.
Since in [1] they implemented WAN and PINN, we will implement DRM and compare the results. These three types of techniques differ from their optimization process:

- PINN aims to minimize the l2 or some other norm of the error

$$MSE = \frac{1}{N_u}\sum_{i=1}^{N_f}\left|u(x_u^i, t_u^i) - u^i\right|^2 + \frac{1}{N_f}\sum_{i=1}^{N_f}\left|f(x_f^i, t_f^i)\right|^2, \tag{4}$$

- WAN uses weak formulation of PDE and introduces the test function ϕ, it aims to solve a minmax problem

$$min_{\gamma,u} max_{\phi}\{|\langle\nabla\cdot(\gamma\nabla u), \phi\rangle| + \lambda||u - a(x)||_{\partial\Omega}\} \tag{5}$$

- DRM uses the variational formula of elliptic PDE and aims to minimize

$$\min_{u\in H}\int_{\Omega}\left(\frac{1}{2}|\nabla u|^2 - f(x)u(x)\right)dx, \tag{6}$$

We model the functions u, γ with neural networks u_θ, γ_θ. Generally they compose of several layers of linear maps and activation functions. The size of parameter θ can be really large so they have strong approximation abilities. We will study the influence of the number of layers, number of neurons and as well as the type of activation functions on the final results.
In details, we define $f_i(x) = \sigma(Ax + b)$, here A is a matrix and b is a vector, σ is some activation function. Then we set $f(x) = f_n(f_{n-1}(...f_1(x)))$. Intuitively, the neural networks look like as

1.3 Platforms of development

We will use Tensorflow and Pytorch for the implementation. They provide many packages and functions, and are designed for machine learning problems.

1.4 Division of labor

All team members have equal contributions to the modeling part.

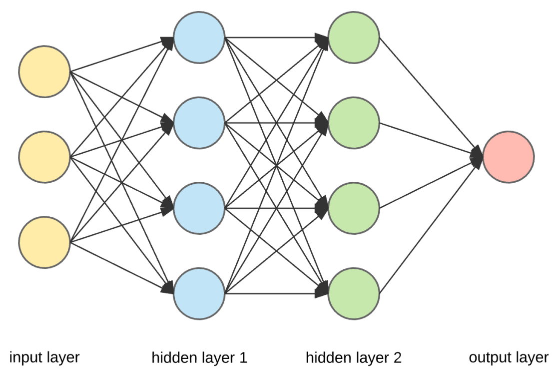


Figure 2: Structure of neural networks

2 Literature Review

2.1 Problem Statement

Many physical problems can be formulated as differential equations (ODE or PDE). They are described by a set of equations which may evolve the (time/space) derivatives of functions. We aim to solve the functions from the given information which is typically the boundary condition or initial condition.
For example, the transfer of heat is described by the heat equation:

$$\frac{\partial u}{\partial t} = \alpha \Delta u \tag{7}$$

Here $u(x, t)$ is the function that gives temperature at time t and position x, α is the thermal diffusivity of the medium.
And the propagation of wave is described by another type of equations with the following form:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u \tag{8}$$

We can get some qualitative results by analyzing the equations. For example, it's well known that heat propagation doesn't take time while the propagation of wave has speed c.
However, we need to do numerical simulations to get more detailed information. Nowadays there are many numerical methods available, including traditional PDE solvers like finite difference method or finite element method, and modern machine learning based approaches. In this project, we plan to study and simulate some physical systems with these techniques and compare the results. Hopefully, we can gain insights about the real physical system from the numerical solutions.

2.2 Previous Work

Traditional numerical methods often divide the space with many grids. The function value at these grid points are unkowns, and the equations are discretized to get a linear system. Solving the linear system can give us the values at each grid point. However, as dimensional goes higher, the number of grid points required grows exponentially, and the computation cost will become

extremely expensive. That's the so called 'curse of dimensionality'. On the hand, most machine learning appoaches use sample points instead of grids, and the functions are more flexible. This can reduce he computational cost and make the problems solvable. That's one of the advantages of machine learning approaches against traditional PDE solvers.
Each type of differential equations has its own properties, so people developed different neural network based approaches for each type.

2.2.1 PINN (Physics-Informed Neural Networks)

In [2], the authors trained the network u as the solution of the PDE, where they consider parametrized and nonlinear differential equations of general form

$$u_t + \mathcal{N}[u; \lambda] = 0. \tag{9}$$

Denote $f(x,t) := u_t(x,t) + \mathcal{N}[u(x,t); \lambda]$, one can obtain the solution u by minimizing the mean squared error

$$MSE = \frac{1}{N_u} \sum_{i=1}^{N_f} \left| u(x_u^i, t_u^i) - u^i \right|^2 + \frac{1}{N_f} \sum_{i=1}^{N_f} \left| f(x_f^i, t_f^i) \right|^2, \tag{10}$$

where $\{x_u^i, t_u^i, u^i\}_1^{N_u}$ denotes the initial and boundary training data for $u(x,t)$, and $\{x_f^i, t_f^i\}_1^{N_f}$ specifies the collocation points for $f(x,t)$.

2.2.2 DRM (Deep Ritz Method)

In [3]. The authors use the variational form of elliptic PDEs to derive the formulation and design the algorithm.

Consider the variational form of PDE problem

$$\min_{u \in H} \int_\Omega \left(\frac{1}{2} |\nabla u|^2 - f(x)u(x) \right) dx, \tag{11}$$

and H is the set of admissible functions (also called trial function, here represented by u), f is a given function, representing external forcing to the system under consideration. u is approximated by a neural network, and the authors use SGD to minimize the loss. The minimizer gives solution to the original PDE. Problems of this type are fairly common in physical sciences.

2.3 Our plan

Among the works mentioned above, they all aim to solve some challenging physical problems such as inverse conductivity problem in electrical impedance tomography (EIT) where the goal is to discover coefficients of the PDE from boundary conditions. We plan to choose one challenging real world problem and apply one of the approaches above as a basis, analysis the result and seek for possible improvement.

References

[1] Gang Bao, Xiaojing Ye, Yaohua Zang, and Haomin Zhou. Numerical solution of inverse problems by weak adversarial networks. *Inverse Problems*, 36(11):115003, 2020.

[2] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational physics*, 378:686–707, 2019.

[3] Bing Yu et al. The deep ritz method: a deep learning-based numerical algorithm for solving variational problems. *Communications in Mathematics and Statistics*, 6(1):1–12, 2018.